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

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# Introduction: Big picture

Many experimental investigations require matrix elements of atomic nuclei:

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

$$\langle \Psi_f | \hat{O} | \Psi_i \rangle \tag{1}$$

# Introduction: A problem with large dimensions

$$\hat{H}\Psi = E\Psi \tag{2}$$

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

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

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

# Introduction: Truncate the basis?

$$\{|\alpha\rangle\}, \ \alpha = 1, 2, 3, ..., dim. \tag{4}$$

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

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

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

perhaps in some other basis?

# Background: Shell model calculations

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

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

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

where $i = 1, ..., k$ , $j = 1, ..., N$.

- Inspired by mean-field theory. (H.O., Woods-Saxon, etc.)
- Carry quantum numbers: $n$, $l$, $j$, $j_z = m$.

# Background: Single particle state basis

Harmonic oscillator basis has infinite single-particle states:

$$\{\phi_i\} = \{0s_{1/2}, 1p_{3/2}, 1p_{1/2}, 1d_{5/2}, 2s_{1/2}, 1d_{3/2}, 1f_{7/2}, ...\}, \tag{8}$$

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

- Leave out states with low occupation probability
- Leave out states with extremely high occupation probability

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

# Background: Example shell model space: sd-shell

*sd*-shell: The infinite space of all 'oscillator' states

$$\{\phi_i\} = \{0s_{1/2}, 1p_{3/2}, 1p_{1/2}, 1d_{5/2}, 2s_{1/2}, 1d_{3/2}, 1f_{7/2}, ...\}, \tag{9}$$

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: $1f_{7/2}$,...

# 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

Many-particle states are represented by:

$$|n_1, n_2, n_3, ..., n_k\rangle = |n_1\rangle\,|n_2\rangle\,|n_3\rangle\,...\,|n_k\rangle \tag{10}$$

Creation/annihilation operator formalism encodes fermion statistics:

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

Bit representation of many-particle states:

$$\hat{c}_1^\dagger \hat{c}_2^\dagger \hat{c}_4^\dagger\,|0\rangle = |110010\rangle \rightarrow 110010 \tag{11}$$

# Background: Wavefunctions with two species of nucleon

Two copies of the single-particle space, one for protons, one for neutrons. Then

$$\begin{aligned} |\pi\rangle &= |0101101011\rangle \in \mathcal{H}_{proton} \\ |\nu\rangle &= |1110111000\rangle \in \mathcal{H}_{neutron} \end{aligned} \tag{12}$$

Nuclear wavefunctions:

$$|\Psi\rangle = \sum_i^{d_\pi} \sum_j^{d_\nu} \Psi_{ij} |\pi_i\rangle \otimes |\nu_j\rangle \,, \tag{13}$$

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

# Background: Wavefunctions with two species of nucleon

Nuclear wavefunctions:

$$|\Psi\rangle = \sum_{i}^{d_\pi} \sum_{j}^{d_\nu} \Psi_{ij} \, |\pi_i\rangle \otimes |\nu_j\rangle \,, \tag{14}$$

$d_\pi \times d_\nu = dim.$

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|---|---|---|---|
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Table 3: Dimensions of the nuclear matrix eigenvalue problem. [4]

# Background: Many-proton many-neutron coupling scheme

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

$$\langle M_i | \hat{H} | M_j \rangle = \delta_{M_i, M_j} \tag{15}$$

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

$$[|\pi_i\rangle \otimes |\nu_j\rangle]_M, \tag{16}$$

- "M-scheme" basis
- "J-scheme" also possible

# Purpose: Approximating wavefunctions with a truncated basis

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

$$\sum_{\beta}^{Q \ll dim.} H_{\alpha\beta}\Psi_{\beta} \approx E\Psi_{\alpha}, \tag{17}$$

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

$$|\Psi\rangle \approx \sum_{ij}^{Q \ll \min[d_\pi, d_\nu]} \Psi_{ij} \, |\pi_i\rangle \otimes |\nu_j\rangle \,, \tag{18}$$

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

# First study: Entanglement entropy

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

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

$$|\Psi\rangle = \sum_i^{d_\pi} \sum_j^{d_\nu} \Psi_{ij} \, |\pi_i\rangle \otimes |\nu_j\rangle = \sum_i \gamma_i \, |\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle \, . \tag{19}$$

- We can compute the eigenvalues of

$$\underline{\Psi} * \underline{\Psi}^\dagger = UDV^\dagger VD^\dagger U^\dagger = UD^2 U^\dagger, \tag{20}$$

  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

$$|\Psi\rangle = \sum_{i}^{d_\pi} \sum_{j}^{d_\nu} \Psi_{ij} |\pi_i\rangle \otimes |\nu_j\rangle = \sum_i \gamma_i |\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle . \tag{21}$$

- 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 postulate that $\gamma_i^2$ will fall off even faster for nuclei with unequal numbers of protons and neutrons.

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

Will $\gamma_i^2$ will fall off even faster in nuclei with unequal numbers of protons and neutrons?

$$|\Psi\rangle = \sum_i^{d_\pi} \sum_j^{d_\nu} \Psi_{ij} |\pi_i\rangle \otimes |\nu_j\rangle = \sum_i \gamma_i |\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle . \tag{22}$$

Let's compare two sets of nuclei:

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

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

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

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

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

- Proton-neutron entanglement entropy

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

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

$d_\pi \leq d_\nu$.

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

$$|\Psi\rangle = \sum_i^{d_\pi} \sum_j^{d_\nu} \Psi_{ij} |\pi_i\rangle \otimes |\nu_j\rangle = \sum_i \gamma_i |\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle . \tag{26}$$

$$S_{pn} = -\sum_i \gamma_i^2 \ln \gamma_i^2 \tag{27}$$

Wavefuntion normalization: $1 = \sum_i^{d_\pi} \gamma_i^2$.

- If $\{\gamma_i^2\} = \{1, 0, 0, ...\}$, $S_{pn} = S_{min} = 0$
- If $\{\gamma_i^2\} = \{\frac{1}{d_\pi}, \frac{1}{d_\pi}, \frac{1}{d_\pi}, ...\}$, $S_{pn} = S_{max} = \ln(d_\pi)$

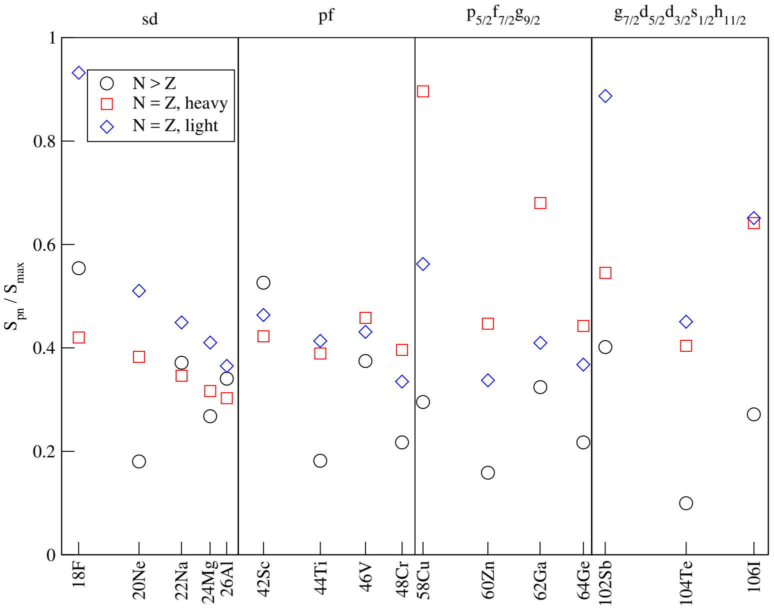


Figure 1: Proton-neutron entanglement entropy for particle-hole conjugate nuclei

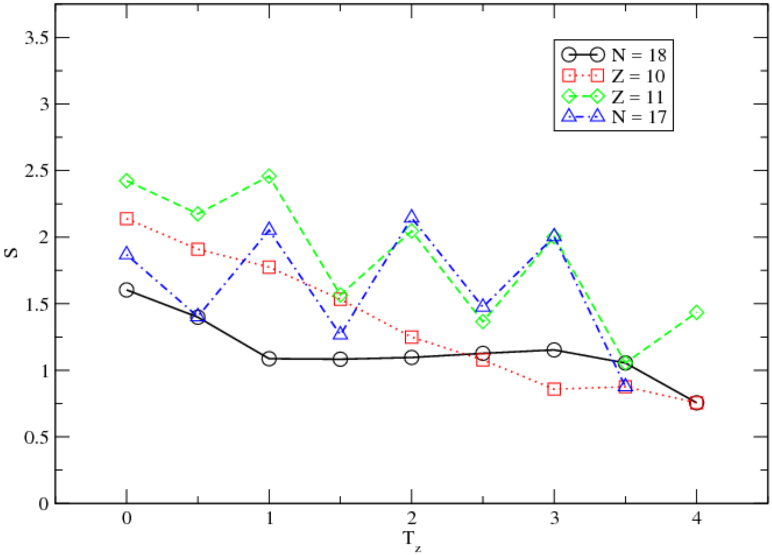


Figure 2: Proton-neutron entanglement entropy versus isospin in the sd-shell

# First study: Entanglement entropy (Continued...)

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

Nuclear Hamiltonian:

$$\hat{H} = \hat{H}_{proton} + \hat{H}_{neutron} + \lambda \hat{H}_{proton-neutron} \tag{28}$$

How does the parameter $\lambda$ affect $S_{pn}$?

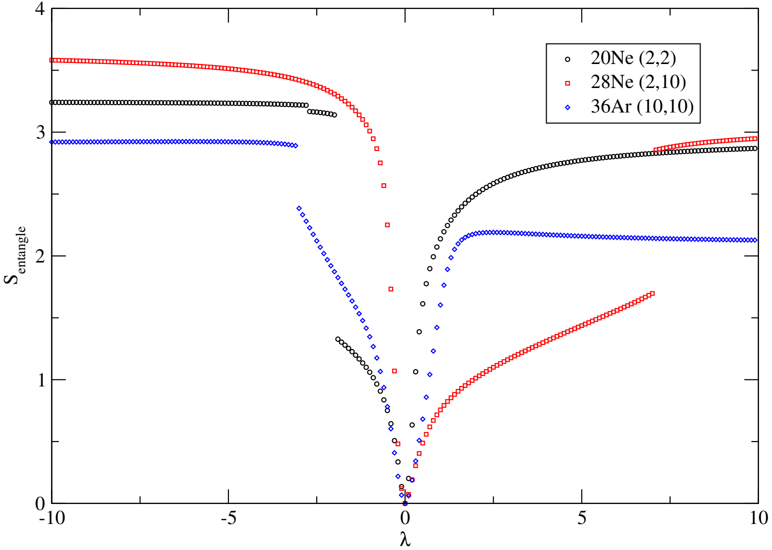


Figure 3: Proton-neutron entanglement entropy versus proton-neutron interaction strength

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

Toy model Hamiltonian:

$$\begin{aligned} \hat{H} &= \hat{H}_A + \hat{H}_B + \lambda \hat{H}_{AB} \\ &= \hat{D}_A + \hat{D}_B + \lambda \sum V \otimes W, \end{aligned} \tag{29}$$

with random interactions. Will this exhibit the same behavior?

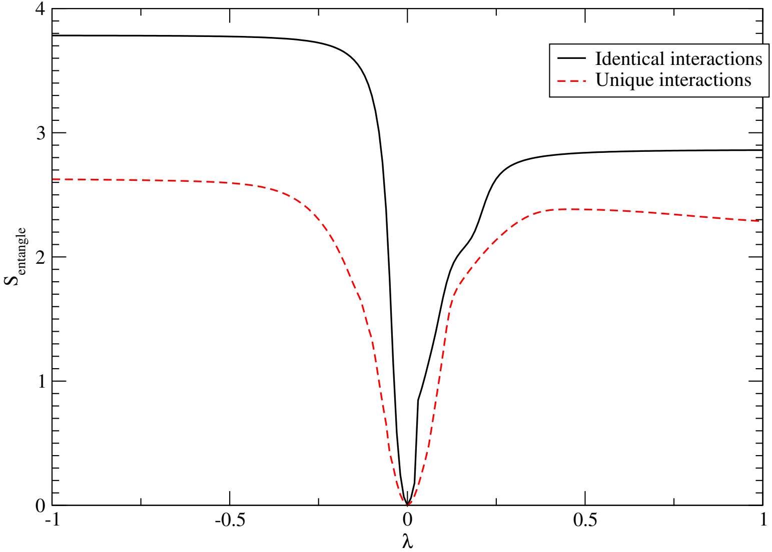


Figure 4: Toy model

# Second study: Specific framework

# Method: Strength function decomposition

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

$$|\Psi\rangle = \sum_{ij} \tilde{\Psi}_{ij} |PP\rangle \otimes |NN\rangle , \tag{30}$$

$$|\Psi\rangle \tag{31}$$

$$c_\alpha = \langle \alpha | \Psi \rangle \tag{32}$$

$$|\Psi\rangle = \sum_\alpha c_\alpha |\alpha\rangle \tag{33}$$

$$c_\alpha^2 = \langle \Psi | \alpha \rangle \langle \alpha | \Psi \rangle \tag{34}$$

Generalize to bipartite system, guess a basis, and examine $c_\alpha^2$.

# Method: Strength function decomposition

Our guess: eigenstates of the proton-proton interaction and of the neutron-neutron interaction:

$$\hat{H}_{proton} |PP\rangle = E_p |PP\rangle ,$$
$$\hat{H}_{neutron} |NN\rangle = E_n |NN\rangle . \tag{35}$$

Plot the strength function coefficients:

$$\langle \Psi | PP \rangle \langle PP | \Psi \rangle = \sum_P |\tilde{\Psi}_{NP}|^2 \equiv c_N^2 \tag{36}$$

$$\langle \Psi | NN \rangle \langle NN | \Psi \rangle = \sum_N |\tilde{\Psi}_{NP}|^2 \equiv c_P^2. \tag{37}$$

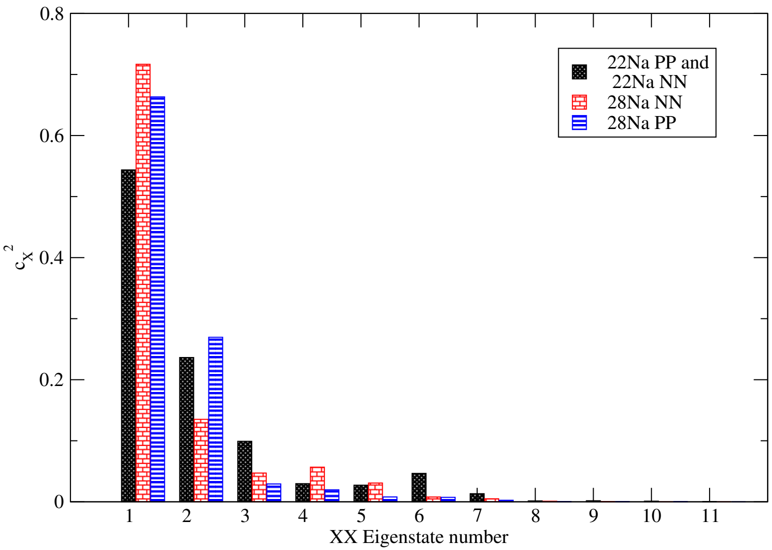


Figure 5: Proton-proton and neutron-neutron strength decomposition of nuclear wavefunctions

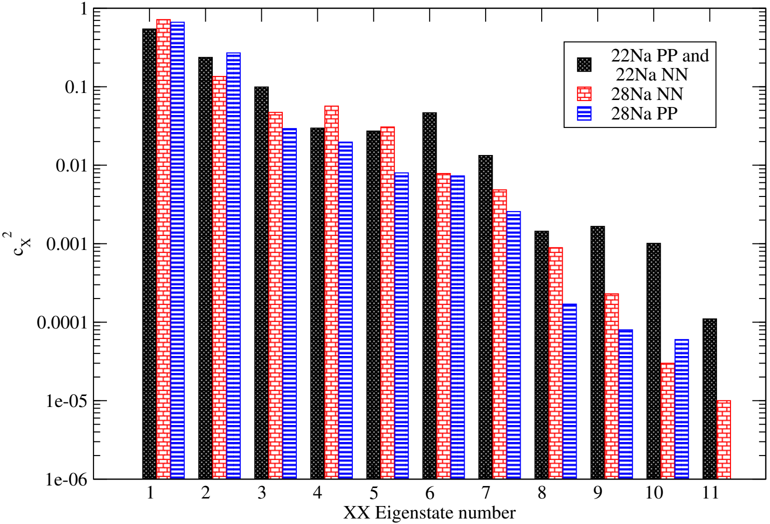


Figure 6: Proton-proton and neutron-neutron strength decomposition of nuclear wavefunctions

# Recap

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

- How do we select states to keep/leave out?
- Can we still use the M-scheme?

# A new shell model code: PNISM

# PNISM: Create the proton-neutron coupled basis and truncate

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

- Use existing ISM code to solve:

$$\begin{aligned} \hat{H}_{proton} \left| j_p \alpha_p \right\rangle &= E_p \left| j_p \alpha_p \right\rangle \\ \hat{H}_{neutron} \left| j_n \beta_n \right\rangle &= E_n \left| j_n \beta_n \right\rangle , \end{aligned} \tag{38}$$

  dimension $d_\pi$ and $d_\nu$ problems (and not $d_\pi \times d_\nu$).

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

$$[\left| j_p \alpha_p \right\rangle \otimes \left| j_n \beta_n \right\rangle]_J \tag{39}$$

# PNISM: Create the proton-neutron coupled basis and truncate

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

$$|a\rangle = [|j_p\alpha_p\rangle \otimes |j_n\beta_n\rangle]_J, \tag{40}$$

has $d_\pi \times d_\nu$ states. But we truncate to compute:

$$\sum_b^{N^2 \ll d_\pi \times d_\nu} H_{ab}\Psi_b = E\Psi_a, \tag{41}$$

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

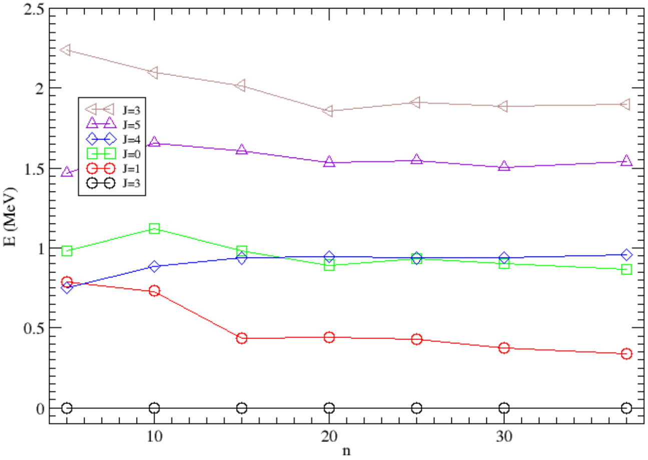


Figure 7: Excitation spectra for $^{22}$Na

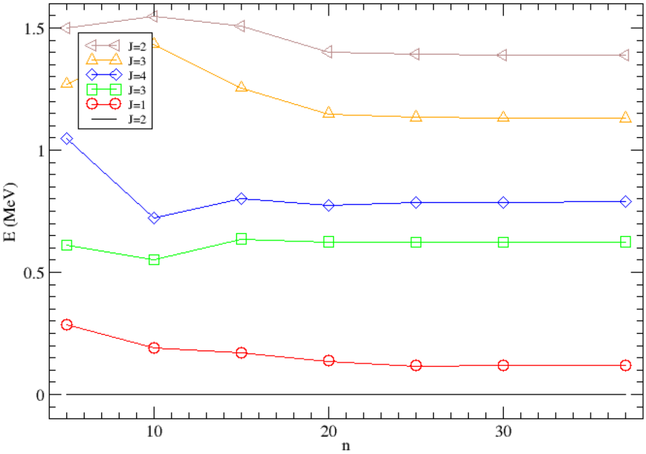


Figure 8: Excitation spectra for $^{28}Na$

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

Table 4: M-scheme dimensions for nuclei in the ($p_{1/2}$, $p_{3/2}$, $f_{5/2}$, $f_{7/2}$) model space.

| Val. protons | Val. neutrons | M-scheme dim. |
|---|---|---|
| 0 | 8 | 12022 |
| 8 | 0 | 12022 |
| 12 | 0 | 12022 |
| 0 | 12 | 12022 |

Table 5: M-scheme dimensions for $\hat{H}_{proton}$ and $\hat{H}_{neutron}$ which are used by PNISM to build the J-scheme basis for nuclei in the ($p_{1/2}$, $p_{3/2}$, $f_{5/2}$, $f_{7/2}$) model space.

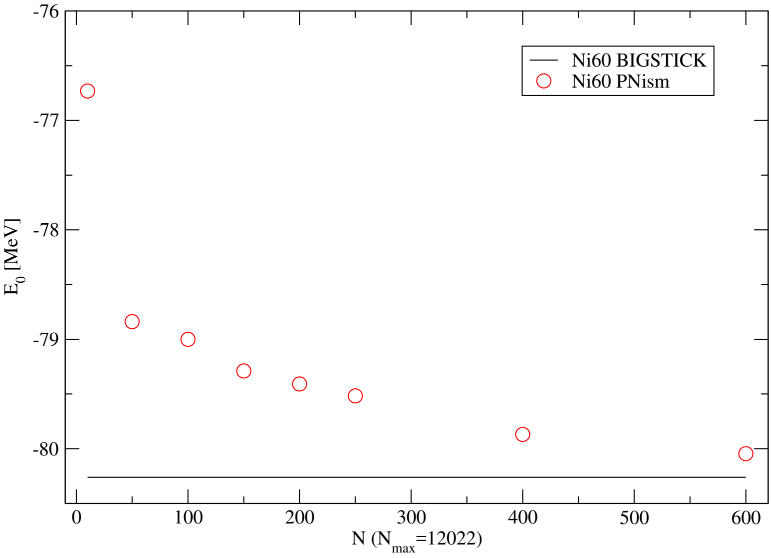


Figure 9: Ground state energy for $^{60}Ni$

| $N$ | 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 6: $^{60}$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.

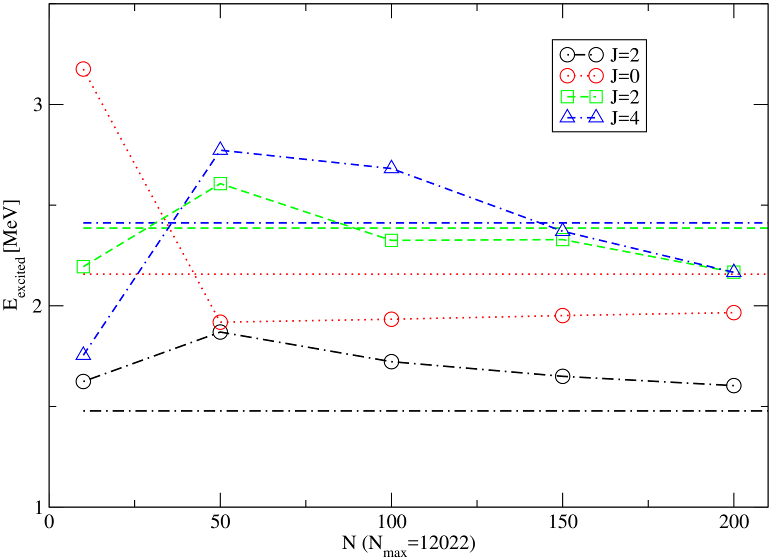


Figure 10: Excitation spectra for $^{60}Ni$

# Summary

- 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
- Investigate convergence of transition rates

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

# Sources

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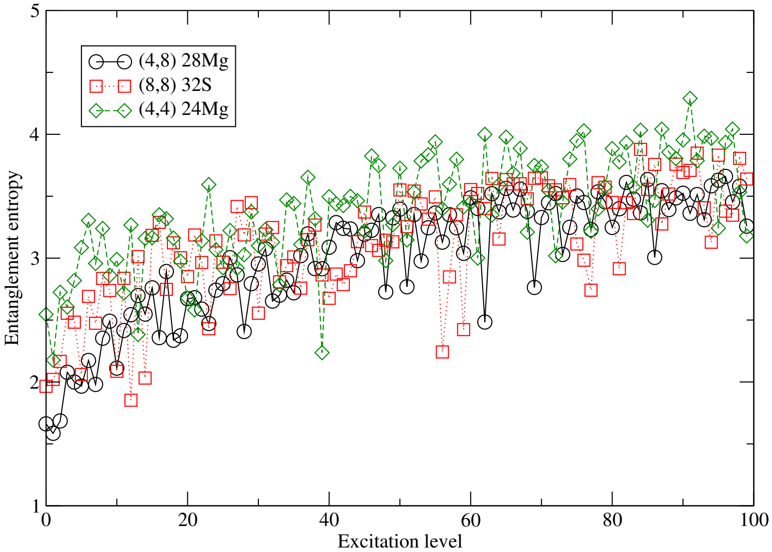


Figure 11: Proton-neutron entanglement entropy versus isospin in the sd-shell

# 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

$$|\Psi\rangle = \sum_i \gamma_i \, |\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle \,, \tag{42}$$

  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

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  in some unknown basis $|\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle$.
- We can compute the eigenvalues of

$$\underline{\Psi} * \underline{\Psi}^\dagger = UDV^\dagger VD^\dagger U^\dagger = UD^2 U^\dagger, \tag{44}$$

  to find $\gamma_i^2$.