

# Nuclear physics in the coming decade

**D J Dean**

Oak Ridge National Laboratory, Oak Ridge, TN 37831-6369, USA

E-mail: [deandj@ornl.gov](mailto:deandj@ornl.gov)

**Abstract.** The summary talk for this conference is actually a brief status report on the physics of nuclei and what advances we may anticipate during the next decade. We are making progress on multiple fronts to tackle the nuclear quantum many-body problem. Due to the continuing expansion and use of computational science in our field, and due to the new experimental facilities that will soon be available, progress will continue.

## 1. Introduction

In summarizing this conference in honor of Jerry Draayer's 70<sup>th</sup> birthday, I tried to perform an extrapolation of the next 10 years (when we celebrate HITES2022) of the physics of nuclei based on where we are today. This kind of discussion is, of course, difficult, as we all know that extrapolation is far more uncertain than interpolation. We heard many excellent presentations at this conference, and one surmises from them that the field is making substantial progress in developing a theoretical understanding of nuclei. I will attempt to briefly indicate some of the progress that is being made and some of the developments that will occur during the next few years.

One goal of our field is to understand nuclei. To that end we develop a comprehensive theory of nuclei; we experimentally determine rare isotope properties and use these as benchmarks to validate our theories and approximations; and we use this validated theory to make predictions where experimental data are not available (e.g., for nucleosynthesis). We have witnessed in the last decade an increasingly sophisticated approach to the nuclear many-body problem. During the next decade, the field will continue to develop effective field theory approaches, computationally scalable many-body techniques, and increasingly accurate energy density functionals for nuclear density functional theory approaches.

During the next decade we should see the completion of second-generation rare isotope experimental facilities such as GSI/FAIR, SPIRAL-II, and HIE-ISOLDE in Europe, FRIB in the US, and an upgraded TRIUMF in Canada, and the continuation of the experimental program at RIBF in Japan and other facilities. Experiments will probe many aspects of neutron-rich nuclei. Furthermore, they should enable a substantial experimental description of nuclear properties along the r-process — the process that creates half of the heavy elements from iron to uranium and is believed to occur during supernova explosions or neutron star mergers.

In developing a comprehensive theory for nuclei, we have increasingly relied on high-performance computing. With calculations performed on these machines, we should be able to constrain theoretical parameters and we should be able to quantify uncertainties of the calculations. Uncertainty quantification, admittedly a buzz word today, is a way of performing numerical analysis to determine the accuracy of a given calculation.

In the following sections, I will expand on each of the areas mentioned in the previous four paragraphs: progress in theory, experiment, computing, and uncertainty quantification.

## 2. Progress in the theory of nuclei

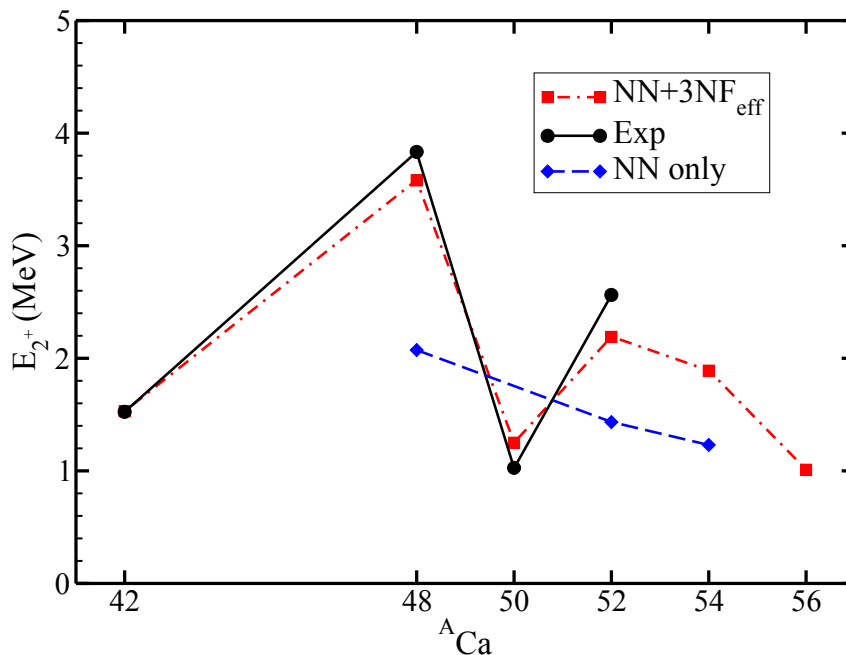
In her Nobel Lecture, Maria Goeppert-Mayer stated [1] that “[T]he first, basic approach, is to study the elementary particles, their properties, and mutual interaction. Thus one hopes to obtain knowledge of the nuclear forces. If the forces are known, one should, in principle, be able to calculate deductively the properties of individual nuclei.” From a different perspective, eloquently expressed by another Nobel Laureate, Philip Anderson [2], the behavior of large and complex aggregates of elementary particles is not easily understood in terms of simple extrapolations. We are making progress in understanding nuclei precisely because of the tension between these two points of view.

The nuclear shell model rests on the idea that for certain nuclei identifiable and relatively large single-particle energy gaps exist between the highest occupied and lowest unoccupied single-particle orbitals in a nucleus. These gaps yield magic numbers in neutrons and protons. Experimental evidence suggests that “shells” as defined in the classical nuclear sense (at particle numbers 2, 8, 20, 50,...) disappear in neutron rich nuclei while others may appear. Part of the reason for this change in structure is the rather simple explanation that the mean field exhibited by very neutron-rich nuclei is not a simple oscillator well. The continuum plays an important role in the very neutron-rich nuclei, and should be incorporated into calculations. In the past few years, progress has been made in this direction across a number of efforts.

The appropriate degrees of freedom that we use in nuclear physics to describe phenomena depend on the energy scale in which we are interested. The theory of quantum chromodynamics (QCD) describes quarks and gluons that make up protons and neutrons (nucleons), and the strong force that we measure between nucleons is the residual of QCD. Significant progress has been made through the applications of effective field theory [3]. Effective field theories describe the nuclear interactions through diagrammatic expansions of a Lagrangian that possesses the symmetries of QCD and also describes the interactions between nucleons and pions. Interestingly, from this approach one naturally obtains three-body forces. One fits parameters of the expansion such that nucleon-nucleon phase-shift scattering data and deuteron properties are obtained [4], and one adjusts the three-body force parameters to obtain the binding of the triton and  $^4\text{He}$  [5]. Thus far, the two-body forces have been fit at the next-to-next-to-next-to-leading-order ( $\text{N}^3\text{LO}$ ), while the three-body forces are fit at the next-to-next-to-leading-order [5].

We have come a long way from the initial nucleon-nucleon interactions of the 1950’s. The situation changed dramatically for the better in the mid-1990s when new nucleon-nucleon interactions were accurately fit to scattering data [6, 7]. Today’s nucleon-nucleon interactions all fit scattering data with  $\chi^2/\text{dof} \approx 1$ . Green’s Function Monte Carlo (GFMC) calculations [8] utilizing two- and three-body forces paved the way for a modern look at the nuclear many-body problem and have been extremely successful into the p-shell [9]. The three-nucleon force can have a significant effect on nuclear properties. For example, consider calculations of the lifetime of  $^{14}\text{C}$  [10] which is anomalously long compared to its neighbors. The no-core shell model calculations utilizing only two-body forces failed to reproduce the lifetime, but one could show that inclusion of the three-body force indeed reproduced the long lifetime. This interesting result shows that more than just a few low-lying states may be affected by the three-nucleon interactions.

Work with coupled-cluster theory also demonstrates three-nucleon force and continuum effects on shell closures in Ca nuclei. Calculations show that the closure at  $^{48}\text{Ca}$  cannot be reproduced with the two-body  $\text{N}^3\text{LO}$  interaction [11, 12]. However, inclusion of a three-body force solves this problem. These coupled-cluster calculations utilize an effective three-body potential that



**Figure 1.** Coupled-cluster results from Ref. [11] for first excited states in Ca isotopes. Results dramatically indicate the effect of a three-body force on the shell closure at  $^{48}\text{Ca}$ .

results from integrating one nucleon in the leading-order chiral three-nucleon force over the Fermi sphere with Fermi momentum  $k_F$  in symmetric nuclear matter. While not an exact treatment of the three-nucleon potential in coupled-cluster theory (see e.g. [13] for an example of a full coupled-cluster implementation with a three-body interaction), the calculations in Ca isotopes show that the three-body force strongly affects the shell closure at  $^{48}\text{Ca}$ , as illustrated in Fig. 1. The coupled-cluster results also point to a neutron drip-line that may reside around  $^{60}\text{Ca}$  where continuum effects will be important.

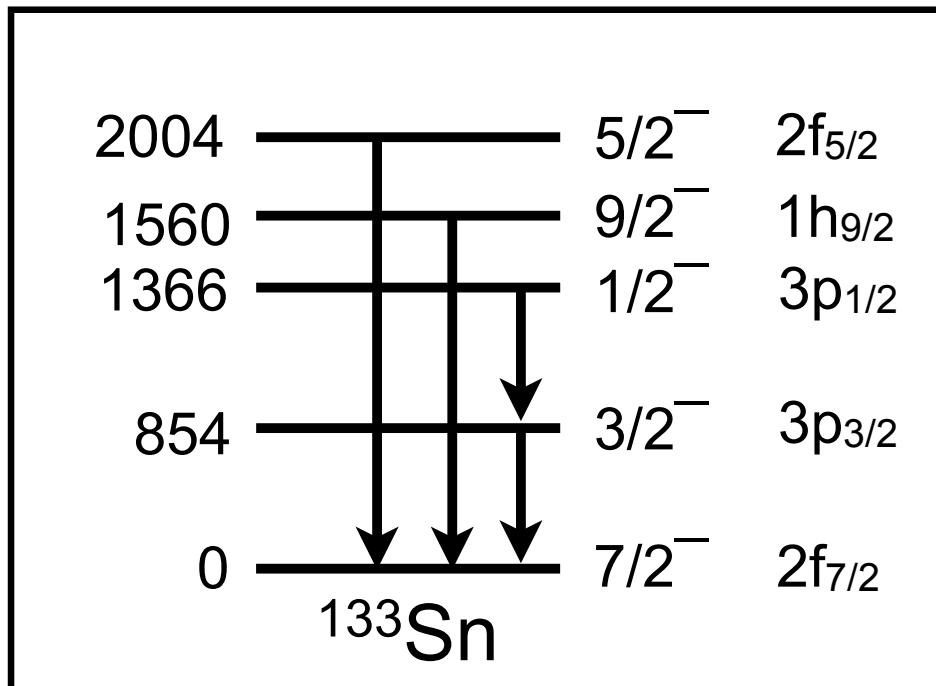
In most cases, the basis used in no-core shell model or coupled-cluster calculations is spherical. The basis lends some simplicity but also requires large numbers of basis states to properly describe highly deformed configurations. Draayer and his colleagues [14] are beginning to pursue the marriage of symmetry-adapted single-particle states and nucleon-nucleon interactions in light nuclei. This nascent approach shows promise to add to our computational tool box for solutions of the nuclear many-body problem.

While some heavier nuclei may be treated within the framework of the no-core shell model or coupled-cluster theory, the full range of nuclei, including well-deformed heavy nuclei, can more naturally be investigated utilizing nuclear density functional theory. Here, the degrees of freedom are quasiparticles and the framework is that of Hartree-Fock-Bogoliubov. Significant progress was made through the Universal Nuclear Energy Density Functional (UNEDF) collaboration in defining the next generation of energy density functionals. The UNEDF-I functional predicts a nuclear landscape with  $6900 \pm 500$  nuclei [15].

### 3. Rare isotope experiments

Space will not allow for me to adequately cover the experimental landscape today. I will however mention two extremes of measurements in the Sn isotopes as illustrative of the recent past and likely things to come, and a third example from super-heavy nuclei.

The first example is from work performed at the Holifield Radioactive Ion Beam Facility



**Figure 2.** Tentative single-particle states assignments measured in  $^{133}\text{Sn}$ . These states were excited through  $^{132}\text{Sn}(d,p)^{133}\text{Sn}$  reactions at HRIBF. Data are from [16].

(HRIBF) at Oak Ridge [16]. It was long a goal of the facility to produce beams of  $^{132}\text{Sn}$  impinging on various targets. Some of the last experiments at the facility included discoveries of the single particle energies of states in  $^{133}\text{Sn}$ . These states serve as benchmarks for various theories and models of nuclei. Experiments showed very clearly that  $^{132}\text{Sn}$  is indeed doubly-magic. Furthermore,  $^{132}\text{Sn}$  is one of the few heavy nuclei experimentally accessible and also close to the r-process path. Fig. 2 represents preliminary level scheme and spin assignments extracted from several  $^{132}\text{Sn}(d,p)^{133}\text{Sn}$  reactions [16]. Data taken during March, 2012 also indicates evidence for an excited  $i_{13/2}$  state in  $^{133}\text{Sn}$  [17].

A second example concerns  $^{100}\text{Sn}$ . Experiments performed at GSI utilized a  $^{124}\text{Xe}$  beam directed at a beryllium target to identify  $^{100}\text{Sn}$  and its decay to  $^{100}\text{In}$  via a strong Gamow-Teller transition [18]. The measurement of a  $B(\text{GT})$  strength of  $9.1^{+2.6}_{-3.0}$  to the single  $1^+$  state in  $^{100}\text{In}$  that resides below the  $Q$ -window represents years of effort to determine this transition. Future experiments will require more intensity in order to obtain more experimental precision. This experiment was originally motivated by a desire to study more carefully the effects of the nuclear medium on the ratio of the axial-to-vector coupling constants. This rate also feeds into the Sn-Sb-Te cycle which is likely the end-point of the rapid proton capture process.

We are beginning to see confirmation of long-standing predictions (for a review of theoretical efforts see [19]) related to the island of stability in the super-heavy region of elements. Recently, element 117 was discovered at Dubna through the bombardment of a  $^{249}\text{Bk}$  target (produced at ORNL's High Flux Isotope Reactor) by a  $^{48}\text{Ca}$  beam [20]. Theory predicts a super-heavy island of stability around  $N = 184$  and  $Z = 118$ . Indeed, for the two isotopes known, the half-life of  $^{293}\text{Uus}$  is about 14 ms while the half life of  $^{294}\text{Uus}$  is about 78 ms (although both numbers have large experimental error bars). Taken as a whole, the super-heavy region from element 105-117

display a trend of increasing stability with larger neutron number. This may be an experimental indication that we have reached the beaches of the island of stability.

#### 4. Trends in Computing

We live in a time of continuing growth in computational capability. Approximately every two years computing power doubles [21]. Twenty years ago, only a few people in our field knew how to extract some physics from the high-performance computers of that day. The fastest of these machines computed at 500 gigaflops (see <http://www.top500.org> for the first Top500 list in June, 1993). Today, access to 1-10 petaflop (PF) computers is routine.

The hardware changes can be summarized as going from a single vector processor (in the early to late 1980s) to parallel processing in the 1990s and early 2000s. The first wave of change introduced us to parallel computing and message passing protocols such as MPI. The high end computers continued to become larger, with more processors, but also the clock speeds increased regularly, until about the mid-2000s. At that time, multi-core technology began to take over. Today's largest machines utilize multicore processors with graphical processor units (GPUs) attached to each core. Programming languages and algorithms have to continuously evolve in order to keep up with these kinds of hardware changes. This means that the underlying algorithms we utilize to solve our physics problems will also need to evolve. Development of algorithms that can utilize flops efficiently while minimizing data movement will be essential for scalability on these hybrid architecture machines.

The growth in high-end computing power tremendously benefitted the nuclear theory community through a U.S. Department of Energy program called Scientific Discovery through Advanced Computing (SciDAC). The first round of SciDAC included supernovae efforts with some nuclear physics components. The second round of SciDAC funding came in 2006 and one of the big winners in that round was the UNEDF collaboration. UNEDF made significant contributions to the science of nuclei through computational advances [22]. UNEDF was also extremely successful through engaging and training post-docs and students. The third round of SciDAC grants has just been awarded, and the UNEDF follow-on, the Nuclear Computational Low Energy Initiative (NUCLEI), has already begun work. One of the main goals of NUCLEI will involve implementation of uncertainty quantification into various codes and algorithms of the collaboration. The collaboration will also place an emphasis on generating scalable codes for hybrid architectures.

#### 5. Trends in uncertainty quantification

Uncertainty quantification (UQ) is an old and new area of research across the sciences. In fact, UQ has much in common with statistics and numerical analysis. Today, whole journals are devoted to this topic, and our field is just beginning to apply the techniques and ideas, although I would argue that numerical analysis, a major part of UQ, has been with us for a long time.

The basic idea of UQ is to quantify error coming from the following sources: the accuracy of a mathematical model in describing the underlying physics, and the impacts of those underlying model uncertainties on calculations; the error inherent in the numerical algorithm employed to solve a given model; and, the sensitivity of a given numerical solution of the model to the underlying physical parameters. Thus, different sources of error include model approximations, numerical approximations, and the sensitivity of the outputs to physical parameter inputs. A fourth part of a calculation's error budget may be statistical if the problem is amenable to some form of Monte Carlo simulation. I will use coupled-cluster theory as an example of the first three of these errors.

Coupled-cluster theory starts from an exponential ansatz for the wave function,  $|\Psi\rangle = \exp(T)|\Phi\rangle$  where  $T = T_1 + T_2 + \dots + T_n$  is a n-particle-n-hole (np-nh) excitation operator relative to a Slater determinant state  $|\Phi\rangle$ . One particular approximation truncates the series at

$T_2$  (called coupled-clusters in singles and doubles, or CCSD). This turns out to be an extremely powerful approximation, and gives correlation energies converged to the level of 5-7% [23, 24]. Adding  $T_3$  yields converged results at the level of 0.1-1%, but at significant computational cost. Thus the first source of error, model approximations, arises from the level of truncation utilized within the coupled-cluster theory.

Coupled-cluster theory results rest on the solution of a set of nonlinear, coupled algebraic equations. Inherent in such solutions is the necessity of being close to the solution (thus starting from a good mean-field or Hartree-Fock reference Slater determinant is important). A good method for accelerated convergence becomes necessary, and one must choose a cutoff for convergence. This represents an algorithmic, or numerical, source of error. In the context of coupled-cluster theory, this type of error is usually small. Another source of numerical error is the choice of single-particle basis states. Convergence requires that one use very large model spaces.

The third source of error involves the physical parameters of the model. For nuclear many-body problems, some of these involve the physical choice of Hamiltonian and parameters therein. The nucleon-nucleon and three-nucleon potentials are not observables, and thus their choice is not unique. Thus, it becomes important to perform a sensitivity analysis of the parameters within the Hamiltonian. How well constrained are the parameters? This is most evident today in investigations of three-body forces, where fine tuning is often employed to obtain optimal fits. The choice of oscillator strength ( $\hbar\omega$ ) may also affect results unless one proves numerically  $\hbar\omega$  independence of solutions.

Each of these sources of errors should be accounted for in calculations. In the future, one will see a lot of work in nuclear physics on UQ implementations embedded within computational approaches that describe nuclei.

## 6. Predictions for Jerry's 80<sup>th</sup> birthday

Ten years is not a long time. Some things should happen before 2022. For example, all of the students who attended this meeting should have found gainful employment during the next 10 years. FRIB construction should be either completed or nearing completion. FAIR should be on line. Results from other nuclear physics experiments will have been reported. At the conference, I ended the summary talk by making a few predictions.

- One can hardly fail at predicting that the Higgs will have been discovered. At the time of HITES 2012 a  $2\sigma$  bump at the right energy had made the news. In September 2012 the ATLAS collaboration at the LHC reported [25] a  $5.9$  sigma effect at an energy of  $125 \pm 0.4$  (stat)  $\pm 0.4$  (sys) GeV, impressively confirming the standard model. A modified prediction would be that the various branching ratios for Higgs decay will be accurately determined. We may find that indeed at these energy scales the standard model is extremely solid.
- We are going to figure out dark matter. Either it is neutralinos (requiring physics beyond the standard model) or something else. Thus far, dark matter searches are coming up empty handed, and significantly constraining minimal supersymmetric extensions to the standard model.
- The 12 GeV upgrade at JLab will have enabled the discovery of the gluonic excitations. These states are considered QCD exotica. They will either be observed with the upgrade, or there is something seriously wrong with our understanding of QCD.
- The r-process will be better understood, but the astrophysical site will continue to be less well understood. Better data closer to the r-process path will enable better modeling of the process.
- There will be an exascale computer somewhere in the world. We are only a factor of 50 away. Someone will find a solution to the energy costs of moving bits around on these larger

machines. Hopefully, this will happen in the U.S., but international competition may yield a different result.

- The largest  $0\nu\beta\beta$  decay experiments will have just been built, but finding a signal may not have occurred. A lot will be learned from current generation of experiments and technology developments.
- Jerry and his students and post-docs will continue to make significant progress in applying the symmetry-adapted model spaces to nuclear many-body problems.

Some of these predictions will come true, and we are looking forward to the next birthday party for Jerry to once again measure our progress toward the goal of understanding nuclei.

### Acknowledgments

Oak Ridge National Laboratory is managed for the U.S. Department of Energy by UT-Battelle, LLC under contract number DE-AC05-00OR22725.

### References

- [1] Goeppert-Mayer M 1963 *The shell model* (Nobel Lectures: Physics, IV (Amsterdam: Elsevier)) p 20
- [2] Anderson P W 1972 More is different *Science* **177** 393
- [3] Weinberg S 1990 Nuclear Forces from chiral Lagrangians *Phys. Lett. B* **251** 288
- [4] Machleidt R and Entem D R 2011 Chiral effective field theory and nuclear forces *Phys. Repts.* **533** 1
- [5] Gazit D, Quaglioni S and Navratil P 2009 Three nucleon low-energy constants from the consistency of interactions and currents in chiral effective field theory *Phys. Rev. Lett.* **103** 102502
- [6] Wiringa R B, Stoks V G J, and Schiavilla R 1995 Accurate nucleon-nucleon potential with charge-independence breaking *Phys. Rev. C* **51** 38
- [7] Machleidt R 2001 High-precision, charge-dependent Bonn nucleon-nucleon potential *Phys. Rev. C* **63** 024001
- [8] Pudliner B S, Pandharipande V R, Carlson J, and Wiringa R B 1995 Quantum Monte Carlo calculations of  $A \leq 6$  nuclei *Phys. Rev. Lett.* **74** 4396
- [9] McCutchan E A *et al* 2009 Precise electromagnetic tests of ab initio calculations of light nuclei: states in  $^{10}\text{Be}$  *Phys. Rev. Lett.* **103** 192501
- [10] Maris P, Vary J P, Navratil P, Ormand W E, Nam H, and Dean D J 2011 Origin of the anomalous long lifetime of  $^{14}\text{C}$  *Phys. Rev. Lett.* **106** 202502
- [11] Hagen G, Hjorth-Jensen M, Jansen G R, Machleidt R, and Papenbrock T 2012 Evolution of shell structure in neutron-rich calcium isotopes *Phys. Rev. Lett.* **109** 032502
- [12] Holt J W, Kaiser N, and Weise W 2010 Density-dependent effective nucleon-nucleon interaction from chiral three-nucleon forces *Phys. Rev. C* **81** 024002
- [13] Hagen G, Dean D J, Hjorth-Jensen M, Papenbrock T, and Schwenk A 2007 *Phys. Rev. C* **76** 034302
- [14] Draayer J P, Dytrych T, Launey K D, and Langr D 2012 Symmetry-adapted no-core shell model applications for light nuclei with QCD-inspired interactions *Progress in Particle and Nuclear Physics* **67** 516
- [15] Erler, J Birge N, Kortelainen M, Nazarewicz N, Olsen E, Perhac A M, and Stoitsov M 2012 The limits of the nuclear landscape *Nature* **486** 509
- [16] Jones K L *et al* 2010 The magic nature of  $^{132}\text{Sn}$  explored through the single-particle states of  $^{133}\text{Sn}$  *Nature* **465** 454
- [17] Beene J R *et al* 2013 in preparation
- [18] Hinke C B *et al* 2012 Superaligned Gamow-Teller decay of the doubly magic nucleus  $^{100}\text{Sn}$  *Nature* **486** 341
- [19] Cwiok S, Heenen P H, and Nazarewicz W 2005 Shape coexistence and triaxiality in the superheavy nuclei *Nature* **433** 705
- [20] Oganessian Yu Ts *et al* 2010 Synthesis of a new element with atomic number  $Z = 117$  *Phys. Rev. Lett.* **104** 142502
- [21] Moore G E 1965 Cramming more components onto integrated circuits *Electronics* **38** 4
- [22] Bertsch G F, Dean D J, and Nazarewicz W 2007 Computing atomic nuclei *SciDAC Review* **6** 42
- [23] Hagen G, Papenbrock T, Dean D J, and Hjorth-Jensen M 2010 Ab initio coupled-cluster approach to nuclear structure with modern nucleon-nucleon interactions *Phys. Rev. C* **82** 034330
- [24] Bartlett R J and Musial M 2007 Coupled-cluster theory in quantum chemistry *Rev. Mod. Phys.* **79** 291
- [25] ATLAS Collaboration 2012 Observation of a new particle in the search for the Standard Model Higgs boson with the ATLAS detector at the LHC *Phys. Lett. B* **716** 1