FURTHER PROGRESS IN SHELL-MODEL MONTE CARLO STUDIES

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During the past several years, an alternative method for the exact solution of the shell model based on Auxiliary Field Monte Carlo techniques has been developed. The shell-model Monte Carlo (SMMC) method can calculate both ground-state and finite-temperature properties. The accuracy of its results is limited only by easily controlled sampling and discretization errors. Because the numerical effort scales only as a low power of the problem size, much larger (and hence more realistic) calculations are possible. Further, because the calculations are compute-intensive, with relatively modest memory or I/O, they are ideally suited to take advantage of developments in parallel computing.

These calculations are performed by taking the quantum mechanical trace of the imaginary-time many-body propagator $U = \exp(-\beta H)$, where H is the Hamiltonian of the system, and beta is the inverse temperature. The trace of U gives the partition function. Since the Hamiltonian contains two-body terms, beta must be discretized (the Trotter approximation), and each resulting exponential must be linearized using the Hubbard-Stratonovich transformation. The resulting problem becomes one of many-dimensional quadrature. We can calculate the canonical expectation value for any one- or two-body observable, such as the energy (the expectation of the Hamiltonian), the Gamow-Teller strength (a two-body spin operator), or the B(E2) strengths (two-body quadrupole and deformation operators). Additionally, we calculate response functions for various operators, and thus obtain detailed information on strength functions.

As this is a continuing project with multiple publications per year, we briefly describe our goals for the next several years. Several interesting calculations may be performed with the existing technology.

1) In previous work we calculated the total strength of pair removal from N=Z even-even and odd-odd nuclei. This work may be extended to pair transfer strength distributions by calculating the response of the nucleus to a pair transfer operator. These calculations should be useful in determining more precisely the nature of the pair correlations in nuclei.

2) A continuing study of γ-soft nuclei in the Xe region is under way. These nuclei exhibit interesting changes in symmetry as one investigates an isotopic chain of nuclei. For example, moving from ^{124}Xe to ^{114}Xe, preliminary calculations indicate that the shape changes from γ-soft to fairly well deformed and that the change is gradual. This project is being pursued in collaboration with Yoram Alhassid.

3) Multi-major shell calculations open up several new areas of application for SMMC. One particular area of research will be in understanding giant-dipole and giant-quadrupole resonances in nuclei. We will calculate the GDR as a function of temperature to study the thermal broadening. This will be a first for interacting shell-model studies.

Realistic interactions often have a Monte Carlo sign problem; that is, they have complex actions. We have found that a certain class of Hamiltonians has good Monte Carlo sign properties, and one performs calculations with these Hamiltonians. Fortunately in

nuclear physics good Hamiltonians, such as pairing plus quadrupole, are not too far removed from realistic Hamiltonians so that the extrapolation is a gentle function of the coupling constant, g. Recently, constrained path integral methods have been developed and used in Hubbard-model calculations[1] which circumvent the sign problem. We will adapt this algorithm to the SMMC technique to understand whether this may be a useful way to alleviate our extrapolation scheme.

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[1] S. Zhang, J. Carlson, and J. E. Gubernatis, *Phys. Rev.* B **55**, 7464 (1997).