COMPUTATIONAL NUCLEAR STRUCTURE:
CHALLENGES, REWARDS, AND PROSPECTS

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Computational Nuclear Structure: Challenges, Rewards, and Prospects

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The shell model Monte Carlo technique (SMMC) transforms the traditional nuclear shell model problem into a path-integral over auxiliary fields. Applications of the method to studies of various properties of fp-shell nuclei, including Gamow-Teller strengths and distributions, are reviewed. Part of the future of nuclear structure physics lies in the study of nuclei far from beta-stability. I will discuss preliminary work on proton deficient Xe isotopes, and on neutron rich nuclei in the sd-fp shells.

1 Introduction: nuclear structure and computing

Studies of nuclei far from stability have long been a goal of nuclear structure science. Nuclei on either side of the stability region, either neutron rich or deficient, are being produced at new radioactive beam facilities across the world. Some of the key questions concern: mapping of the neutron and proton drip lines, thus finding the limits of stability; understanding effects of the continuum on weakly bound nuclear systems; understanding the nature of shell gap melting in very neutron rich systems; determination of nuclear masses and the density of states for nuclei of astrophysical interest; and investigating deformation, spin, and pairing properties of systems far from stability.

The range and diversity of nuclear behavior, as indicated in the above list of ongoing and planned experimental investigations, have naturally engendered a host of models. Short of a complete solution to the many-nucleon problem, the interacting shell model is widely regarded as the most broadly capable description of low-energy nuclear structure, and the one most directly traceable to the fundamental many-body problem. Difficult though it may be, solving the shell-model problem is of fundamental importance to our understanding of the correlations found in nuclei. New and improved computational techniques should allow these theoretical studies to continue and expand.

This symposium has placed an emphasis on the link between nuclear theory and computing. This link is clearly evident in the sub-field of nuclear structure and dynamics. One quote from a paper co-authored by our conference summary speaker should indicate this intricate interplay: "With Skyrme's
force each iteration of the Hartree-Fock equations for $^{208}$Pb takes less than 30 seconds on the Univac 1108. The simplicity of the calculations... suggest that Skyrme's interaction might be useful for extrapolating to properties of nuclei off the $\beta$-stability line and to super heavy nuclei." ¹ Of course, today these same calculations may be performed on a personal computer.

Increasingly we rely on computation to guide us in our understanding of the basic nature of the nucleus. This is true both at the structural level, as well as at very high collision energies needed to study quark-gluon plasma formation and hadronization. With the continuing advances in computational technology, we will certainly be able to study problems that until a few years ago were simply unapproachable. We have a very hopeful future since large scale computing today is typically commonplace tomorrow.

My research over the past few years has been in the area of the nuclear shell model solved not by diagonalization, but by integration. In what follows, I will describe the shell-model Monte Carlo (SMMC) method, and discuss some interesting results obtained from the model. These include properties of the Gamow-Teller resonance in fp-shell nuclei, and properties of nuclei far from $\beta$-stability.

2 The SMMC method

Investigations into both ground state and thermal properties of nuclei have been described using the SMMC technique²,³. This method offers an alternative way to calculate nuclear structure properties, and is complementary to direct diagonalization. SMMC cannot find, nor is it designed to find, every energy eigenvalue of the Hamiltonian. It is designed to give thermal or ground-state expectation values for various one- and two-body operators. Indeed, for larger nuclei, SMMC may be the only way to obtain information on the thermal properties of the system from a shell-model perspective. The partition function of the imaginary-time many-body propagator, $U = \exp(-\beta \hat{H})$ where $\beta = 1/T$ and $T$ is the temperature of the system in MeV, is used to calculate the expectation values of any observable $\hat{\Omega}$ with

$$\langle \hat{\Omega} \rangle = \frac{\text{Tr} \hat{U} \hat{\Omega}}{\text{Tr} \hat{U}}.$$  \hspace{1cm} (1)

Since $\hat{H}$ contains many terms that do not commute, one must discretize $\beta = N_\beta \Delta \beta$. Finally, two-body terms in $\hat{H}$ are linearized through the Hubbard-Stratonovich transformation, which introduces auxiliary fields over which one
must integrate to obtain physical answers. The method can be summarized as

$$Z = \text{Tr} U = \text{Tr} \exp(-\beta \hat{H}) \to \text{Tr} \left[ \exp(-\Delta \beta \hat{H}) \right]^{N_t}$$

$$- \int D[\sigma] G(\sigma) \text{Tr} \prod_{n=1}^{N_t} \exp \left[ \Delta \beta \hat{h}(\sigma_n) \right],$$

(2)

where \(\sigma_n\) are the auxiliary fields (there is one \(\sigma\)-field for each two-body matrix-element in \(\hat{H}\) when the two-body terms are recast in quadratic form), \(D[\sigma]\) is the measure of the integrand, \(G(\sigma)\) is a Gaussian in \(\sigma\), and \(\hat{h}\) is a one-body Hamiltonian. Thus, the shell-model problem is transformed from the diagonalization of a large matrix to one of large dimensional quadrature. Dimensions of the integral can reach up to \(10^5\) for rare-earth systems, and it is thus natural to use Metropolis random walk methods to sample the space. Such integration can most efficiently be performed on massively parallel computers. Further details are discussed in Koonin, et al.\(^3\).

Realistic interactions often have a Monte Carlo sign problem, that is they have complex actions. However, a certain class of Hamiltonians has good Monte Carlo sign properties, and one performs calculations with these Hamiltonians, and extrapolates to the realistic case. Fortunately in nuclear physics good Hamiltonians with no sign problems are not too far removed from realistic Hamiltonians so that the extrapolation is a gentle function of the extrapolation parameter\(^4\).

3 Gamow-Teller properties of \(fp\)-shell nuclei

The impact of nuclear structure on astrophysics has become increasingly important, particularly in the fascinating and presently unsolved problem of type-II supernovae explosions. The possibility to detect neutrinos ejected before the infalling matter reaches the neutrino trapping density\(^5\) will allow us for the first time to understand whether models of the precollapse evolution are in reasonable agreement with observation.

One key ingredient of the precollapse scenario is the electron capture cross section on nuclei\(^6,7\). The core of a massive star at the end of hydrostatic burning is stabilized by electron degeneracy pressure as long as its mass does not exceed the appropriate Chandrasekhar mass \(M_{CH}\). If the core mass exceeds \(M_{CH}\), electrons are captured by nuclei\(^6\). Thus, the depletion of the electron population due to weak capture by nuclei is a crucial factor determining the initial collapse phase.

The reduction of the electroweak interaction matrix element to the zero momentum transfer limit for the nuclear sector leads directly to the Gamow-
Figure 1: Shown are strength distributions of the GT+ operator relative to the ground state of the daughter for SMMC calculations (line) as compared to experimental data (dashed histograms). The scale for the $^{56}\text{Ni}$ distributions should be multiplied by a factor of 2.

The Gamow-Teller (GT) operator as a primary ingredient in electron-capture cross section calculations. The GT properties of nuclei in the iron region of the periodic table are known to be crucial for supernova physics. The Kuo-Brown interaction, modified in the monopole terms by Zuker and Poves, was used throughout these fp-shell calculations. This interaction reproduces quite nicely the ground and excited state properties of mid-fp shell nuclei, including the total Gamow-Teller strengths and distributions. Shown in Fig. 1 are the strength distributions calculated in SMMC as a function of excitation energy in the daughter nucleus. The experimental data are shown by the dashed histograms and are taken from pn reaction studies. Note the general overall agreement between theory and experiment. The SMMC technique allows us to probe the complete 0hω fp-shell region, without any parameter adjustments to the hamiltonian, although the Gamow-Teller operator has been renormalized by the standard factor of 0.8. These results may then be used to calculate the electron-capture cross sections for nuclei relevant to pre-supernova collapse.
4 Properties of nuclei far from $\beta$-stability

4.1 Neutron deficient nuclei near $A = 120$

Nuclei with mass number $100 \leq A \leq 140$ are believed to have large shape fluctuations in their ground states. Associated with this softness are spectra with an approximate $O(5)$ symmetry and bands with energy spacings intermediate between rotational and vibrational. In the geometrical model these nuclei are described by potential energy surfaces with a minimum at $\beta \neq 0$ but independent of $\gamma$. Some of these nuclei have been described in terms of a quartic five-dimensional oscillator. In the Interacting Boson Model (IBM) they are described by an $O(6)$ dynamical symmetry. The first fully microscopic calculations were performed for nuclei in this mass region using SMMC techniques.

These calculations have recently been extended to the neutron deficient isotope chain $^{110}$Xe to $^{122}$Xe. The two-body interaction is given by a monopole ($J = 0$) plus quadrupole ($J = 2$) pairing, supplemented by a collective quadrupole term:

$$\hat{H}_2 = -\sum_{\lambda \mu} \frac{\pi g_{\lambda}}{2\lambda + 1} \hat{\lambda}_\mu \hat{\lambda}_\mu - \frac{1}{2} \chi : \sum_{\mu} (-)^\mu \hat{Q}_\mu \hat{Q}_{-\mu} :,$$

where $::$ denotes normal ordering. The single particle energies and the other parameters were determined as described in Alhassid et al. These calculations have recently been extended to the neutron deficient isotope chain $^{110}$Xe to $^{122}$Xe. The two-body interaction is given by a monopole ($J = 0$) plus quadrupole ($J = 2$) pairing, supplemented by a collective quadrupole term:

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Shown in Fig. 2 (top) are the calculated and experimental $B(E2)$ values for the Xe isotope chain. Note that an overall agreement between theory and experiment exists, although the experimental error bars are still fairly large. The calculation is scaled by 1.67, which may in the future be eliminated by including additional subshells and an isovector quadrupole interaction. The isovector quadrupole will certainly help in reproduction of the first excited $2^+$ energies (bottom figure). Still, in this preliminary attempt to study the global properties of this region, the results are quite encouraging.

Shown in Fig. 3 is the shape evolution of the system as one moves from $^{110}$Xe to $^{120}$Xe. These calculations were performed at a $\beta = 3.0$ MeV$^{-1}$. For each Monte Carlo sample, the expectation of the quadrupole operator, $Q_{2\mu}$, is used to construct the quadrupole tensor $Q_{ij}$. This tensor is then diagonalized, and its eigenvalues may be related to $\beta$, and $\gamma$, which gives the deformation and the angle of deformation. Note that the $\gamma$-softness builds up from $^{112}$Xe to $^{120}$Xe. Furthermore, $^{110}$Xe, behaves qualitatively differently, and indicates an onset of sphericity. This is also evident in the strong decrease of the $B(E2)$ in $^{110}$Xe, and the increase in the $2^+$ excitation energy for this system. The study of these nuclei experimentally, especially those that are far from stability should
Figure 2: Shown are the $B(E2)$ values for the Xe isotope chain (top), and the corresponding excitation energy of the first $2^+$ state in these systems (bottom).

shed light on the evolution of intrinsic shapes as one approaches the proton drip line. These properties are presently under further investigation, and will be reported in a future publication 25.

4.2 Neutron rich nuclei

Studies of extremely neutron-rich nuclei have revealed a number of intriguing new phenomena. Two sets of these nuclei that have received particular attention are those with neutron number $N$ in the vicinity of the $1s0d$ and $0f7/2$ shell closures ($N \approx 20$ and $N \approx 28$). Experimental studies of neutron-rich Mg and Na isotopes indicate the onset of large deformation, as well as the disappearance of the $N = 20$ shell gap for $^{32}$Mg and nearby nuclei 26. In order to investigate these neutron rich systems, a study of nuclei in the full sd-fp shell model space using SMMC has been undertaken 27. These calculations are complicated by the lack of a well tested interaction, and by the need for center of mass removal. The center of mass is partially removed using a Gloeckner-Lawson approach 28. The interaction is comprised of the USD interaction 29 in
the $sd$-shell, the KB3 interaction\textsuperscript{10} in the $fp$-shell, and the cross-shell matrix elements are given by a Millener-Kurath potential\textsuperscript{39}. The monopole terms are modified in the cross-shell interaction in order to obtain reasonable properties of typical $sd$ or $fp$ shell nuclei. Shown in Fig. 4 are our results for the $B(E2)$ values in this region, and in particular for $^{32}$Mg. Clearly the $fp$-shell plays a major role in $^{32}$Mg, as the $fp$-shell occupation is approximately 1.5 neutrons. Note that without the inclusion of the $fp$-shell, one is not able to describe the deformation of $^{32}$Mg.

5 Conclusions

The expansion of studies in nuclear theory that touch areas of nuclear astrophysics, and into regions of nuclei far from $\beta$-stability continues at a rapid pace. The computational power needed to understand these complicated many-body systems continues to grow. In this proceedings I have attempted to show just a few of the interesting problems where SMMC has been recently applied, and for which large-scale computation has played major role. The future is indeed filled with new and exciting possibilities for stochastic computational techniques.

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Figure 4: Shown are the calculated $B(E2)$ values compared to experiment for neutron rich nuclei in the sd-fp shell region.

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References

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