

# Efficient Modeling of Nuclei Through Coupling of Proton and Neutron Wavefunctions

Oliver Gorton

Physics Department, SDSU

April 6, 2018

# Introduction: Big picture

Many experimental investigations require nuclear matrix elements of atomic nuclei:

- Direct detection of dark matter ( $^{131}\text{Xe}$ ) [1]
- Matter-antimatter asymmetry in the early universe ( $^{199}\text{Hg}$ ) [2]
- Parity violating nuclear 'anapole moment' ( $^{133}\text{Cs}$ ) [3]

$$\langle \Psi_f | \hat{O} | \Psi_i \rangle \quad (1)$$

# Introduction: A problem with large dimensions

Time-independent Schrödinger equation for nuclei:

$$\hat{H}\Psi = E\Psi \quad (2)$$

Solve as:

$$\sum_{\beta}^{dim.} H_{\alpha\beta} \Psi_{\beta} = E_{\alpha} \Psi_{\alpha}, \quad (3)$$

using a computer. Unfortunately,

Nucleus	Model space	dim.	Typical memory req.
$^{28}\text{Si}$	sd	$9.4 \times 10^4$	0.2 GB
$^{52}\text{Fe}$	pf	$1.1 \times 10^8$	720 GB
$^{56}\text{Ni}$	pf	$1.1 \times 10^9$	9600 GB

Table 1: Dimensions of the nuclear matrix eigenvalue problem. [4]

# Introduction: Truncate the basis?

We have some basis:

$$\{|\alpha\rangle\}, \alpha = 1, 2, 3, \dots, \dim. \quad (4)$$

That we use to compute matrix elements of the Hamiltonian and solve:

$$\sum_{\beta}^{\dim.} H_{\alpha\beta} \Psi_{\beta} = E \Psi_{\alpha}, \quad (5)$$

Is it possible to find some subset  $\{|\alpha\rangle\}$   $\alpha = 1, \dots, Q$  with  $Q \ll \dim.$  such that

$$\sum_{\beta}^{Q \ll \dim.} H_{\alpha\beta} \Psi_{\beta} \approx E \Psi_{\alpha}, \quad (6)$$

perhaps in some other basis?

# Background: Quick notes on configuration interaction / shell model calculations. What's our basis?

- N-particle wavefunction  $\Psi(r_1, r_2, \dots, r_N)$  made up of antisymmetric products\* of...
- Single-particle (single-fermion) states

$$\phi_i(r_j), \tag{7}$$

where  $i = 1, \dots, k$  (labels  $k$  single-particle states),  $j = 1, \dots, N$  (labels  $N$  particles).

- These are mean-field approximations to nucleon-nucleon interaction. (H.O., Woods-Saxon, or Phenomenological\*\*.)
- Single-particle states carry quantum numbers:  $n, l, j, j_z = m$ .

# Background: Single particle state basis

Harmonic oscillator basis has infinite single-particle states:

$$\{\phi_i\} = \{0s_{1/2}, 1p_{3/2}, 1p_{1/2}, 1d_{5/2}, 2s_{1/2}, 1d_{3/2}, 1f_{7/2}, \dots\}, \quad (8)$$

read:  $nl_j$  and  $l = 0, 1, 2, 3, 4, \dots = s, p, d, f, g, \dots$

- Want to leave out higher level states that are unlikely to be filled
- Want to leave out low lying states that will always be filled, non-interacting

Shell structure indicates a way to do this: “Magic numbers”  
2,8,20,28,50,82,126, where binding energy is especially high.

## Background: Example shell model space: $sd$ -shell

Shell model space example:  $sd$ -shell. The infinite space of all 'oscillator' states

$$\{\phi_i\} = \{0s_{1/2}, 1p_{3/2}, 1p_{1/2}, 1d_{5/2}, 2s_{1/2}, 1d_{3/2}, 1f_{7/2}, \dots\}, \quad (9)$$

is divided into:

- 1 An inert core of inactive states:  $0s_{1/2}, 1p_{3/2}, 1p_{1/2}$
- 2 An active space of accessible "valence" single-particle states:  
 $1d_{5/2}, 2s_{1/2}, 1d_{3/2}$
- 3 The remaining and excluded inaccessible single particle states:  $1f_{7/2}, \dots$

# Background: Example shell model space: sd-shell

$1d_{5/2}, 2s_{1/2}, 1d_{3/2}$

Orbit	State #	n	l	j	m	Energy
$1d_{5/2}$	1	1	2	5/2	5/2	$E_1$
	2	1	2	5/2	3/2	$E_1$
	3			...		
	4					
	5					
	6					
$2s_{1/2}$	7	2	0	1/2	1/2	$E_2$
	8	2	0	1/2	-1/2	$E_2$
$1d_{3/2}$	9	1	2	3/2	3/2	$E_3$
	10			...		
	11					
	12					

Table 2: sd-shell model single-particle states  $\phi_i$



# Background: Quick notes on occupation representation

Single-particle states  $\phi_i$  carry quantum numbers  $n, l, j, j_z = m$ , many-particle states are represented by:

$$|n_1, n_2, n_3, \dots, n_k\rangle = |n_1\rangle |n_2\rangle |n_3\rangle \dots |n_k\rangle \quad (10)$$

Creation/annihilation operator formalism encodes fermion statistics:

- $\{\hat{c}_i^\dagger, \hat{c}_j\} = \delta_{ij}$  and  $\{\hat{c}_i^\dagger \hat{c}_j^\dagger\} = \{\hat{c}_i \hat{c}_j\} = 0$
- $n_i = 0, 1$ .
- $\Psi(\dots, r_i, \dots, r_j, \dots) = -\Psi(\dots, r_j, \dots, r_i, \dots)$ .

Bit representation of many-particle states:

$$\hat{c}_1^\dagger \hat{c}_2^\dagger \hat{c}_4^\dagger |0\rangle = |110010\rangle \rightarrow 110010 \quad (11)$$

# Background: Wavefunctions with two species of nucleon

Nuclear wavefunctions:

$$|\Psi\rangle = \sum_i^{d_\pi} \sum_j^{d_\nu} \Psi_{ij} |\pi_i\rangle \otimes |\nu_j\rangle, \quad (12)$$

with many-proton basis  $\{|\pi_i\rangle\}$ , many-neutron basis  $\{|\nu_j\rangle\}$ .

- For example,  $|\pi\rangle = |0101101011\rangle$
- Two copies of the single-particle space, one for protons, one for neutrons

# Background: Many-proton many-neutron coupling scheme

Taking advantage of symmetry:  $[\hat{H}, \hat{J}_z] = [\hat{H}, \hat{J}^2] = 0$ .

$$\langle M_i | \hat{H} | M_j \rangle = \delta_{M_i, M_j} \quad (13)$$

- Choose to construct basis states with fixed total  $J_z = M$ :

$$[|\pi_i\rangle \otimes |\nu_j\rangle]_M \quad (14)$$

- $M$  is an additive quantum number.  $J$  take more work for the same result.
- “M-scheme” codes can reduce the effective dimension by an order of magnitude or more.



# Purpose: Approximating wavefunctions with a truncated basis

Can we leave out certain states and retain a good approximation?

$$\sum_{\beta}^{Q \ll \dim.} H_{\alpha\beta} \psi_{\beta} \approx E \psi_{\alpha}, \quad (15)$$

Related question: can we approximate wavefunctions in a truncated basis?

$$|\psi\rangle \approx \sum_{ij}^{Q \ll \min[d_{\pi}, d_{\nu}]} \psi_{ij} |\pi_i\rangle \otimes |\nu_j\rangle, \quad (16)$$

Answer: It depends on the distribution of  $\psi_{ij}$ .

# Method: Entanglement entropy: A measure of $\Psi_{ij}$ distributions

Without going into the details...

- Any matrix (e.g.  $\Psi_{ij}$ ) can be written  $\underline{\Psi} = UDV^\dagger$
- Diagonal elements of  $D$ ,  $\gamma_i$ , tell us about

$$|\Psi\rangle = \sum_i \gamma_i |\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle, \quad (17)$$

in some unknown basis  $|\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle$ .

- If  $\gamma_i$  are distributed such that just a few terms make up most of  $|\Psi\rangle$ ...
- At least we know such a basis exists, even if we can't find it yet.

(We should check this before searching for the basis!)

# Method: Entanglement entropy: A measure of $\Psi_{ij}$ distributions

- Any matrix (e.g.  $\Psi_{ij}$ ) can be written  $\underline{\Psi} = UDV^\dagger$
- Diagonal elements of  $D$ ,  $\gamma_i$ , tell us about

$$|\Psi\rangle = \sum_i \gamma_i |\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle, \quad (18)$$

in some unknown basis  $|\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle$ .

- We can compute the eigenvalues of

$$\underline{\Psi} * \underline{\Psi}^\dagger = UDV^\dagger VD^\dagger U^\dagger = UD^2 U^\dagger, \quad (19)$$

to find  $\gamma_i^2$ .

# Method: Entanglement entropy: A measure of $\Psi_{ij}$ distributions

- In some unknown basis  $|\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle$ :

$$|\Psi\rangle = \sum_i^{d_\pi} \sum_j^{d_\nu} \Psi_{ij} |\pi_i\rangle \otimes |\nu_j\rangle = \sum_i \gamma_i |\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle. \quad (20)$$

- We can compute the eigenvalues of

$$\underline{\Psi} * \underline{\Psi}^\dagger = U D V^\dagger V D^\dagger U^\dagger = U D^2 U^\dagger, \quad (21)$$

to find  $\gamma_i^2$ .

- The distribution of  $\gamma_i^2$  will tell us if its possible to find an accurate truncation.



# Method: Entanglement entropy: A measure of $\psi_{ij}$ distributions

- Someone has already done this and have shown that the  $\gamma_i^2$  fall off exponentially. [5,6,7]
- They showed this for light nuclei with equal numbers of protons and neutrons.
- We hypothesize that  $\gamma_i^2$  will fall off even faster in nuclei with unequal numbers of protons and neutrons.

# Method: Entanglement entropy: A measure of $\psi_{ij}$ distributions

Hypothesis:  $\gamma_i^2$  will fall off even faster in nuclei with unequal numbers of protons and neutrons.

*Define:* Proton-neutron entanglement entropy:

$$S_{pn} = - \sum_i \gamma_i^2 \ln \gamma_i^2 \quad (22)$$

Let's compare two sets of nuclei:

- $N > Z$
- $N = Z$

( $Z$  = number of protons,  $N$  = number of neutrons)

# Review: Entanglement entropy: A measure of $\Psi_{ij}$ distributions

- In some unknown basis  $|\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle$ :

$$|\Psi\rangle = \sum_i^{d_\pi} \sum_j^{d_\nu} \Psi_{ij} |\pi_i\rangle \otimes |\nu_j\rangle = \sum_i \gamma_i |\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle. \quad (23)$$

- Proton-neutron entanglement entropy

$$S_{pn} = - \sum_i \gamma_i^2 \ln \gamma_i^2 \quad (24)$$

$$S_{max} = \ln(d_\pi), \quad (25)$$

$$d_\pi \leq d_\nu.$$

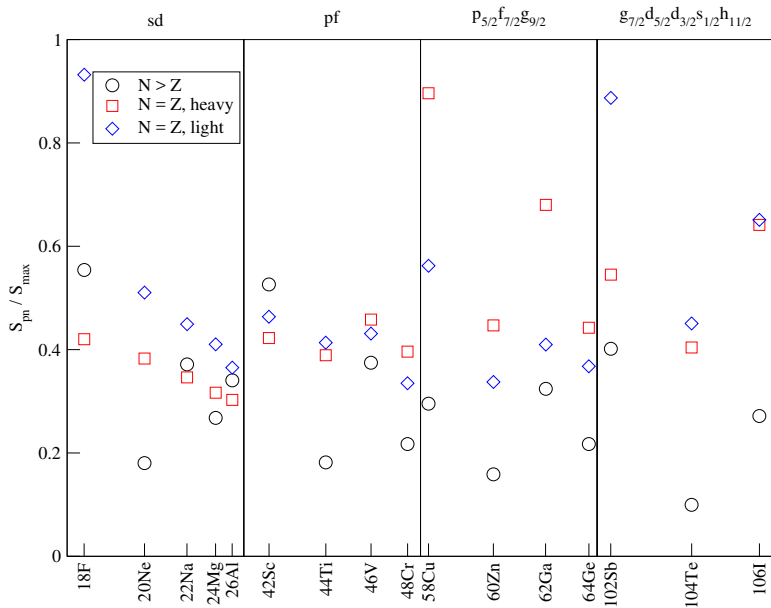


Figure 1: Proton-neutron entanglement entropy for particle-hole conjugate nuclei

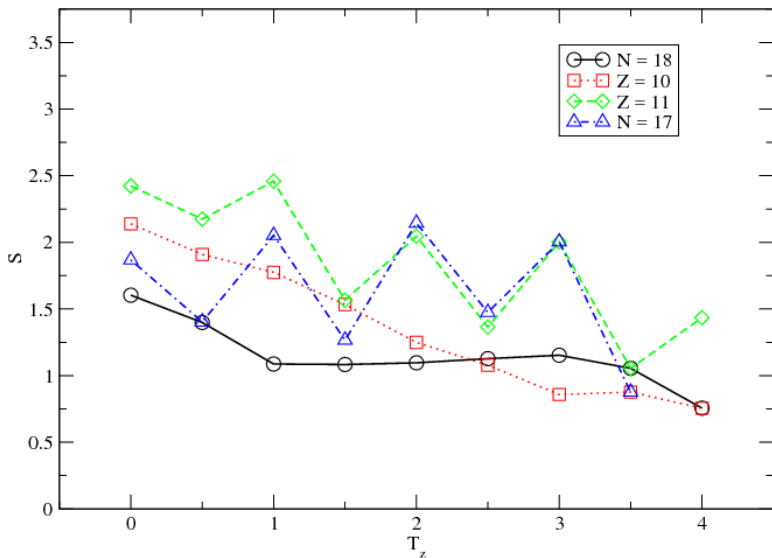


Figure 2: Proton-neutron entanglement entropy versus isospin in the sd-shell

# Study: Varying the strength of the proton-neutron interaction

Nuclear Hamiltonian:

$$\hat{H} = \hat{H}_{proton} + \hat{H}_{neutron} + \lambda \hat{H}_{proton-neutron} \quad (26)$$

Toy model Hamiltonian:

$$\begin{aligned} \hat{H} &= \hat{H}_A + \hat{H}_B + \lambda \hat{H}_{AB} \\ &= \hat{D}_A + \hat{D}_B + \lambda \sum V \otimes W \end{aligned} \quad (27)$$

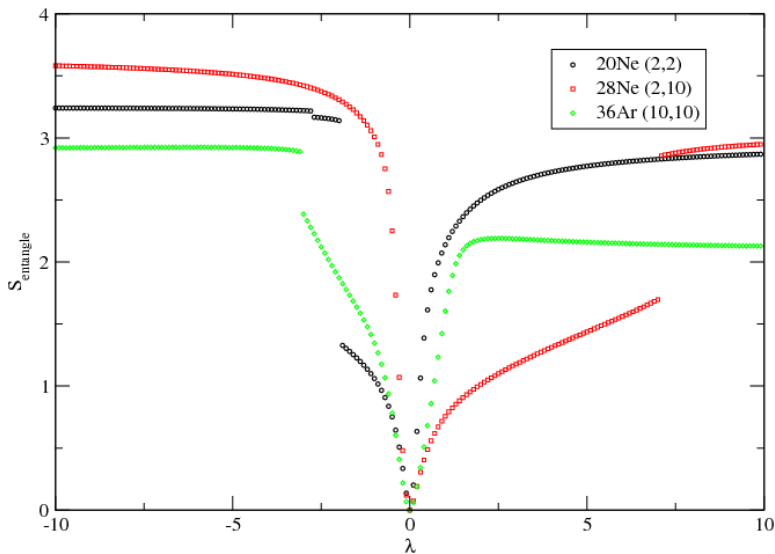


Figure 3: Proton-neutron entanglement entropy versus proton-neutron interaction strength

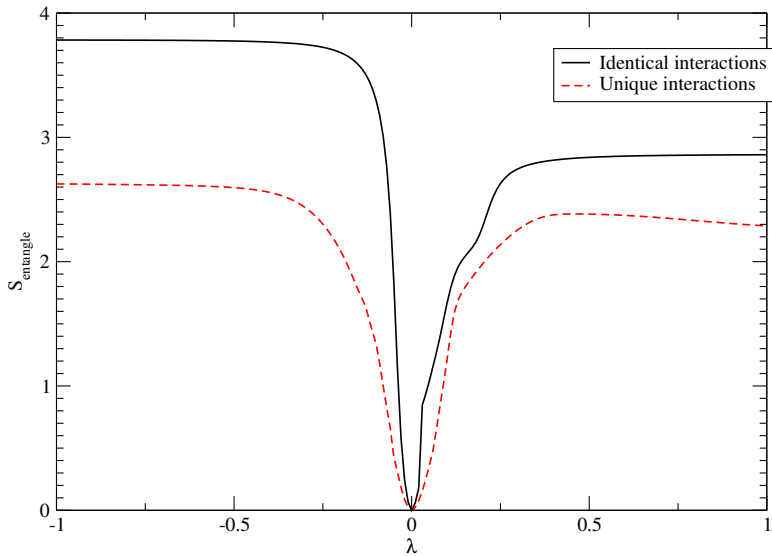
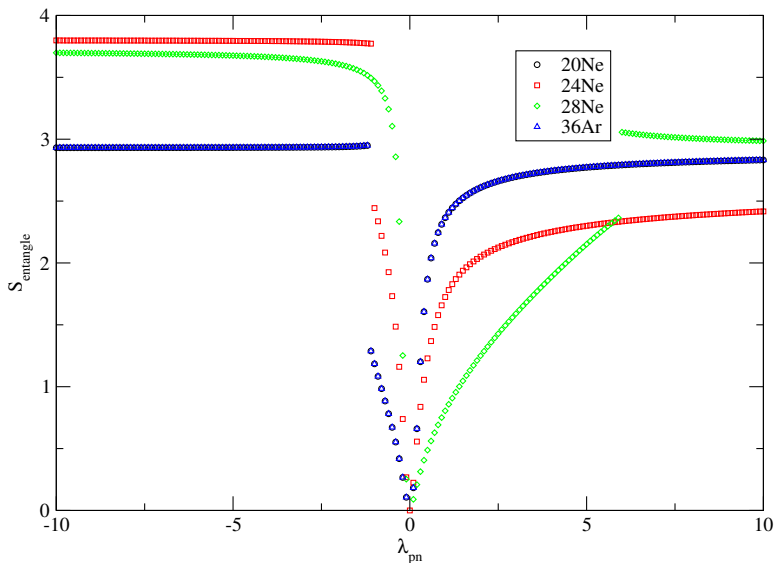


Figure 4: Toy model





**Figure 5:** Proton-neutron entanglement entropy versus proton-neutron interaction strength with monopole terms removed (responsible for shell structure)



# Method: Strength function decomposition

In principle, there exists a basis that we could truncate to approximate our wavefunctions:

$$|\Psi\rangle = \sum_{ij} \tilde{\Psi}_{ij} |PP\rangle \otimes |NN\rangle, \quad (28)$$

can be truncated.

## Method: Strength function decomposition

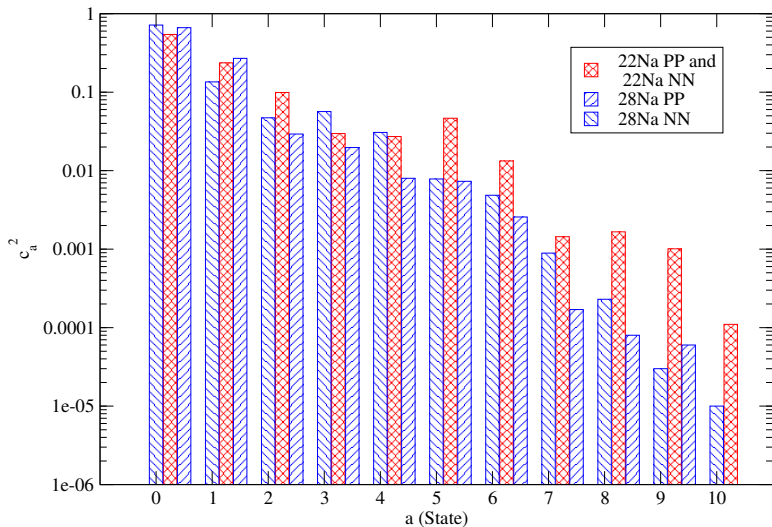
Decompose existing wavefunctions into eigenstates of the proton-proton interaction and of the neutron-neutron interaction:

$$\begin{aligned}\hat{H}_{PP} |PP\rangle &= E_p |PP\rangle, \\ \hat{H}_{NN} |NN\rangle &= E_n |NN\rangle.\end{aligned}\tag{29}$$

Plot the strength function coefficients:

$$\langle \Psi | PP \rangle \langle PP | \Psi \rangle = \sum_P |\tilde{\Psi}_{NP}|^2 \equiv c_N^2\tag{30}$$

$$\langle \Psi | NN \rangle \langle NN | \Psi \rangle = \sum_N |\tilde{\Psi}_{NP}|^2 \equiv c_P^2.\tag{31}$$



**Figure 6:** Proton-proton and neutron-neutron strength decomposition of nuclear wavefunctions

## Addressed questions

- Is it possible to find approximate wavefunctions in a truncated basis?  
YES
- Can we expect that truncating in a basis of coupled proton and neutron wavefunctions is such a basis? YES

## Un-addressed questions

- What coupling scheme do we choose?
- How do we select states to keep/leave out?

## Method: Create the coupled basis, which we truncate

Recall:  $\hat{H} = \hat{H}_{proton} + \hat{H}_{neutron} + \hat{H}_{proton-neutron}$

- Use existing ISM code to solve:

$$\begin{aligned}\hat{H}_{proton} |j_p \alpha_p\rangle &= E_p |j_p \alpha_p\rangle \\ \hat{H}_{neutron} |j_n \beta_n\rangle &= E_n |j_n \beta_n\rangle ,\end{aligned}\tag{32}$$

dimension  $d_p$  and  $d_n$  problems (and not  $d_p \times d_n$ ).

- Use these to build our many-proton many-neutron J-scheme basis:

$$[|j_p \alpha_p\rangle \otimes |j_n \beta_n\rangle]_J\tag{33}$$

Method: Create the coupled basis, which we truncate

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

Our basis,

$$|a\rangle = [|j_p\alpha_p\rangle \otimes |j_n\beta_n\rangle]_J, \quad (34)$$

where  $\hat{H}_{proton} |j_p\alpha_p\rangle = E_p |j_p\alpha_p\rangle$ , has on the order of  $d_p \times d_n$  states. We truncate to compute:

$$\sum_b^{N \ll \min[d_p, d_n]} H_{ab} \Psi_b = E \Psi_a, \quad (35)$$

Using  $\hat{H} = \hat{D}_{proton} + \hat{D}_{neutron} + \hat{H}_{proton-neutron}$ . I wrote a code that does this, PNISM.



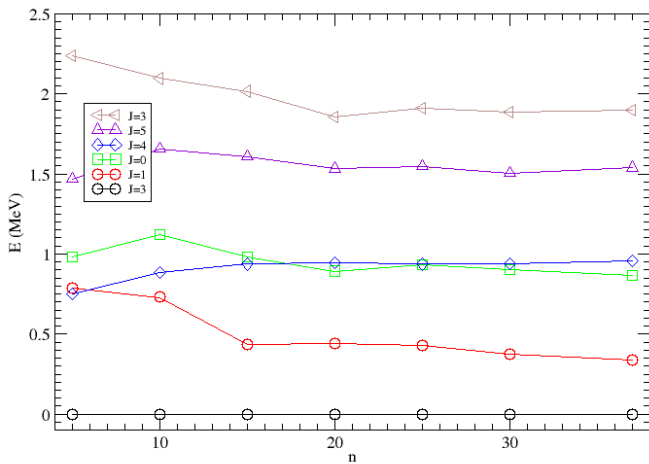


Figure 7: Excitation spectra for  $^{22}\text{Na}$

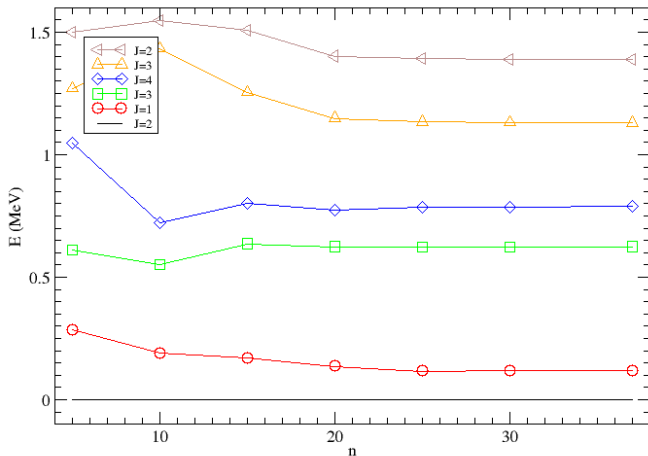


Figure 8: Excitation spectra for  $^{28}\text{Na}$

Nuclide	Zval	Nval	M-scheme dim.	Ground state E [MeV]
$^{56}\text{Ni}$	8	8	$1.09 \times 10^9$	-72.56190
$^{60}\text{Ni}$	8	12	$1.09 \times 10^9$	-80.26105
$^{64}\text{Ge}$	12	12	$1.09 \times 10^9$	-98.81734

**Table 3:** M-scheme dimensions for nuclei in the  $(p_{1/2}, p_{3/2}, f_{5/2}, f_{7/2})$  model space.

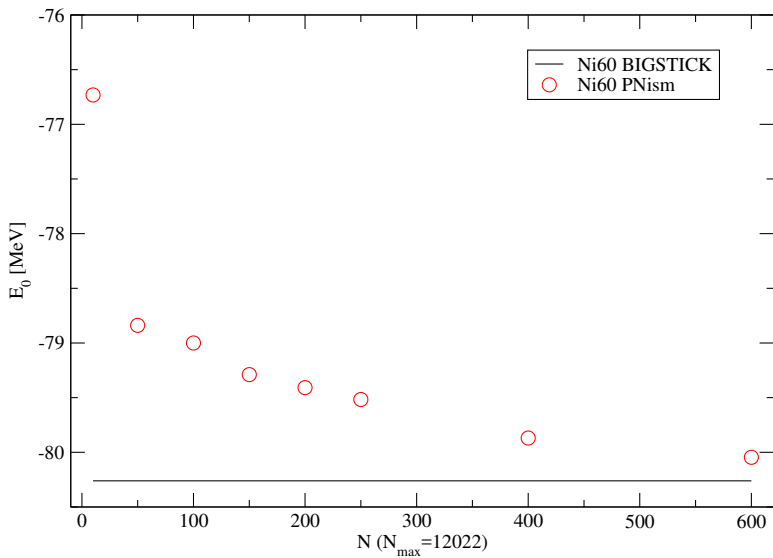


Figure 9: Ground state energy for  $^{60}\text{Ni}$

$N$	J-scheme dim.	Ground state E [MeV]	Abs. error	% error
10	20	-76.731	3.5400	4.398
50	412	-78.839	1.4221	1.778
100	1477	-79.000	1.2611	1.571
200	5424	-79.408	0.8531	1.063
400	20459	-79.869	0.3921	0.4885
600	45086	-80.046	0.2151	0.2679

**Table 4:**  $^{60}\text{Ni}$  ground state energy as a function of number  $N$  of proton and neutron wavefunctions retained for coupled J-scheme basis using M-scheme solutions in the  $(p_{1/2}, p_{3/2}, f_{5/2}, f_{7/2})$  model space.  $N_{\max} = 12022$ . J-scheme dimension is the size of the Hamiltonian for fixed  $J$ . Absolute error and percent error are computed relative to M-scheme solution from BIGSTICK.

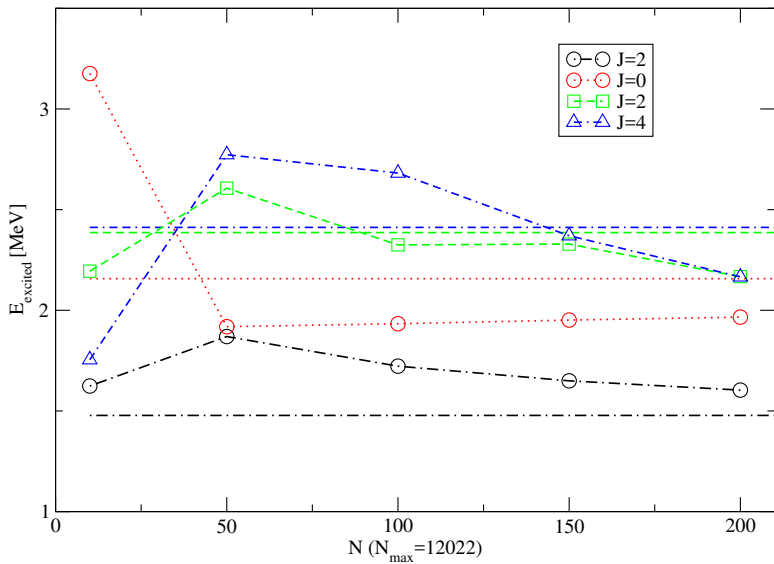


Figure 10: Excitation spectra for  $^{60}\text{Ni}$

- Showed that the distribution of nuclear wavefunction coefficients points the existence of a truncateable basis
- Studied the properties of proton-neutron entanglement entropy in shell model spaces. ( $S$  versus  $T_z$ ,  $S$  versus  $\lambda$ .)
- Demonstrated progress towards a J-scheme interacting shell model code to efficiently model nuclei.

# Future work

Short term:

- Optimize memory usage
- Parallel computing

Long term:

- Need to improve convergence of our results
  - Account for basis states left out with effective interaction
- Apply this code to very heavy nuclei



- [1] V.A. Bednyakov and F. Simkovic, "Nuclear spin structure in dark matter search: The zero momentum transfer limit," *Phys.Part.Nucl.* 36 (2005) 131-152. arXiv:hep-ph/0406218.
- [2] L. Willmann and K. Jungmann, "Matter-antimatter Asymmetry - Aspects at low energy," *Annalen der Physik* (2015). arXiv:1506.03001.
- [3] W. C. Haxton, C. P. Liu, and M. J. Ramsey-Musolf, "Nuclear anapole moments," *Physical Review C* 65 (045502), 045502–1–045502–30 (2002).
- [4] C. W. Johnson, W. E. Ormand, and P. G. Krastev, "Factorization in large-scale many-body calculations," *Comp. Phys. Comm.* 184 (2761), 1–34 (2013)
- [5] T. Papenbrock, and D. J. Dean, "Factorization of shell-model ground states," *Physical Review C* 67 (051303), 1–5 (2003).
- [6] T. Papenbrock, A. Juodagalvis, and D. J. Dean, "Solution of large scale nuclear structure problems by wave function factorization," *Physical Review C* 69 (024312), 1–12 (2004). 62
- [7] T. Papenbrock, and D. J. Dean, "Density matrix renormalization group and wavefunction factorization for nuclei," *J. .Phys. G: Nucl. .Part. Phys.* 31 (S1377S1383), S1377S1383 (2005).

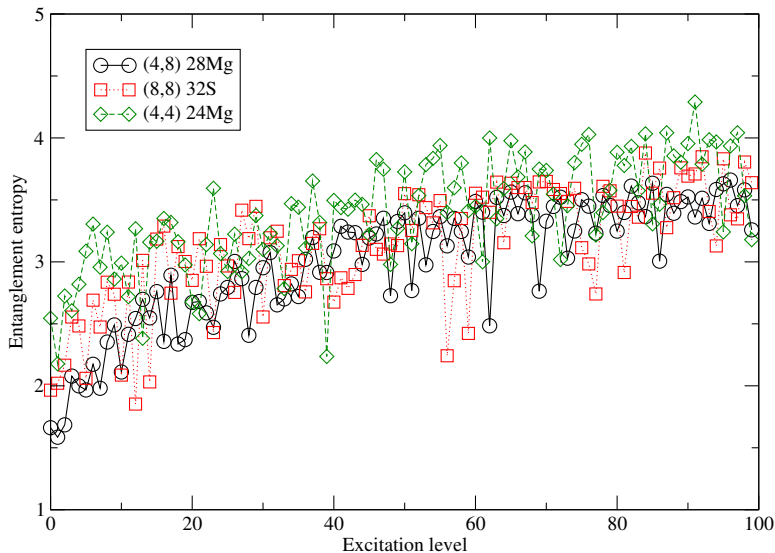


Figure 11: Proton-neutron entanglement entropy versus isospin in the sd-shell