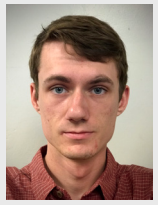
Proton Neutron Interacting Shell Model: Order of Magnitude Reduction in Dimension for Medium Mass Nuclei



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Detailed information about the structure and properties of atomic nuclei (the center of atoms) are critical for a number of scientific and even national security interests. Much of what is needed can be measured in a laboratory, but for a significant number of calculations, nuclear scientists have to rely on theoretical predictions from quantum mechanics. The problem theorists have is that the quantum N-body problem is a non-trivial computational task, with millions or billions of basis dimensions. In one approach to solving the nuclear Schrodinger equation, we represent the system as a matrix eigenvalue problem in what is called the shell model (SM) approach. In this work I present preliminary work by myself and my advisor Dr. Johnson to intelligently truncate the basis space in which we frame the computational problem. We partition the Hilbert space and use solutions to its (much smaller) partitions to select the most important basis states for the full space. By leaving out the least important basis states, it is possible to reduce the computational and memory requirements of this problem by an order of magnitude.

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The Schrödinger equation is a matrix eigenvalue problem:

$$\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle\,. \tag{1}$$

To approximate (1) for our nuclear wave functions, we separate the nuclear Hamiltonian by nucleon species:

$$\hat{H} = \hat{H}_{proton} + \hat{H}_{neutron} + \hat{H}_{proton-neutron}, \tag{2}$$

and solve the proton and neutron parts independently:

$$\begin{aligned} \hat{H}_{proton}\,|\pi\rangle &= E_p\,|\pi\rangle\,, \\ \hat{H}_{neutron}\,|\nu\rangle &= E_n\,|\nu\rangle\,. \end{aligned} \tag{3}$$

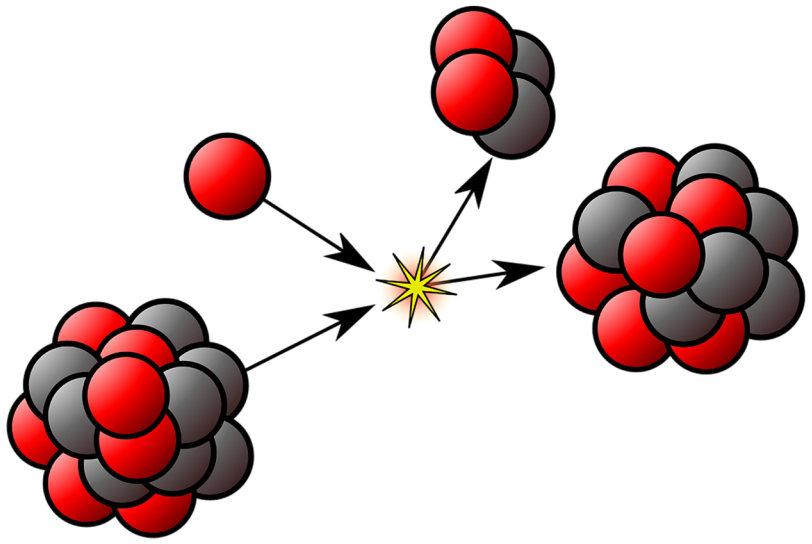
The many body basis states are then constructed by coupling together the resulting eigenstates:

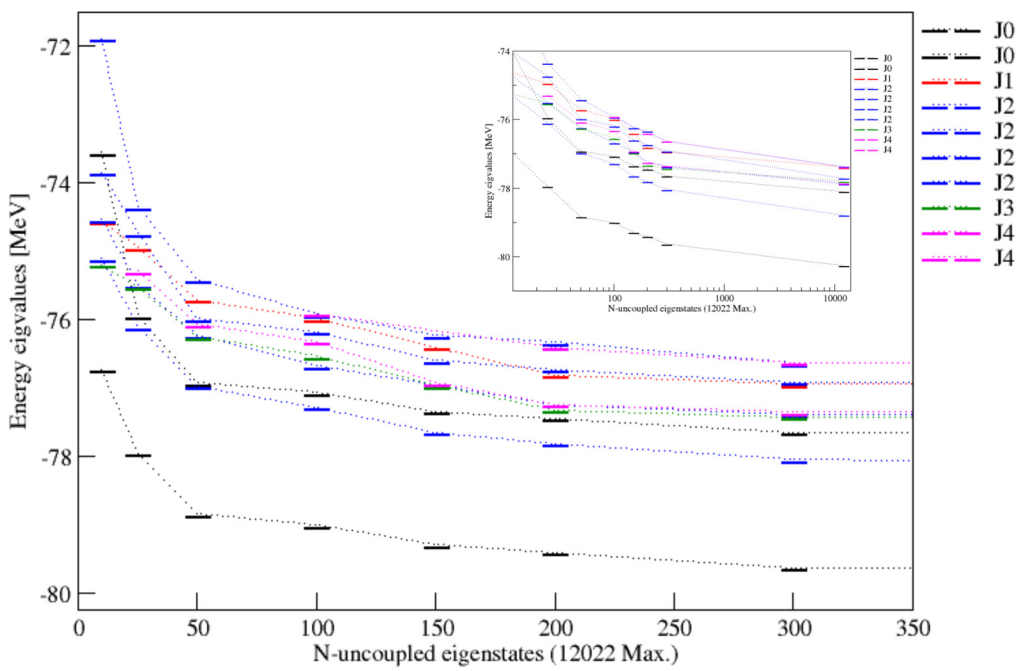
$$|\phi\rangle = \sum_i^{d_\pi}\sum_j^{d_\nu} \phi_{ij}\,|\pi_i\rangle \otimes |\nu_j\rangle\,, \tag{4}$$

where d_π and d_ν are the dimensions of the proton and neutron spaces, respectively. Finally, the full Hamiltonian matrix is computed in a truncated (subset) of the full basis:

$$\sum_b^{N^2<<d_\pi d_\nu} \langle\phi_a|\,\hat{H}\,|\phi_b\rangle\,\Psi_b = E\Psi_a. \tag{5}$$

Standard diagonalization techniques are used to solve for the extremal eigenvalues of this system. These solutions are guaranteed to converge to the un-truncated solutions by the *variational principle.*





Ni 60 Low-Lying Energy Spectra

Here we see the convergence trend of the approximation method for low-lying excitation spectra for Ni60. Each 'stack' of parallel lines represents the ten lowest energy levels of the Ni 60 nucleus. As you move from left to right, the number of eigenstates used to construct the model space basis increases, thus increasing the accuracy of the approximation. The rightmost spectra with N=12022 was computed on a supercomputer using another interacting shell model code and is guaranteed to be the final converged value of these calculations.