

Efficient Modeling of Nuclei Through Coupling of Proton and Neutron Wavefunctions

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Introduction: Nuclear structure

- 1 Introduction: Nuclear structure
- 2 Background: Shell Model calculations
- 3 First study: Entanglement entropy
- 4 Second study: Specific framework
- 5 A new shell model code: PNISM
- 6 Summary and future work

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]

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

Introduction: A problem with large dimensions

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

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

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

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

Introduction: Truncate the basis?

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

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

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

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

perhaps in some other basis?

Background: Shell model calculations

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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 states

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

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

- 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:

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

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

- 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

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

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 ϕ_i

Background: Quick notes on occupation representation

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

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:

$$|\Psi\rangle = \sum_i^{d_\pi} \sum_j^{d_\nu} \Psi_{ij} |\pi_i\rangle \otimes |\nu_j\rangle, \quad (14)$$

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

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

$$\langle M_i | \hat{H} | M_j \rangle = \delta_{M_i, M_j} \quad (15)$$

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

$$[|\pi_i\rangle \otimes |\nu_j\rangle]_M, \quad (16)$$

- “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?

$$\sum_{\beta}^{Q \ll \dim.} H_{\alpha\beta} \psi_{\beta} \approx E \psi_{\alpha}, \quad (17)$$

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

$$|\psi\rangle \approx \sum_{ij}^{Q \ll \min[d_{\pi}, d_{\nu}]} \psi_{ij} |\pi_i\rangle \otimes |\nu_j\rangle, \quad (18)$$

Answer: It depends on the distribution of ψ_{ij} .

First study: Entanglement entropy: A measure of Ψ_{ij} distributions

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Method: Entanglement entropy: A measure of Ψ_{ij} distributions

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

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

- We can compute the eigenvalues of

$$\underline{\Psi} * \underline{\Psi}^\dagger = U D V^\dagger V D^\dagger U^\dagger = U D^2 U^\dagger, \quad (20)$$

to find γ_i^2 .

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

Method: Entanglement entropy: A measure of Ψ_{ij} distributions

$$|\Psi\rangle = \sum_i^{d_\pi} \sum_j^{d_\nu} \Psi_{ij} |\pi_i\rangle \otimes |\nu_j\rangle = \sum_i \gamma_i |\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle. \quad (21)$$

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

Method: Entanglement entropy: A measure of ψ_{ij} distributions

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

$$|\Psi\rangle = \sum_i^{d_\pi} \sum_j^{d_\nu} \psi_{ij} |\pi_i\rangle \otimes |\nu_j\rangle = \sum_i \gamma_i |\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle. \quad (22)$$

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 Ψ_{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:

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

Method: Entanglement entropy: A measure of Ψ_{ij} distributions

$$|\Psi\rangle = \sum_i^{d_\pi} \sum_j^{d_\nu} \Psi_{ij} |\pi_i\rangle \otimes |\nu_j\rangle = \sum_i \gamma_i |\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle. \quad (25)$$

$$S_{pn} = - \sum_i \gamma_i^2 \ln \gamma_i^2 \quad (26)$$

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

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

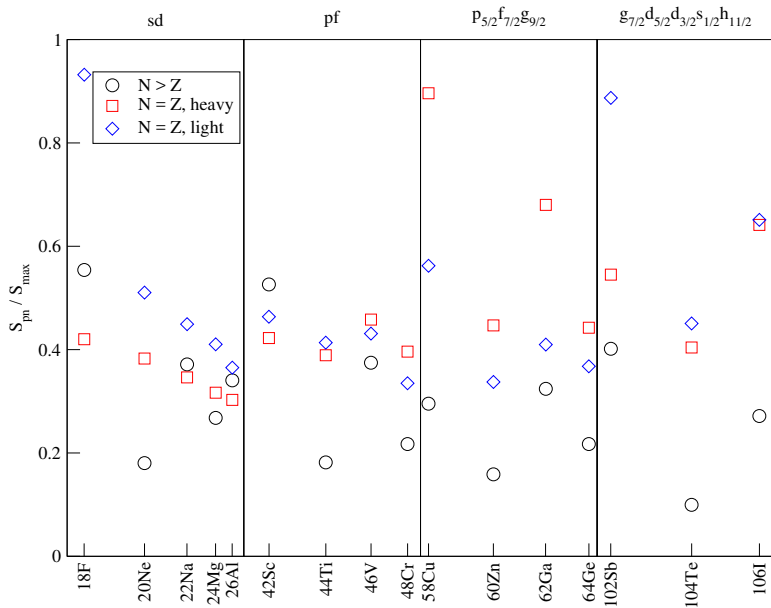


Figure 1: Proton-neutron entanglement entropy for particle-hole conjugate nuclei

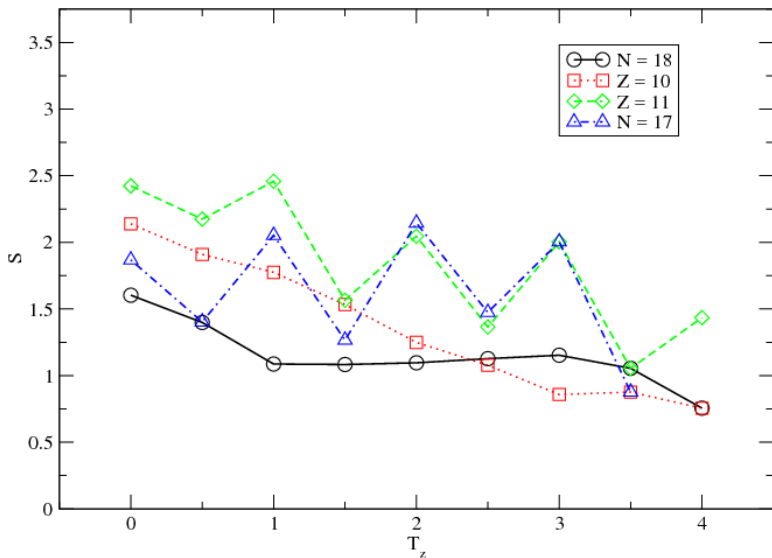


Figure 2: Proton-neutron entanglement entropy versus isospin in the sd-shell

First study: Entanglement entropy (Continued...)

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Study: Varying the strength of the proton-neutron interaction

Nuclear Hamiltonian:

$$\hat{H} = \hat{H}_{proton} + \hat{H}_{neutron} + \lambda \hat{H}_{proton-neutron} \quad (27)$$

How does the parameter λ affect S_{pn} ?

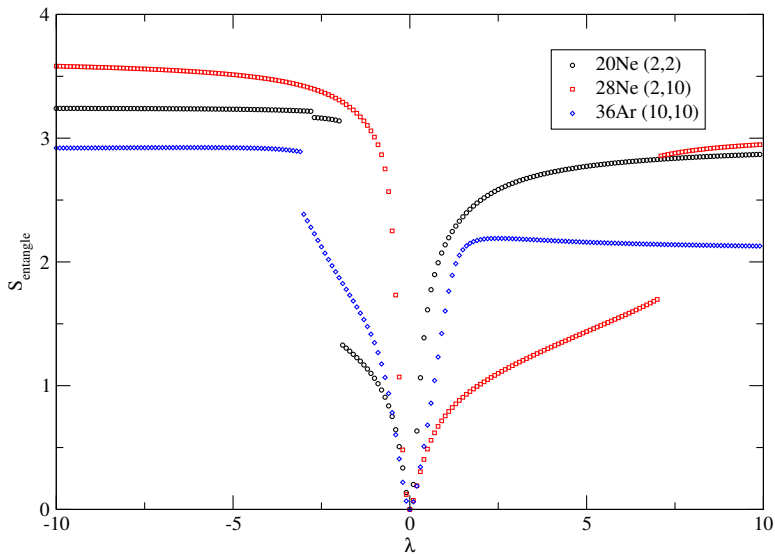


Figure 3: Proton-neutron entanglement entropy versus proton-neutron interaction strength

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

Toy model Hamiltonian:

$$\begin{aligned}\hat{H} &= \hat{H}_A + \hat{H}_B + \lambda \hat{H}_{AB} \\ &= \hat{D}_A + \hat{D}_B + \lambda \sum V \otimes W,\end{aligned}\tag{28}$$

with random interactions. Will this exhibit the same behavior?

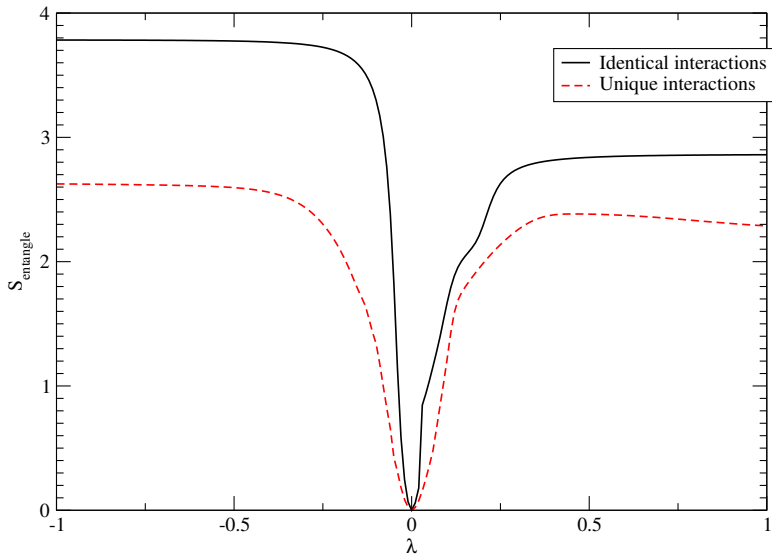


Figure 4: Toy model

Second study: Specific framework

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Method: Strength function decomposition

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

$$|\Psi\rangle = \sum_{ij} \tilde{\Psi}_{ij} |PP\rangle \otimes |NN\rangle, \quad (29)$$

$$|\Psi\rangle \quad (30)$$

$$c_\alpha = \langle \alpha | \Psi \rangle \quad (31)$$

$$|\Psi\rangle = \sum_{\alpha} c_{\alpha} |\alpha\rangle \quad (32)$$

$$c_{\alpha}^2 = \langle \Psi | \alpha \rangle \langle \alpha | \Psi \rangle \quad (33)$$

Generalize to bipartite system, guess a basis, and examine c_{α}^2 .

Method: Strength function decomposition

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

$$\begin{aligned}\hat{H}_{proton} |PP\rangle &= E_p |PP\rangle, \\ \hat{H}_{neutron} |NN\rangle &= E_n |NN\rangle.\end{aligned}\tag{34}$$

Plot the strength function coefficients:

$$\langle \Psi | PP \rangle \langle PP | \Psi \rangle = \sum_P |\tilde{\Psi}_{NP}|^2 \equiv c_N^2\tag{35}$$

$$\langle \Psi | NN \rangle \langle NN | \Psi \rangle = \sum_N |\tilde{\Psi}_{NP}|^2 \equiv c_P^2.\tag{36}$$

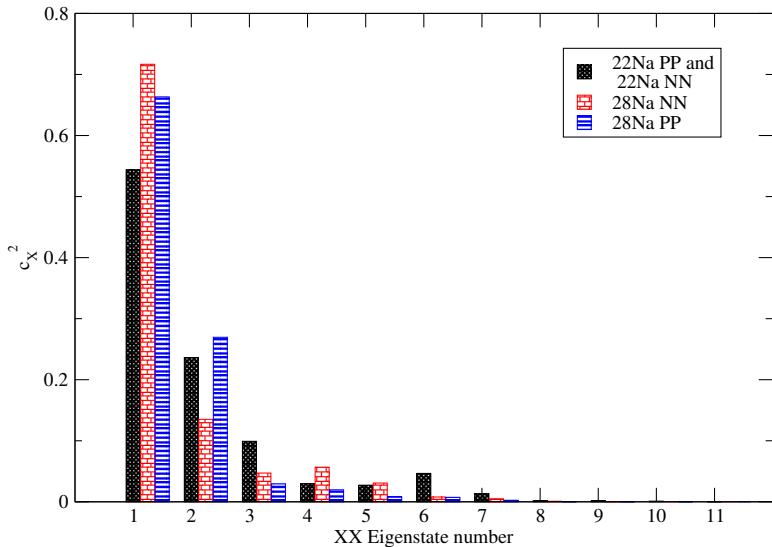


Figure 5: Proton-proton and neutron-neutron strength decomposition of nuclear wavefunctions

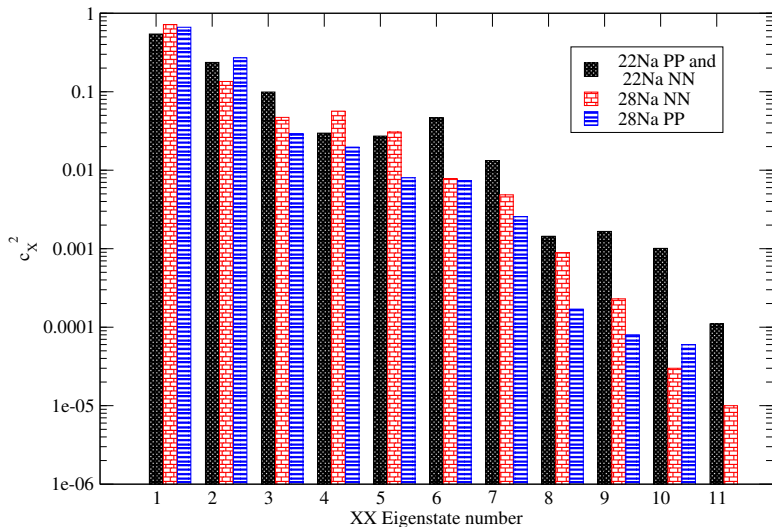


Figure 6: Proton-proton and neutron-neutron strength decomposition of nuclear wavefunctions

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

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

A new shell model code: PNISM

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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:

$$\begin{aligned}\hat{H}_{proton} |j_p \alpha_p\rangle &= E_p |j_p \alpha_p\rangle \\ \hat{H}_{neutron} |j_n \beta_n\rangle &= E_n |j_n \beta_n\rangle,\end{aligned}\tag{37}$$

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

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

$$[|j_p \alpha_p\rangle \otimes |j_n \beta_n\rangle]_J\tag{38}$$

PNISM: Create the proton-neutron coupled basis and truncate

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

Our basis,

$$|a\rangle = [|j_p \alpha_p\rangle \otimes |j_n \beta_n\rangle]_J, \quad (39)$$

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

$$\sum_b^{N^2 \ll d_\pi \times d_\nu} H_{ab} \Psi_b = E \Psi_a, \quad (40)$$

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

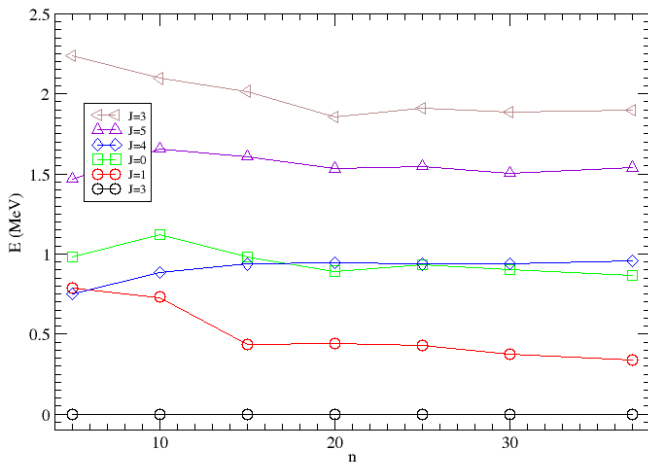


Figure 7: Excitation spectra for ^{22}Na

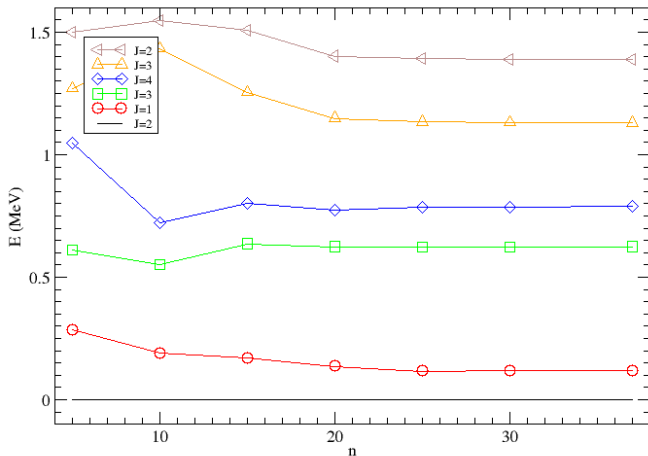


Figure 8: Excitation spectra for ^{28}Na

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

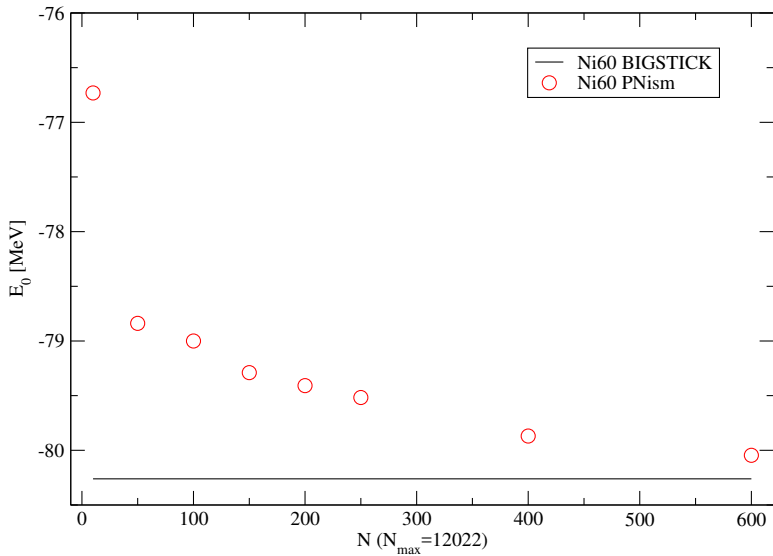


Figure 9: Ground state energy for ^{60}Ni

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.

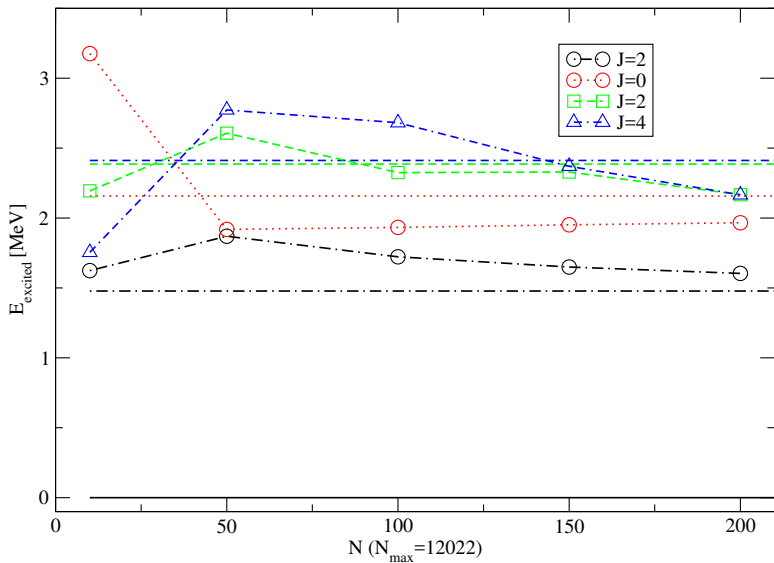


Figure 10: Excitation spectra for ^{60}Ni

Summary and future work

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- Showed that the distribution of wavefunction coefficients points to the existence of an efficient basis (can truncate it)
- Studied the properties of proton-neutron entanglement entropy in shell model spaces. (S versus T_z , S versus λ .)
- Demonstrated progress towards a J-scheme interacting shell model code to efficiently model nuclei

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

- [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](#).
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- [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)
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- [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).

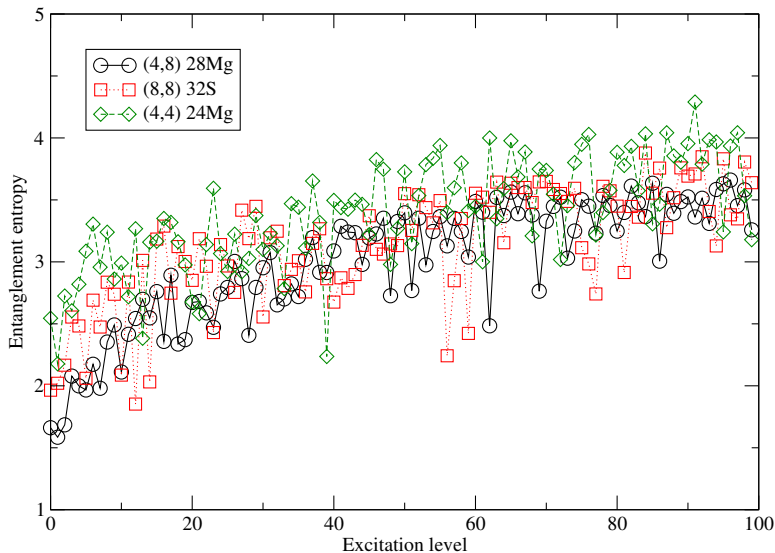


Figure 11: Proton-neutron entanglement entropy versus isospin in the sd-shell

Method: Entanglement entropy: A measure of Ψ_{ij} distributions

Without going into the details...

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

$$|\Psi\rangle = \sum_i \gamma_i |\tilde{\pi}_i\rangle \otimes |\tilde{\nu}_i\rangle, \quad (41)$$

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

- If γ_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 Ψ_{ij} distributions

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

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

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

- We can compute the eigenvalues of

$$\underline{\Psi} * \underline{\Psi}^\dagger = UDV^\dagger VD^\dagger U^\dagger = UD^2 U^\dagger, \quad (43)$$

to find γ_i^2 .