Nuclear Structure

The nucleus is a fascinating quantum mechanical system exhibiting diverse and rare phenomena. Governed by the strong interactions between nucleons, nuclei exhibit strong correlations resulting in both single-particle and collective modes of excitation; examples of the latter include Goldstone modes like rotation and tunneling between spherical and deformed intrinsic nuclear configurations. Nuclear theory attempts to understand these excitations and the response of nuclei to diverse external probes within a coherent framework. This framework must encompass a wide range of energy and momentum scales for nuclei ranging from the deuteron to the superheavy elements. Nuclear theorists strive to describe the structure and dynamics of these often-disparate systems, and to apply our knowledge of these systems to help unravel mysteries of our Universe.

One of the primary goals of nuclear physics is to explain the properties and reactions of nuclei in terms of interacting nucleons (protons and neutrons). There are two fundamental aspects to this problem: (1) determining the interactions between nucleons, and (2) given the interactions (i.e., the Hamiltonian), making accurate calculations of many-nucleon systems. The Argonne/Urbana/Los Alamos group uses NERSC computing resources to evaluate six- through ten-nucleon systems with realistic interactions also developed by that group [see e.g., Wiringa et al., Phys. Rev. C62, 14001 (2000), Pieper et al.,Phys. Rev. C64, 14001 (2001), S.C. Pieper, et al., Phys. Rev. C 66, 044310 (2002)] . The accuracy of these calculations is at the 1% level for the binding energies. The resulting wave functions can be used to compute properties measured at electron and hadron scattering facilities (in particular Jefferson Laboratory), and to compute astrophysical reaction rates, many of which cannot be measured in the laboratory.

This year the GFMC group studied the effects of new three-nucleon potential terms on multiple states of the same angular momentum and parity [S.C. Pieper, R.B. Wiringa, and J. Carlson, Phys. Rev. C70, 054325 (2004)]. Previously the GFMC group demonstrated that the Hamiltonian that has been used successfully for more than a decade in studies of s-shell nucleon is inadequate in the p-shell. Some of the possible new potential terms, whose forms are derived from meson-exchange arguments, result in considerable additional complications in the Green's function propagator. New potential models were developed that reproduce all of the known stable or narrow-width levels of up to ten-body nuclei with an average error of only 300 keV.

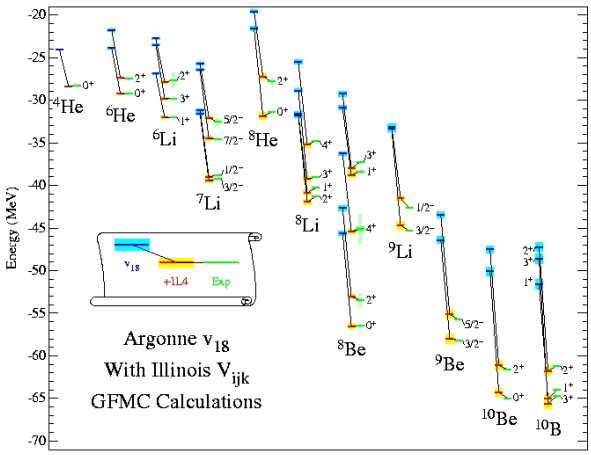

Figure 1: GFMC calculations of mass 4-10 systems.

This project uses Green's function (GFMC) and variational (VMC) Monte Carlo methods to compute ground state and low-lying excited state expectation values of energies, densities, structure functions, astrophysical reaction rates, etc., for light nuclei and neutron drops. Realistic two- and three-nucleon potentials are used. The group is developing

new computational techniques, optimizing them for different computer architectures, and improving the nuclear Hamiltonian used in the calculations. An area of increasing interest is the use of GFMC or VMC generated wave functions to compute reaction rates of astrophysical interest.

Other approaches to the nuclear many-body problem involve expansion in a basis of single-particle states. Much in the same way that chemists expand single-particle wave functions in the atomic-orbital basis, nuclear physicists typically invoke an oscillator basis in which to perform either Hamiltonian diagonalization or coupled-cluster calculations which we will discuss in the following.

The No-Core-Shell Model (NCSM) approach involves diagonalization of a very large dimensional matrix (typically with a rank of 1 billion) using Krylov space techniques (Lanczos or Davidson-Liu algorithms). These demanding calculations begin from a bare Hamiltonian consisting of two-nucleon and three-nucleon interactions. The implementation of a many-body model space requires that the interactions be renormalized to the model-space in which one performs the diagonalization. This process of 'decimation' removes the hard-core potentials normally associated with the bare nucleon-nucleon interaction and yields an effective interaction appropriate for the model space in which calculations are to be performed. The diagonalization procedure yields the energy spectrum of the nucleus and the resulting wave functions may be used to obtain information on transition properties of the Hamiltonian. The method is currently being appled (using only two body interactions) to ^{16}O (see the figure). Recently this method was applied to neutrino-nucleus scattering [A.C. Hayes et al., Phys. Rev. Lett. 91, 12502 (2003)]. The neutrino scattering cross section on ^{12}C remains one of the only measured neutrino-nucleus events. This weak interaction requires very accurate descriptions of nuclear ground- and excited state wave functions in order to be accurately obtained from theory. The NCSM calculations included both two- and three-nucleon interactions and, with no adjustable parameters, recovered more than 60% of the experimental cross section from a theory that included NO adjustable parameters. This represents a significant advance in our understanding of neutrino-nucleus scattering cross sections on nuclei.

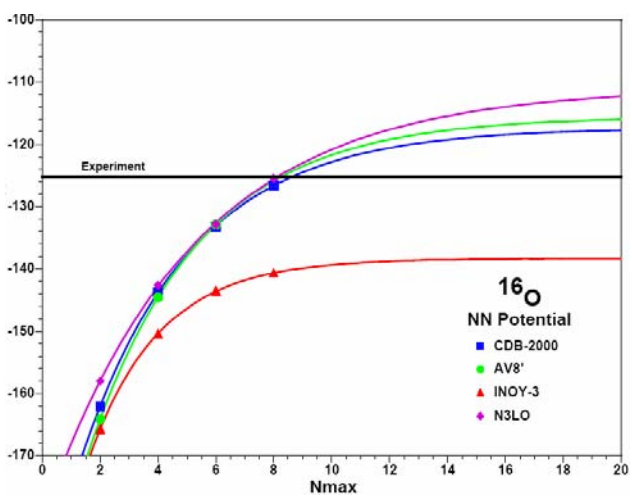

Figure 2: No core shell model results the ^{16}O ground state using two-body interactions.

While the NCSM diagonalizes a Hamiltonian in a given many-body basis, coupled-

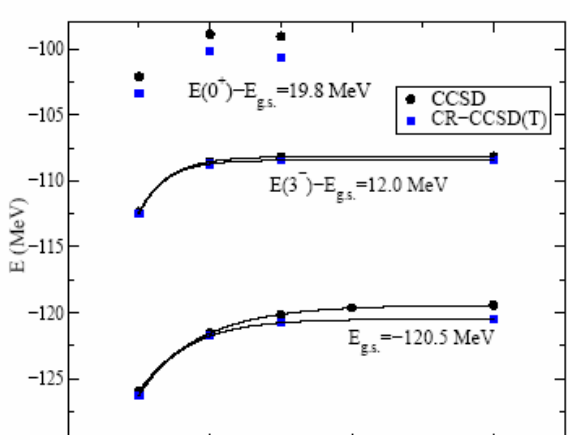

Figure 3: Nuclear coupled-cluster results for ground-and excited states of ^{16}O.

cluster theory obtains information on nuclear correlations through the solution of coupled-nonlinear algebraic equations for particle-hole excitation amplitudes generated by a given effective Hamiltonian appropriate for the chosen single-particle model space. The application of this technique to closed-shell nuclei was described in K. Kowalski et al., Phys. Rev. Lett. 92, 132501 (2004). Recent large scale applications of the method including non-iterative triples corrections to ground- and excited-state energies yielded converged results for the ground-state of ^{16}O and for the first excited negative-parity J=3 state (the positive parity J=0 state is not well described at this level of the theory). See the figure where we plot both ground-state and excited state energies as a function of increasing model space. The nuclear two-body interaction was taken from chiral effective field theory. We know from GFMC and NCSM calculations in mass 10 systems that three-body forces significantly affect spin-orbit splitting of the single-particle states. The negative-parity J=3 state is essentially a one-particle-one-hole state and should be well described by our coupled-cluster techniques. We can therefore surmise that three-body forces will also play a significant role in determining the nuclear structure of these systems. Therefore in the future, we will necessarily need to develop coupled-cluster algorithms that incorporate three-body forces.

Nuclear structure studies in medium mass nuclei require an implementation of Auxiliary Field Monte Carlo (AFMC) techniques to calculate ground state and thermal properties of these systems. The calculation of the heat capacity of a finite interacting nuclear system including correlations is a difficult problem. The residual interaction among nucleons generates correlations that must be taken into account. The interacting nuclear shell model is an appropriate framework for such calculations, but very large model spaces are necessary to obtain reliable results. AFMC methods developed for the nuclear shell model enable zero- and finite-temperature calculations in large model spaces. One interesting effect involves breaking of pairs and the melting deformation as temperature is increased in a nucleus. Recent calculations suggest that peaks will appear in the nuclear specific heat (around T=0.5-1.0 MeV) when pairing correlations are destroyed by temperature. Deformations wipe out this effect. [Langanke et al, to appear in Nucl. Phys. A]. Shown in Figure 3 are deformation plots for several nuclei in the mass 70-80 region with 40 neutrons. In the figure β describes how deformed the nucleus is while g indicates whether the nucleus is

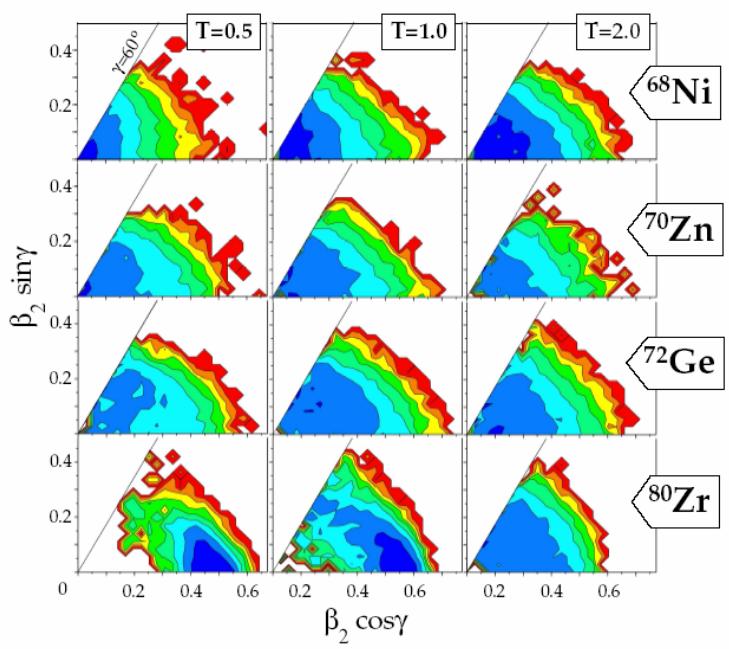

Figure 4: Nuclear deformation as a function of temperature in the mass 80 region.

oblate (γ=0) oblate (γ=60) or soft (uniform filling in γ). ^{68}Ni and ^{70}Zn are fairly spherical nuclei while ^{72}Ge exhibits shape-coexistence. ^{80}Zr is very well deformed (and prolate) as is seen in the figure. At intermediate temperatures (middle column) all nuclei retain some of their ground-state character, but the shape distributions become softer in the g-direction. At the higher temperature of T=2.0 MeV the four N=40 systems considered become soft in both β and γ, filling uniformally the phase space in the β–γ plot.

Electron capture on protons nuclei is an important process that occurs during the early stages of the evolution of core-collapse supernovae. These weak captures serve to deleptonize the core of the massive star and determine the final electron fraction within the core. Therefore they set the size of the homologous core that must then collapse. The size of the core influences the amount of energy required to explode the star. Accurate nuclear structure calculations are required to understand these processes, and such calculations require also significant computational resources. While the iron region has been sufficiently investigated, the distinct possibility exists for electron capture to occur in nuclei beyond this region. Historically, this possibility has not been included in core-collapse simulations where most capture took place on protons. Inclusion of newly calculated electron-capture rates (calculated with a combination of AFMC and RPA theories) on nuclei indicate that nuclei up to mass 120 dominate electron capture on protons, thus leading to significant modifications of the evolution of core collapse models [see Langanke et al., Phys. Rev. Lett. 90, 241102 (2003); Hix et al., Phys. Rev. Lett. 91, 201102 (2003)].

Computational Needs

Calculations of high priority during the next 5 years include the following: (1) GFMC needs 150×10^{15} operations for one state in ^{12}C when the nuclear three-body interaction is included in the calculation. For something of both astrophysical and nuclear interest, calculation of the first excited 0^+ will require 1-2 million Seaborg processor hours. Upgrades to the processor speed, while keeping memory per processor at current, or enhanced, levels, is important for this effort. (2) The no-core shell model approach would run optimally with 4 Gigabytes of memory per processor. The NCSM effort will require approximately 5 million Seaborg equivalent processor hours at NERSC to continue production runs through mass 16 nuclei. These runs will also include realistic three-nucleon forces. While some of these cycles will be obtained from other resources, NERSC remains an important part of the NCSM effort. (3) The nuclear coupled-cluster calculations would benefit from an increased memory per processor (to 8 Gbytes) and an increased processor speed. Current plans include calculations of mass 40 nuclei and the inclusion of three-body terms into the Hamiltonian. Compared to today (mass 16 nuclei in 8 oscillator shells) mass 40 nuclei will require at least 9 oscillator shells for convergence. While the largest ^{16}O runs (with 2-body interactions) cost 2 Tflop-hours, the largest ^{40}Ca runs will require 36 Tflop-hours. For the same number of basis states, we estimate that an ^{16}O calculation including a three-body interaction will require roughly 500 Tflop-hours per calculation. Memory needs for a three-body interaction are also significant. For an 8-oscillator shell run, the memory required to store the three-body interaction matrix elements is well over 10 Tbytes.