Coupled-cluster approach to an *ab-initio* description of nuclei

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We presents results from *ab-initio* coupled-cluster theory for stable, resonant and weakly bound nuclei. Results for the chain of helium isotopes $^{4-10}$He, ^{16}O and ^{40}Ca are discussed.

Keywords: Nuclear structure calculations; Coupled Cluster theory; Weakly bound nuclei; Ground state resonances

1. Introduction

The theoretical description of bound, weakly bound and unbound quantum many-body systems, together with present and planned experimental studies of such systems, represents a great challenge to our understanding of nuclear systems. Experiments in nuclear physics will address such important topics as how shells evolve, the role of many-body correlations, and the position of the stability lines of nuclei. The proximity of the scattering continuum in these systems implies that they should be treated as open quantum systems where coupling with the scattering continuum can take place. This means that a many-body formalism should contain resonant and continuum states in the basis in order to describe loosely bound systems or unbound systems. Extending the single-particle basis to include such degrees of freedom results in intractable dimensionalities for traditional configuration interaction methods (shell-model in nuclear physics) approaches.

Shell-model codes taylored to the nuclear many-body problem can today reach dimensionalities of approximately 10^{10} basis states. Some of the systems studied here exhibit dimensionalities of some 10^{60} basis states To circumvent this dimensionality problem, we have built a nuclear many-body program based on the coupled-cluster methods. Coupled-cluster theories allow for numerical cost-efficient ways of dealing with large dimensionalities compared with traditional configuration interaction methods.

We report here new results from coupled-cluster theories including both bound, resonant, and continuum states.[1–4] We also show that Coupled cluster theories reproduce benchmark results for light nuclei with minimal numerical cost and provide benchmarks for heavier nuclei.

2. Results and discussions

In addition to the above dimensionality problems, the nuclear many-body problem is riddled by the fact that there is no analytic expression for the underlying nucleon-nucleon (NN) interaction. Furthermore, three-body interactions are important in nuclear physics and need to be included in a systematic way in a many-body formalism. In recent years, quite a lot of progress has been made within chiral effective field theories to construct NN and three-nucleon interactions from the underlying symmetries of QCD. The starting point is then a chiral effective Lagrangian with nucleons and pions as effective degrees of freedom only. Three-body interactions emerge naturally and have explicit expressions at every order in the chiral perturbation theory expansion. In this work we have chosen to work with a nucleon-nucleon interaction derived from effective-field theory, such as the N^3LO model of Entem and Machleidt. In addition, we have also used the more phenomenological V_{18} interaction.

We renormalize the short-range part of the nucleon-nucleon interaction by a similarity transformation technique in momentum space, for details see Ref.[4] This renormalized interaction defines our Hamiltonian which enters the solution of the coupled cluster equations.

To obtain ground state energies of both bound and weakly bound systems, we need a many-body scheme which is (i) fully microscopic and size extensive, (ii) allows to include in a systematic way various many-body correlations to be summed to infinite order, (iii) can account for the description of both closed-shell systems and valence systems and (iv) capable to describe both bound and weakly bound systems. Coupled cluster theories allow for the inclusion of all these features.

Our coupled cluster approaches include $1p-1h$ and $2p-2h$ correlations, normally dubbed single and double excitations (CCSD). Correlations of the $3p-3h$ type are included perturbatively (labelled CCSD(T)) or via other approximations to the full $3p-3h$ correlations (CCSDT). Furthermore, for weakly bound systems we employ complex Gamow-Hartree-Fock single-particle basis and an effective interaction defined by such a single-particle basis[1,2]

In the left panel Fig. 1 we show the coupled-cluster results for ^{4}He and compare them with results from few-body calculations. There is an excellent agreement, showing that coupled-cluster reproduce other ab initio results with a much smaller numerical cost. The right panel shows the corresponding results for ^{16}O, providing a benchmark for this nucleus. The results are given as function of the number of oscillator shells, limited by $2n + l$. Details in Ref.[2] The ^{16}O results show an overbinding,which most likely is due to omitted three-body interactions. Fig. 2 shows results for ^{16}O (left panel) and ^{40}Ca as functions of the oscillator energy $\hbar\omega$ used in computing the oscillator wave function and the number of major shells N used in the coupled cluster calculations. As expected, with increasing size of the model space, the results stabilize as function of the chosen oscillator energy. Our results are converged with a given two-body Hamiltonian and we can therefore claim that lack of agreement with experiment is due to missing physics, such as three-body interactions, in our Hamiltonian.

In Tables 1 and 2 we present our recent CCSD results, see Ref.[3] for details, for the chain of helium isotopes using a complex single-particle basis. The largest model space has 850 single-particle orbitals, distributed among $5s5p5d4f44h4i$ proton orbitals and $20s20p5d4f44h4i$ neutron orbitals. For ^{10} this results in approximately 10^{22} basic states. These are the first ever *ab initio* calculations of weakly isotopes and we see that with a two-body Hamiltonian we are able to reproduce correctly the experimental trend and predict correctly which nuclei have bound ground states and which are resonances. The results are converged within our chosen model spaces. The quantitative lack of agreement with experiment is due to our omission of three-body interactions.

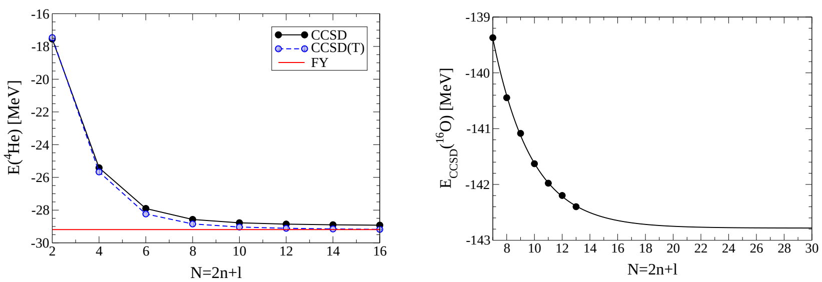

Fig. 1. Left figure is the binding energy for ^{4}He as function of the number of oscillator shells $N = 2n + l$. The maximum orbital momentum was set to $l = 7$. The right panel exhibits the corresponing result for ^{16}O. The V_{18} NN interaction was used.

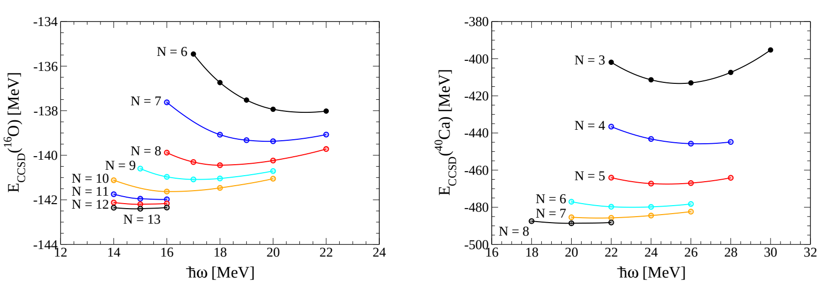

Fig. 2. Left figure is the binding energy for ^{16}O as function of the number of oscillator shells $N = 2n+l$ and oscillator energy $\hbar\omega$. The maximum orbital momentum was set to $l = 7$. The right panel is the corresponing result for ^{40}Ca. The V_{18} NN interaction was used.

Table 1. CCSD calculation of the $^{3-6}$He ground states with the low-momentum N^{3}LO nucleon-nucleon interaction for increasing number partial waves.

	^{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	-20.08	-0.54	-19.03	-0.18
$s-d$	-6.42	0.00	-26.58	0.00	-23.56	-0.22	-23.26	-0.09
$s-f$	-6.81	0.00	-27.27	0.00	-24.56	-0.17	-24.69	-0.07
$s-g$	-6.91	0.00	-27.35	0.00	-24.87	-0.16	-25.16	-0.06
Expt.	-7.72	0.00	-28.30	0.00	-27.41	-0.33(2)	-29.27	0.00

Table 2. CCSD calculation of the $^{7-10}$He ground states. Our calculated width of ^{10}He is ≈ 0.002MeV.

	^{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]
$s-p$	-17.02	-0.24	-16.97	-0.00	-15.28	-0.40	-13.82	-0.12
$s-d$	-22.19	-0.12	-22.91	-0.00	-21.34	-0.15	-20.60	-0.02
$s-f$	-24.13	-0.11	-25.28	-0.00	-23.96	-0.06	-23.72	-0.00
$s-g$	-24.83	-0.09	-26.26	-0.00	-25.09	-0.03	-24.77	-0.00
Expt.	-28.83	-0.08(2)	-31.41	0.00	-30.26	-0.05(3)	-30.34	0.09(6)

In summary, coupled cluster theories held great promises for a quantitative understanding of nuclei. With the possibility to include three-body interactions as discussed in Ref.,[1] we may be able to tell how nuclei evolve as one moves towards the drip line.

3. Acknowledgments

This work was supported in part by the U.S. Department of Energy under Contract Nos. DE-AC05-00OR22725 (Oak Ridge National Laboratory), DE-FG02-96ER40963 (University of Tennessee), DE-FG05-87ER40361 (Joint Institute for Heavy Ion Research), and by the Research Council of Norway (Supercomputing grant NN2977K). Computational resources were provided by the Oak Ridge Leadership Class Computing Facility and the National Energy Research Scientific Computing Facility. Discussions with A. Schwenk are acknowledged.

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