COUPLED-CLUSTER THEORY FOR NUCLEI *

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In these Proceedings, I discuss recent developments and applications of coupled cluster theory to calculations of properties of medium-mass nuclei. I will report on results for both the closed-shell nucleus ^{16}O and its neighbors. I will also discuss future directions involving the implementation of a three-body force and resonant states into the coupled-cluster problem.

1. Current perspectives in the study of nuclei

Six years from now, new nuclear facilities will be churning out experimental data on short-lived nuclei. RIBF at RIKEN in Japan, SPIRAL-II, and GSI-FAIR will all be well on the way to either completion or full schedules of runs. The U.S. will also have an enhanced program established to continue research associated with the physics of nuclei. Today's experimental facilities are paving the way with exciting results concerning the nature of closed shells, the behavior of light nuclei near the drip lines, and the characteristics of very neutron-rich and unstable nuclei. Such results also impact our understanding of element production in the Universe, and have various application-oriented uses.

Nuclear theory during the same time frame faces the continuing challenges of developments that enable answers to the question(s): "Given a lump of nuclear material, what are its properties, where did it come from, and how does it interact?" We seek a unified framework for the description of nuclei and nuclear reaction processes that allows for accurate predictions and quantifiable error estimates for those predictions. Important in this pursuit is the understanding that we will not be able to measure every nuclear property that may be important even with the most sophisticated future experimental facilities. For example, neutron

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cross sections on highly radioactive species may be important in the design of next-generation reactors or in various astrophysical nucleosynthetic processes, but their actual measurement may be difficult to impossible.

The nuclear many-body problem represents unique challenges and yet entails significant similarities with other fields of science. We use techniques to solve the many-body problem that are used in other quantum systems (for example, Green's function Monte Carlo, Hamiltonian diagonalization, many-body perturbation theory, coupled-cluster theory, Bloch-Horowitz, nuclear DFT and extensions to it). All of these methods focus on solutions of a problem filled with difficulty and yet at the same time, in some instances, possessing rather astonishing simplicity (magic numbers, for example). The nuclear quantum many-body problem has the unique feature of being driven by a Hamiltonian that is characteristically short-ranged, with many active operators (spin, angular momentum, isospin, tensor,...). In contrast to atoms and molecules, the nuclear interaction self-binds protons and neutrons in the nucleus. Furthermore, the nuclear interaction is not completely understood, although one may argue that it is, in fact, pretty much understood. Indeed recent progress enabled the community to describe certain nuclear properties through mass 12 in an ab initio many-body framework. The future holds the promise of using these ab initio results to guide one to the appropriate choice of density functional to be used in heavy nuclei calculations.

Theoretical challenges facing our field were outlined in the RIA Theory Blue Book[1] written in 2005 by a large part of the community. That document outlined broadly our efforts to describe nuclei. They include:

- development of ab initio approaches to medium-mass nuclei,
- development of self-consistent nuclear density-functional theory methods for static and dynamic problems,
- development of reaction theory that incorporates relevant degrees of freedom for weakly bound nuclei,
- exploration of isospin degrees of freedom of the density-dependence of the effective interaction in nuclei,
- development and synthesis of nuclear theory, and its consequent predictions, into various astrophysical models to determine the nucleosynthesis in stars,

These bullets represent the community's long-term goals for the pursuit of studies of nuclei. I might add a further applications-oriented bullet: development of robust theory and error analysis for nuclear reactions relevant to various security and energy applications.

In the remainder of these Proceedings, I will touch on work in coupled-cluster theory which is one of the methods tied to the first bullet in the list above. While we are currently developing coupled-cluster theory in closed-shell nuclei, our long-term goal is to develop the theoretical and computational tools of the coupled-cluster method that will be necessary to investigate very neutron-rich nuclei. We seek, with the application of coupled-cluster theory to nuclei, to describe some properties of larger nuclear systems in an ab initio framework. These developments represent one of the paths forward as we seek ultimately to answer the primary question "Given a lump of nuclear material what are its properties....".

2. Current progress in coupled-cluster theory for nuclei

Modern nucleon-nucleon interactions precisely reproduce phase shifts derived from experimental scattering data. They are based either on meson-exchange models[2,3] or generated through applications of effective field theory[4,5] to chiral Lagrangians that maintain the symmetries of QCD.[6] While these interactions reproduce nucleon-nucleon phase shifts up to a typical momentum scale of 350 MeV, they differ in their treatments of short-range interactions, and therefore results obtained from them for binding energies and nuclear spectra can be different. It has long been surmised[7] that a three-body interaction must be invoked to obtain appropriate nuclear binding, and effective field theory work indicates that three-body interactions arise naturally from diagrammatic power counting.[8] While based on slightly more phenomenological terms, the importance of nuclear three-body interactions for both ground-state energies and spectra was demonstrated by Green's Function Monte Carlo (GFMC) calculations.[9]

The GFMC approach[10] will be discussed in other proceedings of the Workshop. The advantage of the GFMC technique is its use of bare nuclear interactions. Its disadvantage, at least at present, is its incapability to treat interactions that are non-local in r-space. Other approaches rely on building a set of many-body basis states from the underlying single-particle basis. Using a basis necessarily leads to the need to renormalize the bare nuclear interactions for the given set of basis states. Furthermore, the above interactions all have a fairly repulsive core and therefore would require for direct implementation enormous basis sets to obtain converged results which capture the high-momentum components of the interaction (i.e., they would have to reach the 1 GeV scale). To avoid this, one resorts to methods that renormalize the interaction so that it may be computed in a small set of basis states. In standard notation, we divide the two-particle space into the P-space and Q-space such that $P + Q = 1$ and P and Q are projection operators. A goal is to make the P-space small enough to both capture the physics and allow for computation within that space.

Various approaches exist to determine the effective interaction for the P-space. We have used the Brueckner G-matrix approach for the renormalization that yields an effective interaction,[11,12] while the similarity-transform approach due to Lee and Suzuki[13,14] has been used in No-Core Shell Model (NCSM) calculations.[15] The advantage of the similarity-transform approach is that it yields a starting-energy independent solution for the two-body effective interaction, whereas the G-matrix contains the starting-energy (ω) as a parameter, since it is the solution to an equation of the form $G(\omega) = V_{NN} + V_{NN}\frac{\tilde{Q}}{\omega - t}G(\omega)$, where $\tilde{Q}$ allows only two-body state scattering, t describes the one-body part of the Hamiltonian, and V_{NN} is the bare two-body interaction. In many of our previous coupled-cluster calculations, we used the G-matrix with the Bethe-Brandow-Petschek theorem[16] to alleviate much of the starting-energy dependence. Quantitatively, ^{16}O calculations indicate that a 20-MeV change in the starting energy results in a 2-MeV change in the total binding energy using this prescription.

Once we have an effective interaction in a given model space, we then need to set up a many-body technique to solve for the correlated wave function, energy levels, and transition operators within a nucleus. One approach to the problem would be to diagonalize the renormalized nuclear Hamiltonian within the set of basis states as is done in the NCSM.[15] Please note, NCSM is a many-body theory, not a model and has been rather successful in describing light nuclear data.

An alternative approach to Hamiltonian diagonalization is coupled-cluster theory[17,18,19,20] which represents the wave function as an exponential rather than a linear combination of particle-hole excitation operators acting on a reference Slater determinant. In coupled-cluster theory the correlated many-body wave function is

$$| \Psi\rangle = \exp(T) \mid \Phi\rangle \ , \tag{1}$$

where $| \Phi\rangle$ is a Slater determinant representing the non-interacting system and $T = T_1 + T_2 + ...$, with T_n being an n-particle-n-hole correlation operator of the form

$$T_n = \sum_{ab\ldots,;ij\ldots} t_{ij\ldots}^{ab\ldots} a_a^\dagger a_b^\dagger \cdots a_j a_i \ . \tag{2}$$

The amplitudes may be determined by solving the non-linear coupled algebraic equations

$$\langle \Phi_{ij\ldots}^{ab\ldots} \mid \exp(-T) H \exp(T) \mid \Phi\rangle = \langle \Phi_{ij\ldots}^{ab\ldots} \mid [H \exp(T)]_C \mid \Phi\rangle = 0 \ , \tag{3}$$

where H is the Hamiltonian, C means only linked diagrams enter, and $| \Phi_{ij\ldots}^{ab\ldots}\rangle$ are excited Slater determinants built upon the uncorrelated ground-state determinant $| \Phi\rangle$. Labels $a, b, c, \cdots$ represent particle states while $i, j, k, \cdots$ represent hole states. If we work within the coupled-clusters in singles and doubles (CCSD) framework, then one simultaneously solves for the t_i^a 1p-1h and t_{ij}^{ab} 2p-2h amplitudes from Eqn. 3, while all other higher-order amplitudes are assumed to be zero. For two-body interactions, the similarity transformed Hamiltonian is given by

$$\bar{H} = (H\exp(T))_C = \left(H + HT_1 + \frac{1}{2}HT_1^2 + HT_2\right)_C \ . \tag{4}$$

Note that although we solve only for the 1p-1h and 2p-2h amplitudes, the wave function contains many higher-order excitations due to the exponential character of the correlation operator $\exp(T)$.

We use Hamiltonians of the form

$$H = T - T_{\rm CoM} + V + \beta_{\rm CoM} H_{\rm CoM} \ , \tag{5}$$

where V is the two-body interaction, $T_{\rm CoM}$ is the center-of-mass kinetic energy, T is the kinetic energy of the particles, and $\beta_{\rm CoM} H_{\rm CoM}$ is a correction term applied such that the expectation value $\langle H_{\rm CoM}\rangle = 0$ at some (on the order of 0.01 in larger model spaces) value of $\beta_{\rm CoM}$.

In several papers[21,22,23,24] we have developed the coupled-cluster techniques for nuclear systems. Our initial results have all been obtained using a G-matrix formalism for model spaces including up to 8 major oscillator shells. We found that the oscillator energy ($\hbar\Omega$) dependence of results decreases significantly around the $\hbar\Omega$ minimum as one increases the model space. We also found convergence of results with model-space size. We showed that for the ^{16}O system, non-iterative triples corrections hardly affect the total binding energy, and using the equation of motion CCSD (EOMCCSD) method,[25,26] we calculated the excitation energy of the first excited 3^- state to be 11.5 MeV (and with excited-state non-iterative triples corrections, 12.0 MeV).

Furthermore, we recently completed a study of the mass $A = 15, 17$ nuclei around ^{16}O using particle-removed and particle-attached EOM methods.[24] We illustrate the results of these calculations for 8 major oscillator shells (480 single-particle basis states) in Table 1. These results illustrate the coupled-cluster capability we have developed during the last three years.

As shown in Table 1, the CD-Bonn and the N^{3}LO models result in the largest spin-orbit splittings (much larger than in the case of V_{18}). While we used the $\hbar\Omega$ which yields the minimum binding energy for ^{16}O at $N = 8$ oscillator shells, and the ^{16}O ground-state has stabilized, there remains some $\hbar\Omega$ dependence in these excited states. For example, for $N = 6$, the excited states of the $A = 15$ system change by approximately 0.4 MeV in the $\hbar\Omega = 11 - 14$ MeV window, while the $A = 17$ states change by approximately 0.7–1.1 MeV in the same $\hbar\Omega$ window. This would indicate a stronger dependence on $\hbar\Omega$ for the $A = 17$ nuclei than

Table 1. A comparison of the energies of the low-lying excited states of ^{15}O, ^{15}N, ^{17}O and ^{17}F, relative to the corresponding ground-state energies (the $(1/2)_1^-$ states of ^{15}O and ^{15}N and the $(5/2)_1^+$ states of ^{17}O and ^{17}F), obtained with the PR-EOMCCSD (^{15}O and ^{15}N) and PA-EOMCCSD (^{17}O and ^{17}F) methods, the N^{3}LO[5], CD-Bonn[3], and V_{18}[2] potentials, and eight major oscillator shells, with the experimental data in the last column[27]. All entries are in MeV. For the CD-Bonn and N^{3}LO interactions, we used $\hbar\Omega = 11$ MeV. For V_{18}, we used $\hbar\Omega = 10$ MeV. For eight major shells $\beta_{\rm CoM} = 0.0$.

	Interaction			
Excited state	N^{3}LO	CD-Bonn	V_{18}	Expt
^{15}O $(3/2)_1^-$	6.264	7.351	4.452	6.176
^{15}N $(3/2)_1^-$	6.318	7.443	4.499	6.323
^{17}O $(3/2)_1^+$	5.675	6.406	3.946	5.084
^{17}O $(1/2)_1^+$	-0.025	0.311	-0.390	0.870
^{17}F $(3/2)_1^+$	5.891	6.677	4.163	5.000
^{17}F $(1/2)_1^+$	0.428	0.805	0.062	0.495

for the states in the $A = 15$ and ^{16}O nuclei. We see a similar, but decreasing, dependence in the $N = 7$ calculations, where we only performed the check at $\hbar\Omega = 14$ MeV. At least for the hole states we obtain results which stabilize as a function of the number of shells. For the excited states of ^{17}O and ^{17}F, there is still a relatively strong dependence on the number of shells and $\hbar\Omega$. The $(3/2)_1^+$ states are known resonances, and we do therefore expect that our approximation at the particle-attached EOMCCSD calculations may miss some important correlations in this case.

Using information we have for the N^{3}LO interaction, including the $A = 15, 17$ results, and the result of EOM calculations that yield the first-excited 3^- state at 11.5 MeV of excitation, we are able to see the nature of the failure of the two-body interaction. Note that experimentally, the first excited 3^- state in ^{16}O lies at 6.1 MeV. In the lowest order approximation, this state should be a 1p-1h excitation from the $0p_{1/2}$ hole state to the $0d_{5/2}$ particle state relative to the ^{16}O ground state. The energy required to produce such an excitation is

$$\Delta\epsilon_\pi = \epsilon_\pi(0d_{5/2}) - \epsilon_\pi(0p_{1/2}) = +[\mathrm{BE}(^{16}\mathrm{O}) - \mathrm{BE}(^{15}\mathrm{N})] = 11.526\ \mathrm{MeV}, \quad (6)$$

for the proton case. Similarly for the neutron case, we obtain $\Delta\epsilon_\nu = 11.521$ MeV. Thus, experimentally, the interactions among nucleons lower the energy of the first excited 3^- state by $11.5 - 6.1 = 5.4$ MeV. For the N^{3}LO interaction, a similar argument yields $\Delta\epsilon_\pi = 15.846$ MeV and $\Delta\epsilon_\nu = 15.789$ MeV. Using our excitation energy of 11.5 MeV, we see that we are off by $15.8 - 11.5 = 4.3$

MeV. While this is an interaction- (and method) dependent result, it represents a fairly stable situation in our calculations. We find that the discrepancy of 4.3 MeV between theory and experiment for the energy gap between the $0p$ and $1s0d$ shells accounts for a large fraction of the missing 6 MeV needed to reproduce the first 3^- state of ^{16}O. In the future, we will investigate both the additional correlations brought in by higher-order coupled-cluster methods, and also the effect on the spin-orbit splitting and major shell splitting of three-body forces.

All of the above calculations were performed within the context of our implementation of the G-matrix.[12] Another avenue of defining the renormalized nuclear potential is known in the literature as $V_{\text{low}k}$.[28] The approach defines a low-momentum interaction (with momentum cutoff $\Lambda \sim 2.0$ fm^{-1}) by following a renormalization group (RG) equation from a very large cutoff to the desired low-momentum cutoff. The RG approach integrates out modes in the interaction with momenta larger than the cutoff. The procedure preserves the half-on-shell T-matrix scattering amplitudes, and therefore the phase shifts. Since the RG equation and Lee-Suzuki approaches are actually equivalent[29] in momentum space, there will necessarily be effective three-body forces that arise from following the RG approach to a low-momentum cutoff Λ.

Since $V_{\text{low}k}$ reproduces phase-shifts by construction, one can investigate whether it is a model-independent interaction. Using CCSD, I calculated the binding energy of ^{16}O using $V_{\text{low}k}$ derived from two different interactions, CD-Bonn and N^{3}LO, using the same cutoff $\Lambda = 2.0$ fm^{-1}. The results of these calculations are shown as a function of $\hbar\Omega$ in Fig. 1. One sees from this figure that the $V_{\text{low}k}$ associated with two different forces yields different binding. The difference is approximately 10 MeV, which compares to an approximately 14-MeV difference we see between the ground-state energies using our G-matrix interactions at the same starting energies.[24] We can conclude that while $V_{\text{low}k}$ may yield phase equivalence at the two-body level, there is still off-shell behavior that does not make the potential model independent. One also sees significant overbinding with $V_{\text{low}k}$ which must be cured by the further inclusion of a three-body force, as was recently done in the few-body systems.[30]

3. Future paths in coupled-cluster theory

For nuclei with realistic interactions, one should also include three-body interactions. Furthermore, even when one applies the Lee-Suzuki theory or the $V_{\text{low}k}$ approach to obtain an effective two-body interaction, one also necessarily generates an effective three-body potential, which one often ignores in calculations. The effects of this effective three-body potential should become larger as the single-

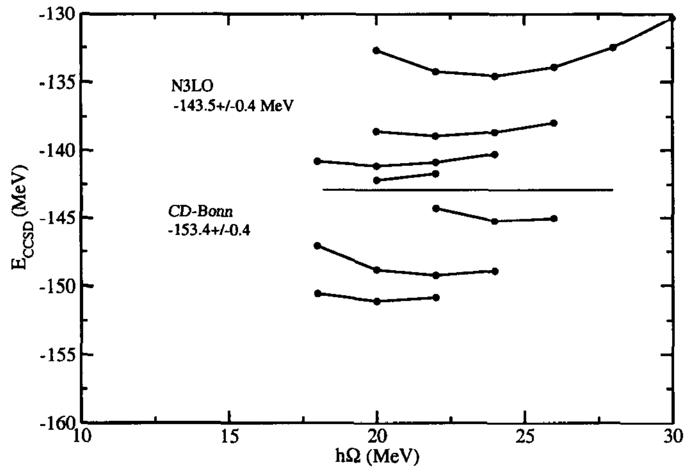

Figure 1. Comparison of $V_{\mathrm{low}k}$ results for the CD-Bonn and N^{3}LO interaction at the same cutoff of $\Lambda = 2.0\ \mathrm{fm}^{-1}$. Lines indicate $N = 5, 6, 7, 8$ shell calculations for N^{3}LO and $N = 5, 6, 7$ shell calculations for CD-Bonn. An extrapolation to the infinite basis was made at using $N = 5, 6, 7$ data in both cases.

particle basis set becomes smaller. Furthermore, we know that real three-body forces should exist in nuclei. We are currently developing coupled-cluster theory at the CCSD level to incorporate three-body interactions.[31] Additional complications come from storage needs and the number of terms that enter Eq. 3. With a three-body interaction included in the Hamiltonian, we obtain for the coupled-cluster similarity-transformed Hamiltonian

$$\bar{H} = \Big[H + HT_1 + \frac{1}{2}HT_1^2 + HT_2 + \frac{1}{6}HT_1^3 + HT_1T_2 + \frac{1}{24}HT_1^4 + \frac{1}{2}HT_1^2T_2 + \frac{1}{2}HT_2^2 + \frac{1}{120}HT_1^5 + \frac{1}{6}HT_1^3T_2 + \frac{1}{2}HT_1T_2^2\Big]_C , \quad (7)$$

where clearly many more terms enter into the amplitude equations.

A second avenue that we are pursuing in coupled-cluster applications involves transforming the nucleon-nucleon interaction problem into a complex basis[32] through a complex rotation. Once the Hamiltonian is transformed to a complex basis, the coupled-cluster technology (also transformed to complex basis states and amplitudes) can then be used to investigate nuclear ground and resonant states.[33]

We are also beginning to work with computer scientists to construct the tensor-multiplies that are carried out within the coupled-cluster algorithm to scale to at least 20,000 processors. Our physics goal is to describe nuclei with 100 particles and 1,000 single-particle basis states. This will require an algorithm change to deal with memory and operation counts, but it is possible during a time when petascale computers will become available.

We should be able to report on each of the above activities in the next 3 years as we move towards ab initio calculations of medium-mass nuclei in the context of coupled-cluster theory. We believe this will be one tool to help us continue our quest to study the physics of nuclei.

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