COMPUTATIONAL SCIENCE&DISCOVERY

Computational aspects of nuclear coupled-cluster theory

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Received 7 April 2008, in final form 15 August 2008
Published 20 November 2008
Computational Science & Discovery **1** (2008) 015008 (11pp)
doi:10.1088/1749-4699/1/1/015008

Abstract. Coupled-cluster (CC) theory represents an important theoretical tool that we use to solve the quantum many-body problem. CC theory also lends itself to computation in a parallel computing environment. In this paper, we present selected results from *ab initio* studies of stable and weakly bound nuclei utilizing computational techniques that we employ to solve CC theory. We also outline several perspectives for future research directions in this area.

Contents

1. Introduction

Nuclei comprise 99.9% of all baryonic matter in the Universe and are the fuel that burns in stars [1]. The rather complex nature of the nuclear forces among protons and neutrons generates a broad range and diversity in the nuclear phenomena that we observe. Experiments indicate that developing a comprehensive description of all nuclei (stable and unstable) and their reactions requires theoretical and experimental investigations of rare and exotic isotopes with unusual neutron-to-proton ratios that are very different from their stable counterparts. These rare nuclei are difficult to produce and study experimentally since they can have extremely short lifetimes. Furthermore, these rare nuclei lie at the heart of nucleosynthesis processes in the Universe and are therefore an important component in the puzzle of matter generation in the Universe. Theoretical approaches to these nuclei involve solving the nuclear quantum many-body problem.

The many-body problem spans nuclei from $A = 2$ (the deuteron) to the superheavy region, and different theoretical techniques are pursued in different regions of the chart of nuclei. This is depicted in figure 1 where the current reach of various theoretical methods is interposed in the chart of nuclei. In this paper, we concentrate on one of the *ab initio* methods for solving the nuclear many-body problem in medium-mass nuclei.

Many-body quantum mechanics deals with the development of stable algorithms and numerical methods for solving Schrödinger's or Dirac's equations for many interacting particles in order to gain information about a given system. Typical examples of popular many-body methods are coupled-cluster (CC) methods [3–9], various types of Monte Carlo methods [10–13], perturbative expansions [14, 15], Green's function methods [16], correlation operator methods [17], the unitary-model-operator approach [18, 19], the density-matrix renormalization group [20–25], density-functional theory [26–28], and large-scale diagonalization methods [29–33]. The numerical algorithms cover a broad range of mathematical methods, from linear algebra problems to Monte Carlo simulations. Furthermore, high-performance computing topics such as efficient parallelization are central to any serious study of many-body problems.

In the context of the various algorithms and approaches referenced above, the challenges for understanding nuclei are to determine the nuclear interactions (which may not be limited to two-nucleon interactions only, but may also include complicated three- or higher-body interactions) and to calculate from these interactions nuclear properties. This may involve including any continuum aspects when necessary. In addition, nuclear theorists are working toward determining an appropriate energy density functional for a nuclear density functional theory approach which should eventually have connections to the *ab initio* approaches. In this paper, we will concentrate on the *ab initio* framework and specifically on our efforts in applications of CC theory to nuclei.

With a given inter-particle interaction and the kinetic energy of the system, one can, in turn, define the so-called many-particle Hamiltonian H that enters the solution of Schrödinger's equation or Dirac's equation in case relativistic effects need to be included. For many particles, Schrödinger's equation is an integro-differential equation whose complexity increases exponentially with increasing numbers of particles and states that the system can access. Unfortunately, there are only a few analytically solvable problems, and virtually exact numerical solutions are at present available only for systems with up to three or four particles via the Faddeev [34] and Faddeev–Yakubowski [35] methods, respectively. For problems involving more particles, one needs reliable numerical many-body methods. Such methods should allow for controlled approximations and provide a computational scheme that accounts for successive many-body corrections in a systematic way.

In the remainder of this paper, we will focus on utilizing CC theory for problems in nuclear physics, a field where comparison between experiment and exact numerical results is still lagging behind the precision obtained in fields like quantum chemistry. One major reason for this is the lack of a proper knowledge of the underlying interaction. In addition, three-body forces play an important role in determining nuclear properties. In some of the currently employed interactions, the three-body interaction provides about 10% of the total binding energy.

This paper is organized as follows. In section 2, we present the basic ingredients for computing the properties of stable and weakly bound nuclei using CC theory, with an emphasis on high-performance computing topics. Section 3 presents selected results from nuclear many-body calculations. We focus in

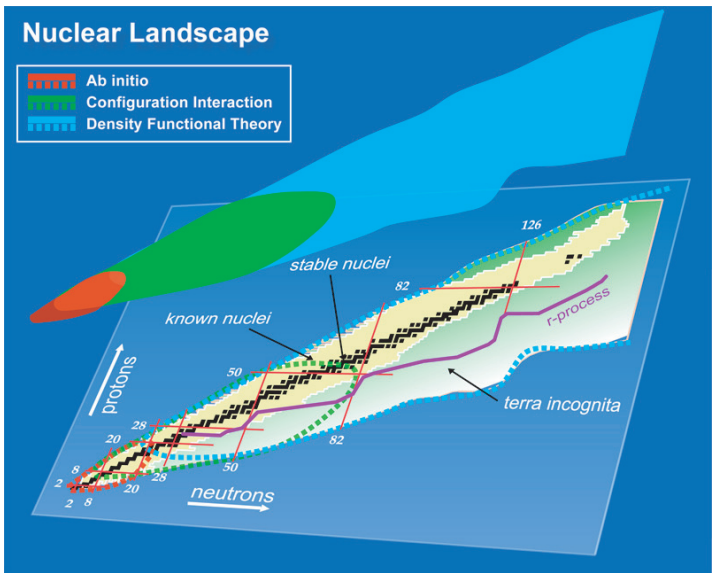

Figure 1. The theoretical methods and computational techniques used to solve the nuclear many-body problem. The red vertical and horizontal lines show the magic numbers, reflecting regions where nuclei are expected to be more tightly bound and have longer half-lives. The anticipated path of the astrophysical r-process responsible for nucleosynthesis of heavy elements is also shown (purple line). The thick dotted lines indicate domains of major theoretical approaches to the nuclear many-body problem. For the lightest nuclei, *ab initio* calculations (GFMC, NCSM and the CC method), based on the bare nucleon–nucleon interaction, are possible (red). Medium-mass nuclei can be treated by configuration interaction (CI) techniques (interacting shell model (green)). For heavy nuclei, the density functional theory, based on self-consistent/mean-field theory (blue), is the tool of choice. By investigating the intersections between these theoretical strategies, one aims to develop a unified description of the nucleus. Taken from [2].

particular on the structure of both stable and weakly bound nuclei. Perspectives and conclusions are discussed in section 4.

2. Nuclear many-body physics

The nuclear many-body problem is particularly difficult to solve due to the complex character of the nucleon–nucleon and three-nucleon interactions. The numerical problems are compounded for rare isotopes with an unusual ratio of proton to neutron number, and for nuclei along the drip lines. These nuclei are the focus of current experimental programs in low-energy nuclear physics. This means that one needs to take into account the fact that many of the nuclei close to the stability line can be weakly bound and therefore the nuclear interactions will couple bound, continuum and resonant states. This leads to a further increase in the dimension of the model space compared with stable nuclei. The current worldwide experimental programs address topics that are of great relevance for our understanding of the stability of matter itself, with applications and relevance to many other fields, including astrophysics (synthesis of elements in the Universe and stellar evolution), particle physics (using nuclei to discover physics beyond the standard model), and societal applications.

We show in table 1 some selected model-space dimensions for configuration interaction (CI, or shell-model in nuclear physics) calculations with various numbers of major shells. These shells are defined by harmonic oscillator single-particle orbits. Four major shells include all possible single-particle orbits of the 0s0p1s0d1p0f shells, and the total number of Slater determinants is constructed by forming all possible direct products of single-particle wavefunctions. Present shell-model codes can today reach dimensions of $d \sim 10^{10}$ basis states [30, 31, 33], and Monte Carlo-based shell-model codes can attack problems with model-space dimensions $d \sim 10^{15}$ [11, 13]. It is rather obvious from table 1 that for weakly bound systems, with many more active single-particle orbits, we cannot use available large-scale diagonalization methods.

Table 1. Shell-model dimensions (single-particle product states) for given numbers of major shells and selected light nuclei.

Nucleus	Four major shells	Seven major shells
^{4}He	4×10^{4}	9×10^{6}
^{8}B	4×10^{8}	5×10^{13}
^{12}C	6×10^{11}	4×10^{19}
^{16}O	3×10^{14}	9×10^{24}

The Green's function Monte Carlo (GFMC) method [10, 36–38] and the no-core shell-model (NCSM) approach [32, 39–44] have been successfully applied for the theoretical description of light nuclei with mass numbers $A \sim 12$, and Hamiltonians based on nucleon–nucleon and three-nucleon interactions. However, present experimental studies of nuclear stability are now being pushed to larger mass regions, with mass numbers from $A = 40$ to 100. Traditionally, this has been the realm of the nuclear shell model (with a smaller number of valence nucleons being the degrees of freedom) and nuclear density-functional theory (an effective single-particle theory). These methods employ Hamiltonians and density functionals with phenomenological corrections and are not directly related to the vacuum nucleon–nucleon interaction employed in *ab initio* calculations. However, in selected medium-mass nuclei, *ab initio* structure calculations can be performed using CC theory. CC methods allow to study ground- and excited-state properties of systems with model-space dimensions beyond the capability of present large-scale diagonalization approaches, with a much smaller numerical effort when compared with diagonalization methods aiming at similar accuracies. Our hope is then that CC methods, which actually originated from nuclear physics, but have found large areas of applications and theoretical developments in quantum chemistry, can be used to shed light on different many-body correlations in nuclear physics. While there are approximations introduced in the theory, the method's accuracy is sufficiently high to attribute an eventual disagreement between experimental data and theoretical results to missing physics in the Hamiltonian. In this way, CC calculations help to increase our understanding of the nuclear interaction on a very fundamental level.

The aim of our recent many-body studies is therefore to delineate a many-body scheme for nuclear physics problems based on CC theory that incorporates as many as possible of the following features.

- The theory should be fully microscopic and employ state-of-the-art two- and three-body interactions.
- It can be systematically improved by the inclusion of more complicated correlations.
- It allows for the description of both closed-shell and open-shell nuclei.
- It is amenable to parallel computing.
- It can be used to compute excitation spectra for nuclei where many shells are involved and describe weakly bound systems with or without resonances and couplings to the continuum.
- It enables the derivation of effective interactions to be used in reduced space appropriate for large-scale diagonalization techniques with model-space dimensions of about 10^{10}. These dimensions should be contrasted with the model spaces that can be reached by our J-coupled code at the level of single and double excitations. In [9], we computed for example the ground state of ^{48}Ca with 15 major shells, corresponding to 10^{80} possible Slater determinants.
- It enables microscopic nuclear structure results to be married with microscopic reaction studies.

In the next subsection, we outline the basic CC equations.

2.1. Coupled-cluster equations

CC theory requires a single-particle basis, and we begin the discussion of the equations by setting up an appropriate single-particle basis for the nuclear problem. We utilize spherical single-particle orbitals $\phi_\alpha(\mathbf{r})$, and the quantum numbers $\alpha = \{n, l, j, j_z, t_z\}$ denote the principal quantum number, orbital angular momentum, total angular momentum, total angular momentum projection, and isospin projection respectively. We split

the total Hamiltonian into a sum over one-body parts H_0, with single-particle operators h_0 and a two-body interaction $H_{\rm I}$. The matrix elements of the two-body interaction are defined as

$$\langle pq \,|\, H_{\rm I} \,|\, rs \rangle = \int {\rm d}^3 r_1 {\rm d}^3 r_2 \phi_p(\mathbf{r}_1)\phi_q(\mathbf{r}_2) H_{\rm I}(\mathbf{r}_1, \mathbf{r}_2)\phi_r(\mathbf{r}_1)\phi_s(\mathbf{r}_2). \tag{1}$$

In second-quantized form, the Hamiltonian can then be written as

$$H = \sum_{pq} \langle p \,|\, h_0 \,|\, q \rangle a_p^\dagger a_q + \frac{1}{4} \sum_{pqrs} \langle pq \,|\, H_{\rm I} \,|\, rs \rangle a_p^\dagger a_q^\dagger a_s a_r. \tag{2}$$

Our one-body part is the kinetic energy operator and since we remove the spurious center of mass energy, by rewriting the internal kinetic energy, we can rewrite the Hamiltonian as

$$H = \left(1 - \frac{1}{A}\right) \sum_{pq} \langle p \,|\, t \,|\, q \rangle a_p^\dagger a_q + \frac{1}{4} \sum_{pqrs} \langle pq \,|\, H_{\rm I} \,|\, rs \rangle a_p^\dagger a_q^\dagger a_s a_r, \tag{3}$$

with A being the number of nucleons and $\langle p|t|q \rangle$ defines the matrix elements of the kinetic energy. The two-body part $H_{\rm I}$ reads

$$\langle pq \,|\, H_{\rm I} \,|\, rs \rangle = \int {\rm d}^3 r_1 {\rm d}^3 r_2 \phi_{\rm p}(\mathbf{r}_1)\phi_q(\mathbf{r}_2) \left(V(\mathbf{r}_1, \mathbf{r}_2) - \frac{\mathbf{k}_1 \cdot \mathbf{k}_2}{mA} \right) \phi_r(\mathbf{r}_1)\phi_s(\mathbf{r}_2), \tag{4}$$

where V is the two-nucleon interaction and $\mathbf{k}_1 \cdot \mathbf{k}_2/mA$ is a two-body operator that arises from our rewriting of the internal kinetic energy. The sums are over all single-particle states in the calculation. We use the notation that p, q, r, s refer to all single-particle states and i, j, k, l index all sums below the Fermi surface. In addition, we let a, b, c, d index all sums above the Fermi surface. The total number of single-particle states in the model space is $N_{\rm s} = N_{\rm p} + N_{\rm h}$, where $N_{\rm p}$ refers to the number of particle states, and $N_{\rm h}$ is the number of hole states.

The single-reference CC theory [3, 45–48] is based on the exponential ansatz for the ground-state wavefunction of the A-body system. CC theory starts with the simple assumption that the correlated ground-state wavefunction can be described by applying an exponentiated correlation operator to an uncorrelated Slater determinant that naively describes the nucleus:

$$|\,\Psi\rangle = \exp(T)\,|\,\Phi\rangle. \tag{5}$$

The correlation operator T induces various np–nh (particle–hole) correlations (up to the number of nucleons, A, in the nucleus):

$$T = T_1 + T_2 + \cdots + T_A. \tag{6}$$

The energy of the ground state is given by

$$\begin{aligned} E &= \langle \Phi \,|\, \exp(-T) H \exp(T) \,|\, \Phi \rangle = \langle \Phi \,|\, \bar{H} \,|\, \Phi \rangle \\ &= \langle \Phi \,|\, (H \exp(T))_{\rm c} \,|\, \Phi \rangle, \end{aligned} \tag{7}$$

where the subscript c means that only connected diagrams enter into the expressions. The T_n operators take the form (as is the case here for the two-body excitation operator)

$$T_2 = \sum_{ab,ij} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i, \tag{8}$$

where t_{ij}^{ab} are the 2p–2h correlation amplitudes.

Table 2. Scaling of the CC methods and comparisons with certain CI truncations. Here n_o is the number of occupied orbitals (the number of particles), n_u is the number of unoccupied orbitals, and $N = n_o + n_u$ is the total number of orbitals in the calculation. We use O_i to indicate that the step requires iteration, while O_n indicates a non-iterative step. The memory requirement $O(N^4)$ stems from the storage of the two-body matrix elements of the interaction.

Methods	Scaling	Memory
CCSD	$O_i(n_o^2 n_u^4)$	$O(n_o^2 n_u^2) + O(N^4)$
CCSD(T)	$O_i(n_o^2 n_u^4) + O_n(n_o^2 n_u^5)$	$O(n_o^2 n_u^2) + O(N^4)$
CCSDT-3	$O_i(n_o^3 n_u^4)$	$O(n_o^2 n_u^2) + O(N^4)$
CCSDT	$O_i(n_o^3 n_u^5)$	$O(n_o^3 n_u^3) + O(N^4)$
CISDT	$O_i(n_o^3 n_u^5)$	$O(n_o^3 n_u^3) + O(N^4)$

One must compute the correlation amplitudes through equations that left-project $\bar{H}$ onto the space of excited Slater determinants. For example, if the theory only contains T_1 and T_2 operators, then the equations to solve for the coefficients t_i^a and t_{ij}^{ab} are

$$\begin{aligned} 0 &= \langle \Phi_i^a \mid \bar{H} \mid \Phi \rangle, \\ 0 &= \langle \Phi_{ij}^{ab} \mid \bar{H} \mid \Phi \rangle. \end{aligned} \tag{9}$$

Equation (7) is exact; however, the power of the CC theory is its highly accurate computation of the energy even when one limits to lower order the number of T_n operators in the theory. For example, at the T_1 and T_2 levels (CC in singles and doubles, or CCSD), approximately 90% of the correlation is obtained, whereas with approximate triples corrections (denoted CCSD(T)), nearly all of the correlation energy is obtained [7]. This contrasts sharply with truncated shell-model calculations where the truncation introduces unconnected diagrams, causing growing errors with particle number [3]. The reader should, however, note that these results are interaction-dependent, since for example the two-nucleon interaction is modeled to fit two-nucleon scattering data and properties of the deuteron. This implies that the off-shell character of the interactions may change, yielding less or more correlation energy. In particular, differing strengths of the two-nucleon tensor force may result in different binding energies in a nuclear medium, see for example the discussions in [15, 49]. Here, we have used the chiral perturbation theory-based interaction N^{3}LO model of Entem and Machleidt [50].

The explicitly connected form of the CC equations guarantees that the process of solving these equations leads to connected terms in cluster components T_n and connected terms in the energy E, independent of the truncation scheme used to define the excitation operator T. The absence of disconnected terms in T and E is essential to obtain the rigorously size-extensive results. The Hamiltonian H_N which enters our equations is discussed in various papers, see for example [4, 6–8].

2.2. High-performance computing topics

The rapid growth in computational hardware that has spanned the last 40 years has enabled continuous and breathtaking advances in the way we attempt to solve our theoretical problems. Not only do computers allow us to solve larger problems in the same framework as on previous systems, but they also allow for innovation and applications of computing to new classes of problems that could not have been previously considered. In considering algorithms currently applied to the nuclear *ab initio* problem, other methods, such as GFMC and the NCSM, scale exponentially with particle number for a given accuracy. CC theory, on the other hand, scales as a polynomial with the number of particles and the number of single-particle basis states. We show in table 2 the computational scaling of various CC implementations.

Memory requirements and scaling for all CI methods follow the same trend as the full CC methods at a given cluster level. Thus, CCSD and CISD are equivalent in terms of computational need. However, in terms of accuracy, the CC methods significantly outperform CI methods for the same system [3]. This is a result of two factors. Firstly, the CC correlation operator is an exponential of the cluster operators rather than a linear combination of cluster operators as in the CI case. This leads to a far more complicated wavefunction

from CCSD, for example, than that obtained in CISD. Secondly, the CC equations are size-extensive, meaning energies and therefore errors in the energy scale linearly with system size. In CI methods, any truncation leads to terms that are not size extensive and whose errors scale far worse than linear with system size. We note that for a given model space and number of nucleons, a full CI calculation will yield a size-extensive result in that model space; see for example the discussion of [3].

2.3. Numerical solution of the nonlinear coupled-cluster equations

The CC equations define a nonlinear set of coupled equations for the t-amplitudes. The typical very large number of unknowns makes a direct solution of the nonlinear equations not feasible, and one has to resort to iterative approaches in order to obtain solutions of the equations. In the largest calculation we have performed to date [7], we solved $\sim 10^8$ nonlinear equations on 1000 2GByte parallel processors. Stable and convergent solutions of such large sets of nonlinear equations require implementation of sophisticated mathematical techniques. We have implemented convergence accelerators such as the direct inversion in the iterative subspace (DIIS) [51] and the modified Broyden method [52]. The aim of these iterative methods is to construct an optimal vector which minimizes the nonlinear equations at each iterative step. The DIIS method assumes a linear mixing between old and new vectors, whereas the typically superior Broyden method uses a quasi-Newton–Raphson method, or Jacobian update procedure to construct new input vectors. We found that combining the iterative convergence accelerators with step-restriction and line-search in each iteration, convergence can be obtained within a reasonable number of iterations. The basic numerical operation is that of a tensor multiplication as demonstrated in the following:

$$t_{ij}^{ab}(\text{new}) = \sum_{kl,cd} \langle kl \,|\, V \,|\, cd \rangle t_{ab}^{kl}(\text{old}) t_{ij}^{cd}(\text{old}). \tag{10}$$

Many similar terms appear in the CC equations. Naively, the basic numerical effort would scale as an $O(N^8)$. Defining appropriate intermediates, one can break the multiplication into two separate multiplications, each of which costs $O(N^6)$ computational cycles. Writing the equations in terms of intermediates, the CC equations take a quasi-linear form, and for the T_1 equation we have:

$$0 = f_a^i + I_a^{'e} t_e^i - \bar{h}_m^i t_a^m - v_{ma}^{ie} t_e^m + \bar{h}_m^e t_{ea}^{mi} - \tfrac{1}{2} \bar{h}_{mn}^{ie} t_{ae}^{mn} + \tfrac{1}{2} v_{am}^{ef} t_{ef}^{im}, \tag{11}$$

where we see that the equation appears linear in the T_1 and T_2 amplitudes. The nonlinearity is hidden in the intermediates which are defined in [53]. In the iterative solution we add the diagonal terms, $-I_a^{'a} t_a^i + \bar{h}_i^i t_a^i$, to the right- and left-hand sides, then multiplying through with $(-I_a^{'a} + \bar{h}_i^i)^{-1}$, we obtain an equation for t_a^i; the same is done for the T_2 equation. It turns out that the equations are typically diagonally dominant, so by this procedure the inverse of the diagonal matrix $-I_a^{'a} + \bar{h}_i^i$ serves to dampen oscillations and divergence of the amplitudes during the iterative process, and convergence is typically much faster compared with the typical procedure of multiplying through with the inverse of the Fock matrix only $-f_a^a + f_i^i$. We typically start the amplitudes using many-body perturbation theory as the guide. By setting all amplitudes to zero in equation (11), we see that only the Fock matrix f_a^i is left, and is therefore the natural initial guess for the amplitudes. Once selected, we feed these amplitudes into the CC equations and solve for new amplitudes. The iteration proceeds until the old and new amplitudes agree to some specified accuracy.

In figure 2, we show the convergence properties of the CCSD ground-state energies of ^{4}He and ^{5}He using standard linear mixing, DIIS and the modified Broyden method for solving the nonlinear CCSD equations. The mixing parameter α is set to 0.5 in all cases. In the DIIS approach, we store the seven previous calculated vectors and initialize DIIS at every seventh iterative step. In the modified Broyden approach, we also store the seven previous vectors. We see that DIIS and Broyden perform superior to the standard linear mixing approach, with typically 20/30 iterations to reach convergence.

One can distribute the CC equations for an efficient parallel implementation by noting that in our current problem sets, the cluster amplitudes (t_1 and t_2) are not memory-intensive, whereas the two-body matrix elements of the interaction require significant memory. If we distribute $\langle ab||cd \rangle$ across processors, but keep the t_1 and t_2 amplitudes in local memory, then we can evenly distribute the work to solve the equations, and

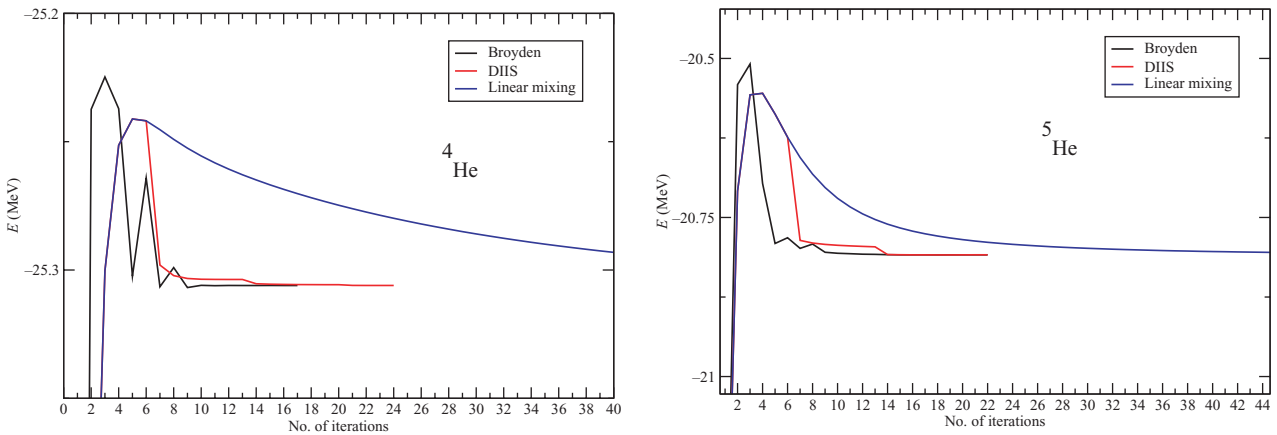

Figure 2. Convergence of the ground-state energies ^{4}He (left figure) and ^{5}He (right figure) for different iterative schemes in solving the nonlinear CCSD equations.

we can also have only one parallel communication per iteration of the full equations. This enables us to scale the problem up to about 1000 processors in today's runs (at 25% efficiency, and well load balanced). How to move beyond this limit forms a part of our current research.

3. Selected results for stable and weakly bound nuclei

3.1. Helium isotopes and weakly bound nuclei

We present recent results from a large-scale CC calculation for helium isotopes; for more details, see [6]. The calculations were mainly carried out at the Leadership Class Facility Oak Ridge National Laboratory. The newly upgraded Cray XT4/XT3 supercomputer named Jaguar had at the time of these calculations a computing power of 101.7 Teraflops.

Figure 3 presents CC results with two-particle-two-hole correlations (so-called singles and doubles) for ground-state energies of the $^{3-10}$He isotopes for an increasing number of partial waves. In our largest calculation we include 5s5p5d4f4g4h4i proton orbitals and 20s20p5d4f4g4h4i neutron orbitals, with a complex basis in order to reproduce eventual resonances. Our calculations show excellent convergence with respect to the single-particle basis size. We obtain a convergence within 10 keV for the real part and within 0.1 keV for the imaginary part of the ground-state energy.

Our largest calculation of ^{10}He with $\sim$850 active single-particle orbitals would correspond to a dimension of $\sim 10^{22}$ many-body basis states. In recent work [8], we computed the ground state energy of ^{40}Ca with a single-basis set which results in a dimensionality of 10^{62} basis states.

The computed decay widths of the helium isotopes are in semi-quantitative agreement with experiment. The comparison of binding energies shows that ^{5}He and ^{7}He are unstable with respect to one-neutron emission, whereas ^{8}He is stable with respect to the emission of up to three neutrons. The nucleus ^{6}He is stable with respect to one-neutron emission but unstable with respect to two-neutron emission. It has a nonzero decay width. All helium isotopes are unstable with respect to ^{4}He plus residual neutrons in the continuum. For the sake of completeness, we list in table 3 the experimental and theoretical energies.

Our results here represent the first time that decay widths have been computed in an *ab initio* way for an isotopic chain. The decay widths of unbound nuclei are in semi-quantitative agreement with experimental data, and the binding energies meet expectations for *ab initio* calculations based on two-body Hamiltonians. The calculated masses follow the experimental pattern in that ^{5,7,9}He are unstable with respect to one-neutron emission and ^{6,8}He stable with respect to one-neutron emission. The missing agreement with experiment is probably due to the lack of the inclusion of three-nucleon clusters and three-nucleon forces, or more complicated many-body correlations. With the inclusion of the latter, we may hopefully be able to tell how much of the spectrum is driven by a coupling to resonances and the non-resonant continuum and how much is due to

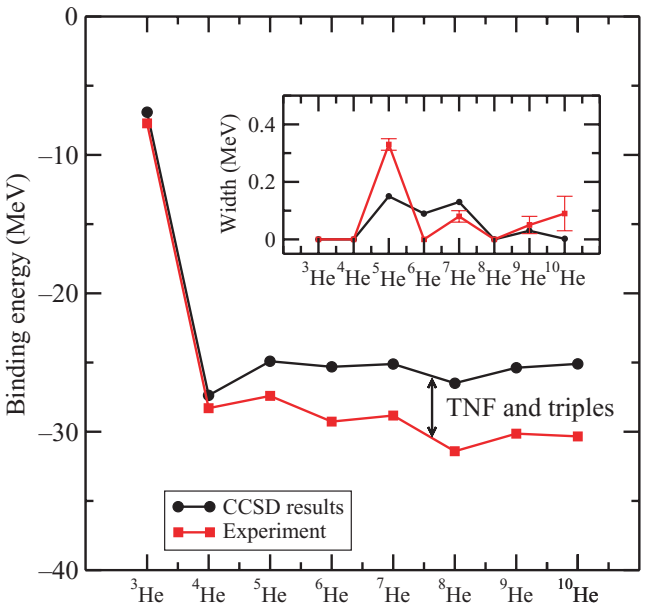

Figure 3. Real (large picture) and imaginary (inset) energies for the chain of helium isotopes up to ^{10}He. Experimental values are included. See text for further details.

possible three-nucleon forces or more complicated terms. The latter would aid us in explaining one of the major unresolved problems in low-energy nuclear physics, namely how nuclei evolve toward the line of stability.

4. Perspective and conclusions

CC theories hold great promise for extending the applicability of *ab initio* methods to heavier nuclei. Furthermore, more complicated many-body correlations such as those resulting from three-nucleon interactions can be included and studied in a systematic way. A preliminary study of three-nucleon forces was done in [8]. This work showed that the main contribution of the three-nucleon forces can be cast as density-dependent one- and two-body forces.

Our recent studies of weakly bound nuclei from [6] represent the first *ab initio* calculation of such systems. The experimental trend was well reproduced, but there remained discrepancy between theory and experiment. Since standard structure calculations seldom include either three-body interactions or the effect of the continuum, with our present formalism, we may therefore be able to answer how much of this discrepancy is due to neglected three-body interactions and how much is due to neglected continuum degrees of freedom. An interesting isotopic chain to study, in this context, are the neutron-rich oxygen isotopes, especially ^{20}O to ^{28}O. ^{24}O is the last bound isotope. Experimenters at RIKEN in Japan and at the National Superconducting Cyclotron Laboratory at Michigan State University are now planning new experiments in order to measure ground states and eventual excited states of ^{24}O and ^{25}O. Finally, the methods we have developed for weakly bound systems can be applied to other self-bound quantum mechanical systems with resonances.

Another future interest is to study the ground-state properties of medium-mass nuclei such as ^{56}Ni and ^{100}Sn. Both nuclei are within computational reach due to more efficient codes. In [9], we obtained recently converged results for the binding energies of ^{4}He, ^{16}O, ^{40}Ca, ^{48}Ca, and ^{48}Ni using 15 major oscillator shells and a bare nucleon–nucleon interaction. In those calculations, we have included only correlations of the one-particle-one-hole and two-particle-two-hole to infinite order. Three-body interactions and more complicated many-body clusters are not included. However, in addition to converged binding energies, we find that the differences in binding energies per particle for all these nuclei between theory and experiment are constant and close to 1 MeV. We ascribe this difference to three-body correlations and possibly other higher-body correlations. The fact that this difference is more or less constant is a welcome feature, as it may allow us to infer that the discrepancies between theory and experiment are mainly due to missing physics beyond a

Table 3. CCSD calculation of the $^{3-10}$He ground states with the low-momentum N^{3}LO nucleon–nucleon interaction [50] for increasing number of partial waves. The energies E are given in MeV for both real and imaginary parts. Our calculated width of ^{10}He is $\approx$0.002 MeV. Taken from [6].

	^{3}He		^{4}He		^{5}He		^{6}He	
lj	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
$s-p$	−4.94	−0.00	−24.97	−0.00	−20.33	−0.56	−19.07	−0.18
$s-d$	−6.44	−0.00	−26.61	−0.00	−23.56	−0.20	−23.25	−0.07
$s-f$	−6.82	−0.00	−27.27	−0.00	−24.53	−0.16	−24.69	−0.07
$s-g$	−6.91	−0.00	−27.35	−0.00	−24.84	−0.15	−25.17	−0.08
$s-h$	−6.92	−0.00	−27.37	−0.00	−24.90	−0.15	−25.28	−0.09
$s-i$	−6.92	−0.00	−27.37	−0.00	−24.91	−0.15	−25.31	−0.09
Expt	−7.72	0.00	−28.30	0.00	−27.41	−0.33(2)	−29.27	0.00
	^{7}He		^{8}He		^{9}He		^{10}He	
lj	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
$s-p$	−17.09	−0.25	−17.02	−0.01	−15.44	−0.28	−13.86	−0.14
$s-d$	−22.22	−0.09	−23.07	−0.00	−21.58	−0.13	−20.69	0.00
$s-f$	−24.19	−0.10	−25.44	−0.00	−24.16	−0.05	−23.67	−0.00
$s-g$	−24.90	−0.12	−26.25	−0.00	−25.10	−0.04	−24.77	−0.00
$s-h$	−25.08	−0.13	−26.45	−0.00	−25.34	−0.03	−25.05	−0.00
$s-i$	−25.11	−0.13	−26.49	−0.00	−25.38	−0.03	−25.10	−0.00
Expt	−28.83	−0.08(2)	−31.41	0.00	−30.14	−0.05(3)	−30.34	−0.09(6)

two-body Hamiltonian and correlations beyond two-particle-two-hole. The net effect of these missing degrees of freedom is roughly 10%. We believe this applies to the chain of helium isotopes as well, but obviously, this remains to be studied. We are now extending these studies to include nuclei such as ^{68}Ni and ^{78}Ni.

These studies will tell us about the saturation properties of modern nuclear interactions. It remains to be seen whether we might extend such calculations even to heavy nuclei such as ^{208}Pb. Calculations in medium-mass and heavy nuclei will also be useful in the construction of effective interactions for the nuclear shell model. We remind the reader that CC theory constructs a similarity transformed Hamiltonian that includes in-medium effects. This might also shed light on the contributions of three-nucleon forces to the single-particle energies and monopole matrix elements. With converged results for the binding energies of presumably good closed-shell nuclei, we plan to compute effective valence–space interactions to be used in standard shell-model calculations limited to one or two major shells.

Acknowledgments

We are much indebted to A Brown, M Horoi, N Michel, W Nazarewicz, T Otsuka, P Piecuch, M Płoszajczak, J Rotureau, and A Schwenk for many discussions on many-body physics. This work was supported in part by the US Department of Energy under contract numbers DE-AC05-00OR22725 (Oak Ridge National Laboratory, managed by UT-Battelle, LLC), DE-FG02-96ER40963 (University of Tennessee) and DE-FG05-87ER40361 (Joint Institute for Heavy Ion Research). Computational resources were provided by the Oak Ridge Leadership Class Computing Facility, the National Energy Research Scientific Computing Facility, and the Research Council of Norway via the Notur project (supercomputing grant NN2977K). This work was also supported by the UNEDF SciDAC Collaboration under DOE grant DE-FC02-07ER41457.

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