International Journal of Modern Physics B

COUPLED CLUSTER THEORY FOR NUCLEI

T. PAPENBROCK
Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA, and Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
tpapenbr@utk.edu

D. J. DEAN
Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

J. R. GOUR
Department of Chemistry, Michigan State University, East Lansing, MI 48824, USA

G. HAGEN
Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA, and Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

M. HJORTH-JENSEN
Department of Physics and Center of Mathematics for Applications, University of Oslo N-0316 Oslo, Norway

P. PIECUCH
Department of Chemistry, Michigan State University, East Lansing, MI 48824, USA

M. WLOCH
Department of Chemistry, Michigan State University, East Lansing, MI 48824, USA

Received Day Month Year
Revised Day Month Year

This presentation focuses on some of the recent developments in low-energy nuclear structure theory, with emphasis on applications of coupled cluster theory. We report on results for ground and excited states in ^{4}He and ^{16}O, and about extensions of coupled cluster theory to treat three-body forces.

Keywords: Nuclear structure, light nuclei, coupled cluster theory

1. Introduction

In recent years, much progress has been made in *ab-initio* nuclear structure calculations. The description of light nuclei can now be based on realistic nuclear interactions and powerful methods that solve the quantum many-body problem. The Greens Function Monte Carlo (GFMC) calculations have established the structure of light nuclei up to mass $A = 12$ [1,2], while the No-Core Shell Model (NCSM) approach has extended *ab-initio* structure calculations to heavier p-shell nuclei [3]. These approaches have led to two main results, namely (i) a unified description of light nuclei starting from nucleons and realistic interactions, and (ii) a much improved understanding and determination of the effective interaction itself. We would like to extend this approach to heavier systems. The coupled cluster method [4] is a very promising candidate for the endeavor, as it scales more favorably with increasing system size than the GFMC or the NCSM.

The progress in *ab-initio* nuclear structure calculations goes hand in hand with progress regarding the effective nuclear interactions. For a recent review, we refer the reader to Ref. [7]. Several realistic nucleon-nucleon potentials fit the two-nucleon phase shifts with a chi-square of one per degree of freedom. These potentials agree in their long range part, and differ in the modeling of the short range part. Note that the latter is presently neither constrained by experimental data on the phase shifts nor by theoretical arguments. As a consequence, different realistic potentials yield different results for many-nucleon systems.

There are at least two possible ways to resolve this dilemma. The first consists in an approach to nuclear interactions that is based on effective field theory [5,6]. Within chiral effective field theory, the effective Hamiltonian is constructed systematically up to a given order of the relative momentum, and the coupling coefficients are fit to reproduce nucleon-nucleon phase shifts and the deuteron bound state [7]. Within this approach, three-body forces naturally enter at higher order. The second way consists in an approach based on the renormalization group. Starting from a realistic potential, one might construct its low-momentum approximation by integrating out momentum modes above a cutoff parameter. This approach leaves the two-nucleon phase shifts unchanged for momenta below the cutoff, and thereby constructs a family of cutoff-dependent potentials that are phase shift equivalent. Interestingly, this approach [8] shows that the realistic potentials collapse onto a "universal" low-momentum potential $V_{\mathrm{low}-k}$. Within this approach, the form of the (cutoff-dependent) three-body force is determined by fit to the three- and four-nucleon system. Like in the chiral potential, the occurrence of three-body forces seems unavoidable. This not surprising: Nucleons are not elementary particles, and the omission of substructure, i.e. the removal of degrees of freedom, is accompanied by the occurrence of many-body forces.

This makes it interesting to test and to further explore the nuclear interaction through *ab-initio* nuclear structure calculations in heavier nuclei. Due to its favorable scaling coupled cluster theory is a promising tool for this endeavor. The

remainder of this article is divided as follows. In the next section, we briefly describe coupled cluster theory. This is followed by presentation of results for ^{4}He and ^{16}O. In the fourth section, we describe coupled cluster theory with effective three-body forces. We finally give a summary.

2. Coupled Cluster Theory

Coupled cluster theory is a very accurate approximation with relative low computational cost. It originated in nuclear physics [4], and saw applications in quantum chemistry a few years later [9]. For reviews, we refer the reader to Refs. [10,11,12,13,14,15]. In recent years, the theory has again been applied to nuclear structure calculations. Guardiola *et al.* performed studies of the center-of-mass problem [16]. Mihaila and Heisenberg [17] employed coupled cluster theory for the ground state calculation of ^{16}O. They obtained a theoretical description of the electron scattering structure function that agrees very well with experimental data [18]. These calculations used a bare nucleon nucleon interaction, and the density-dependent part of the three-body interaction. The approach followed in Refs. [19,20,21] is more conventional in the sense that it utilizes a G-matrix as the interaction, and it employs approximations that have become standards in numerous applications in quantum chemistry.

In coupled cluster theory, the ground state of the A-body system is approximated as

$$|\psi\rangle = e^{\hat{T}}|\Phi\rangle. \tag{1}$$

Here, $|\Phi\rangle$ is a single-particle product state (Slater determinant), and $\hat{T}$ is the cluster operator. It has the form of a particle-hole excitation operator

$$\hat{T} = 1 + \sum_{ia} t_i^a \hat{a}_a^\dagger \hat{a}_i + \sum_{ijab} t_{ij}^{ab} \hat{a}_b^\dagger \hat{a}_a^\dagger \hat{a}_i \hat{a}_j + \ldots, \tag{2}$$

and creates $1p-1h$, $2p-2h$,...,$Ap-Ah$ excitations in the product state $|\Phi\rangle$. Here, $\hat{a}_p^\dagger$ and $\hat{a}_q$ are fermionic creation and annihilation operators, respectively, and we have used the following convention: the labels $i, j, k, \ldots$ refer to single-particle orbitals that are occupied in $|\Phi\rangle$, while $a, b, c, \ldots$ refer to unoccupied orbitals. If the expansion (2) is carried out up to $Ap-Ah$ excitations, coupled cluster theory is exact. The success of coupled cluster theory, however, relies on the finding that a truncation of Eq. (2) at relatively low order already yields quite accurate results for interacting many-body systems. In what follows, we will restrict ourselves to the truncation after $2p-2h$ clusters (CCSD), and will occasionally include $3p-3h$ clusters approximately.

To obtain the coupled cluster equations within the CCSD approximation, one inserts the ansatz (1) into the Schrödinger equation, and left multiplies with $\langle\Phi_{i_1\ldots i_k}^{a_1\ldots a_k}|\exp(-\hat{T})$ for $k = 0, 1, 2$. This yields the CCSD equations

$$\begin{aligned} \langle\Phi|\overline{H}|\Phi\rangle &= E, \\ \langle\Phi_i^a|\overline{H}|\Phi\rangle &= 0, \end{aligned} \tag{3}$$

$$\langle \Phi_{ij}^{ab} | \overline{H} | \Phi \rangle = 0. \tag{4}$$

Here

$$\overline{H} \equiv \exp\left(-\hat{T}\right) H \exp\left(\hat{T}\right) \tag{5}$$

is the similarity transformed Hamiltonian, and $\langle \Phi_{i_1 \dots i_k}^{a_1 \dots a_k}|$ is the adjunct of the $kp-kh$ excited state $|\Phi_{i_1 \dots i_k}^{a_1 \dots a_k}\rangle = \hat{a}_{a_k}^\dagger \dots \hat{a}_{a_1}^\dagger \hat{a}_{i_1} \dots \hat{a}_{i_k} |\Phi\rangle$. The second and third of the Eqs. (3) determine the unknown cluster amplitudes t_i^a and t_{ij}^{ab}, and they constitute a coupled set of nonlinear equations. These equations can be solved iteratively, at the relatively low computational cost $\mathcal{O}(n_o^2 n_u^4)$, where n_o and n_u refer to the number of occupied and unoccupied orbitals, respectively. The energy is obtained by inserting the solution of these equations into the first of the Eqs. (3).

Note that the similarity transformed Hamiltonian (5) is non-Hermitian. This renders coupled cluster theory a non-variational approximation. However, this "disadvantage" is more than compensated by the advantage that $\overline{H}$ can be determined exactly without any further approximation. In a diagrammatic language, only fully connected diagrams enter the expression for $\overline{H}$. For the computation of excited states [22], one diagonalizes the similarity transformed Hamiltonian (5) in the space of all $1p-1h, \dots, kp-kh$ excitations of the product state $|\Phi\rangle$. Within the CCSD approximation one has $k=2$, and the excited states can thus be computed for large model spaces where a full matrix diagonalization would be prohibitively expensive. In principle, one could test the quality of the CCSD approximation by comparing the results with a more expensive calculation that also includes $3p-3h$ cluster excitations. Such a calculation scales as $\mathcal{O}(n_o^3 n_u^5)$, and is thus much more expensive. For this reason, we include the $3p-3h$ cluster only approximately and follow the method that is described in Ref. [23].

3. Results for ^{4}He and ^{16}O

Our calculations on ^{4}He are reported in Ref. [20]. They employ a G-matrix based on the Idaho-A potential [24]. We worked in a spherical harmonic oscillator basis with oscillator frequency Ω, and controlled the center-of-mass problem by adding the center-of-mass Hamiltonian $\frac{\beta}{2}(P^2/M + M\Omega^2 R^2 - 3\hbar\Omega)$ to the Hamiltonian. The Lagrange multiplier β is chosen such that the expectation value of the center-of-mass Hamiltonian is extremal. The calculation was performed in a rather small model space consisting of four oscillator shells. This allowed us to check the quality of the CCSD approximation and to compare with results from exact diagonalizations of the same Hamiltonian. The results are displayed in Table 1. Clearly, CCSD is a good approximation, particularly when compared to CISD – an exact diagonalization in a space of $1p-1h$ and $2p-2h$ excited states which is computationally as expensive as CCSD. This clearly demonstrates that the similarity transformed Hamiltonian (5) contains much more relevant physics that its Hermitian counterpart. The $3p-3h$

corrections denoted by "CR-CCSD(T)" improve the CCSD result, and are close to the exact result. The coupled cluster approximation works equally well for a reference state $|\Phi\rangle$ that is a product of $0s$ oscillator states as for a product state based on the Hartree-Fock (HF) approximation for ^{4}He. For the oscillator basis, both the $1p-1h$ and the $2p-2h$ cluster amplitudes yield considerable contributions to the total binding energy. This is different for the HF basis, where most of the correlation energy stems from the $2p-2h$ cluster amplitudes. The calculations of Ref. [20] also showed that excited states of nuclei can reliably computed within the CCSD approximation.

Table 1. The ground-state energies of ^{4}He calculated using the oscillator (Osc) and Hartree-Fock (HF) basis states. Units are MeV. The reference energies $\langle\Phi|H'|\Phi\rangle$ are -7.211 (Osc) and -10.520 (HF) MeV. Taken from Ref. [20].

Method	Osc	HF
CCSD	-21.978	-21.385
CR-CCSD(T),c	-22.630	-22.450
CR-CCSD(T),c/$\Delta_0 = 1$	-23.149	-22.783
CISD	-20.175	-20.801
Exact	-23.484	-23.484

Our calculations for ^{16}O employ G-matrices based on the Idaho-A and the chiral N3LO potential [25]. The results are reported in Ref. [21]. One of the main questions concerns the convergence of numerical results with respect to the increasing size of the model space. The results of our calculations (See, e.g. Fig. 1 of Ref. [21]) show that the ground state energy converges well for a model space consisting of seven to eight oscillator shells, the difference in binding energy being about 0.5MeV for both model spaces. As previously found for ^{4}He, $3p-3h$ corrections are very small and account for only 0.7MeV additional binding. The binding energies are -109MeV and -112MeV for the Idaho-A and the N3LO potential, respectively. This suggests that the difference to the experimental value of -128MeV must be attributed to deficiencies of the Hamiltonian itself, and it points to the need of three-body forces.

The computation of the excited states of ^{16}O also yielded interesting results. For the Idaho-A potential, we found a $J^\pi = 3^-$ state at about 12MeV excitation energy, and a $J^\pi = 0^+$ state at about 22MeV. Calculations with the N3LO potential yielded similar results. The 3^- state exhibits only small corrections due to $3p-3h$ cluster amplitudes, while the corrections are considerable for the 0^+ state. This is no surprise. The excited 3^- states is known to be mainly a single-particle excitation, while the first excited 0^+ state is thought to be an α-particle excitation and thus of $4p-4h$ character. Within the CCSD approximation, it is impossible to accurately reproduce such a state. Note, that is argument does not apply to the ground state, as the reference Slater-determinant already can be viewed as a cluster of α-particles.

Note also that Nature puts the excitation energy of the 3^- state at about 6.16MeV. Again, the deviation of our theoretical result points to deficiencies of the employed Hamiltonian. This motivates us to consider coupled cluster theory with effective three-body forces.

4. Outlook: Three-Body Forces

The precise description of light nuclei cannot be accomplished with local two-body potentials alone, and the inclusion of three-body forces remedies the situation. Three-body forces affect overall binding as well as level ordering. This occurrence of three-body forces is not surprising. Nucleons, the fundamental degrees of freedom in low-energy nuclear structure theory, are not point particle. Thus, their internal excitations (e.g. the Δ-resonance) are excluded from the model space. This approach is justified by the observation that those excitations are much higher in energy (typically hundreds of MeV) than typical excitations in nuclei (of the order of 1MeV). At low excitation energies, however, the presence of subnuclear degrees of freedom is indistinguishable from three-body forces. This argument is well known from renormalization group theory: integrating out high-momentum (or high-energetic) degrees of freedom creates effective low-momentum Hamiltonians with interactions that have a higher rank than two.

This makes it necessary to use three-body forces in coupled cluster theory. As a first step, one has to derive coupled cluster equations for three-body Hamiltonians. Formally, these are given by Eqs. (3). However, the similarity transformed Hamiltonian (5) has to be evaluated for three-body terms. This introduces a number of new terms to the coupled cluster equations. In practice, $\overline{H}$ can most conveniently be evaluated in a diagrammatic form. The CCSD equations for the energy, and the cluster amplitudes t_i^a and t_{ij}^{ab} consist of two, fifteen, and 51 diagrams, respectively. As an example, Fig. 1 shows the CCSD diagrams of the three-body force that contribute to the energy.

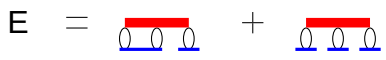

Fig. 1. A diagrammatic equation for the contributions of three-body forces to the coupled cluster energy within the CCSD approximation.

Here, the long bars denote the three-body Hamiltonian, while the shorter bars denote the $1p-1h$ and $2p-2h$ cluster operators. The energy is obtained by fully contracting the Hamiltonian with the cluster operators. The algebraic expression corresponding to Fig. 1 is

$$E = \frac{1}{4}\sum_{klmcde}\langle klm||cde\rangle t_k^c t_{lm}^{de} + \frac{1}{6}\sum_{klmcde}\langle klm||cde\rangle t_k^c t_l^d t_m^e. \qquad (6)$$

Here, $\langle klm||cde\rangle$ denotes the three-body matrix elements. For the efficient numerical implementation we write the CCCD equations in factorized form [26], such that more complex diagrams result from successive contractions of simple sub-diagrams with individual cluster amplitudes. This approach allows us to re-use many sub-diagrams, and to order the contractions such that the computational cycle count is minimal. At present, we have derived and implemented coupled cluster theory for three-body Hamiltonians. Near-future calculations for ^{16}O and ^{40}Ca will unravel the role that three-body forces play for medium mass nuclei, and will also help us to better constrain the three-body force itself. The pending results of these calculations will be reported elsewhere.

5. Summary

We employed coupled cluster theory for nuclear structure calculations, and obtained an *ab initio* description of light nuclei. Within the two-particle two-hole cluster approximation, we obtained results for the ground and excited states of ^{4}He and ^{16}O that are fully converged with respect to the size of the model space, and corrections due to three-particle three-hole clusters are small. The difference between our results for oxygen and experimental values suggest that the microscopic Hamiltonian we employed is deficient, and that three-body forces might be the missing ingredient. We have extended coupled cluster theory to treat three-body interactions, and derived the corresponding coupled cluster equations. This will enable us to explore the role of these forces in medium mass nuclei.

Acknowledgments

Research supported by the U.S. Department of Energy (Oak Ridge National Laboratory, University of Tennessee, Michigan State University), the National Science Foundation (Michigan State University), and the Research Council of Norway (University of Oslo).

References

1. S. C. Pieper and R. B. Wiringa, *Ann. Rev. Nucl. Part. Sci.* **51**, 53 (2001).
2. R. B. Wiringa and S. C. Pieper, *Phys. Rev. Lett.* **89**, 182501 (2002).
3. P. Navrátil and W. E. Ormand, *Phys. Rev. C* **68**, 034305 (2003); *Phys. Rev. Lett.* **88**, 152502 (2002).
4. F. Coester, *Nucl. Phys.* **7**, 421 (1958); F. Coester and H. Kümmel, *Nucl. Phys.* **17**, 477 (1960).
5. S. Weinberg, *Phys. Lett. B* **363**, 288 (1990).
6. U. van Kolck, *Prog. Part. Nucl. Phys.* **43**, 337 (1999).
7. R. Machleidt and I. Slaus, *J. Phys. G* **27**, R69 (2001).
8. S. K. Bogner, T. T. S. Kuo, and A. Schwenk, *Phys. Rep.* **386**, 1 (2003).
9. J. Čížek, *J. Chem. Phys.* **45**, 4256 (1966); *Adv. Chem. Phys.* **14**, 35 (1969).
10. H. Kümmel, K. H. Lührmann, and J. G. Zabolitzky, *Phys. Rep.* **36**, 1 (1978).

11. R. J. Bartlett, *J. Phys. Chem.* **93**, 1697 (1989); J. Paldus and X. Li, *Adv. Chem. Phys.* **110**, 1 (1999).
12. R. F . Bishop, in *Microscopic Quantum Many-Body Theories and Their Applications*, eds.: J. Navarro and A. Polls, Lecture Notes in Physics, Vol. **510** (Springer, Berlin, 1998), p. 1.
13. T. D. Crawford and H. F. Schaefer III, *Rev. Comput. Chem.* **14**, 33 (2000).
14. H.G. Kümmel, in *Recent Progress in Many-Body Theories*, eds.: R. F. Bishop *et al.* (World Scientific, Singapore, 2002), p. 334.
15. P. Piecuch *et al.*, *Theor. Chem. Acc.* **112**, 349 (2004).
16. R. Guardiola, P. I. Moliner, J. Navarro, R. F. Bishop, A. Puente, and N. R. Walet, *Nucl. Phys.* **A609**, 218 (1996).
17. J. H. Heisenberg and B. Mihaila, *Phys. Rev. C* **59**, 1440 (1999); B. Mihaila and J. H. Heisenberg, *Phys. Rev. C* **61**, 054309 (2002).
18. B. Mihaila and J. H. Heisenberg, *Phys. Rev. Lett.* **84**, 1403 (2000).
19. D. J. Dean and M. Hjorth-Jensen, *Phys. Rev. C* **69**, 054320 (2004).
20. K. Kowalski, D.J. Dean, M. Hjorth-Jensen, T. Papenbrock, and P. Piecuch, *Phys. Rev. Lett.* **92**, 132501 (2004).
21. M. Włoch, D. J. Dean, J. R. Gour, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock, and P. Piecuch, *Phys. Rev. Lett.* **94**, 212501 (2005).
22. H. Monkhorst, *Int. J. Quantum Chem. Symp.* **11**, 421 (1977); K. Emrich, *Nucl. Phys. A* **351**, 379 (1981).
23. K. Kowalski and P. Piecuch, *J. Chem. Phys.* **120**, 1715 (2004).
24. D. R. Entem and R. Machleidt, *Phys. Lett. B* **524**, 93 (2002).
25. D. R. Entem and R. Machleidt, *Phys. Rev. C* **68**, 041001 (2003).
26. S. A. Kucharski and R. J. Bartlett, *Theor. Chim. Acta* **80**, 387 (1991).