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

Oliver Gorton[1] and Dr. Calvin Johnson[1]

[1]San Diego State University | ogorton@sdsu.edu
cjohnson@sdsu.edu

***Big Picture: Nuclear Structure***

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 -which you have to solve for each nucleus - is a non-trivial computational task, with millions or *billions of basis dimensions*.

***Specific Question: Truncating the many body basis***

In one approach to solving the Schrodinger equation for the nucleus, 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 truncate the basis space in which we frame the computational problem.

***Method: Importance Truncation***

By selecting the *most important basis states*, and 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. The method for selecting basis states is to construct the mixed-proton-neutron basis out of eigenstates of the pure-proton and pure-neutron solutions of the Hamiltonian*. We present results for the medium mass nucleus Ni 60 which were computed on a desktop workstation, where otherwise a supercomputer would have been necessary.

***For the informed: Some Formalism****

The Schrodinder 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 $d_\pi$ and $d_\nu$ 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:

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

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*.

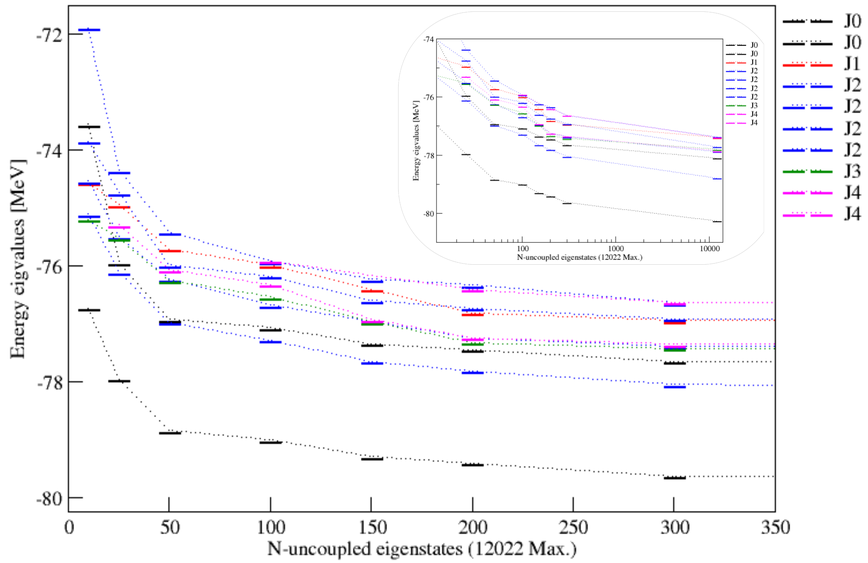


***Figure 1. Ni 60 Low-Lying Energy Spectra***

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.

***Results: Comparison to Full Model Space Solution***

Comparison to the full shell model space calculations: with an approximation reducing the model space to dimensions of roughly $10^5$, we find that our energy levels each fall within 0.25 MeV of the full solution (Table 2). This error is comparable to full solution's typical error of 0.1 MeV (Table 3). The full solution requires a dimension around $10^9$.

***Conclusion***

We have shown an order of magnitude reduction in the basis dimensions of our model, while maintaining the same order of magnitude in the error of our results. This method has potential applications to heavy-mass nuclei, where the full model space dimensions can exceed the capacity of even cutting edge supercomputers.

Table 1. and Table 2. show the results for Ni 60 calculations: errors relative to full model space diagonalization - which would otherwise require a ***1.1 billion x 1.1 billion*** matrix to be diagonalized! For comparison, absolute uncertainties for a full solution are on the order of 0.1 MeV, relative to experiment.

***Table 1. Ni 60 Low-Lying Excitation Spectra (N=200, dimension < 30k)***

| State | J | Eigenvalue [MeV] | Excitation [MeV] | Error [MeV] |
|---|---|---|---|---|
| 1 | 0 | -79.408 | 0.0000 | --- |
| 2 | 2 | -77.809 | 1.5998 | +0.1219 |
| 3 | 0 | -77.442 | 1.9658 | -0.1914 |
| 4 | 3 | -77.321 | 2.0871 | **-0.3786** |
| 5 | 4 | -77.243 | 2.1657 | -0.2462 |
| 6 | 2 | -77.240 | 2.1680 | -0.2182 |
| 7 | 1 | -76.813 | 2.5953 | -0.2770 |
| 8 | 2 | -76.724 | 2.6841 | +0.1330 |
| 9 | 4 | -76.404 | 3.0044 | +0.1256 |
| 10 | 2 | -76.332 | 3.0765 | +0.1820 |

***Table 2. Ni 60 Low-Lying Excitation Spectra (N=300, dimension < 70k)***

| State | J | Eigenvalue [MeV] | Excitation [MeV] | Error [MeV] |
|---|---|---|---|---|
| 1 | 0 | -79.630 | 0.0000 | --- |
| 2 | 2 | -78.047 | 1.5829 | +0.1050 |
| 3 | 0 | -77.646 | 1.9841 | -0.1731 |
| 4 | 3 | -77.419 | 2.2113 | **-0.2544** |
| 5 | 2 | -77.376 | 2.2537 | -0.1325 |
| 6 | 4 | -77.346 | 2.2842 | -0.1277 |
| 7 | 1 | -76.944 | 2.6865 | -0.1858 |
| 8 | 2 | -76.912 | 2.7180 | +0.1669 |
| 9 | 2 | -76.632 | 2.9977 | +0.1032 |
| 10 | 4 | -76.626 | 3.0045 | +0.1257 |

***Table 3. Context for accuracy:***
***Full solution relative to experiment***

| State | J | Error* [MeV] |
|---|---|---|
| 1 | 0 | --- |
| 2 | 2 | +0.145 |
| 3 | 0 | -0.128 |
| 4 | 2 | +0.228 |
| 5 | 4 | -0.094 |
| 6 | 3 | -0.160 |
| 7 | 2 | -0.573 |
| 8 | 1 | -0.322 |
| 9 | 4 | -0.241 |
| 10 | 2 | -0.375 |

***Table 4. Context for dimensions***

| N | J | Dimension | Memory*(GB) |
|---|---|---|---|
| 100 | 4 | 8,000 | $10^{-1}$ |
| 300 | 4 | 70,000 | 20 |
| 500 | 4 | 190,000 | 150 |
| 1000 | 4 | 760,000 | 2300 |

*Memory for Hamiltonian matrix.

***How can we make this better?***

Our next steps will be modify the single-species Hamiltonians to introduce a mean field effect from each species compliment. This will add back in some of the interaction that is left out, thus improving the convergence rate of the results. We would also like to implement MPI for parallel processing.

Computational Science Research Center

Oliver Gorton is a doctoral student with CSRC. His advisor is Dr. Calvin Johnson from the department of physics.