Efficient Modeling of Nuclei Through Coupling of Proton and Neutron Wavefunctions

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April 6, 2018

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	9.4×10^4	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?

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

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

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

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

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 ϕ_i

Background: Quick notes on occupation representation

Many-particle states are represented by:

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

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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^{52}Fe	pf	1.1×10^8	720 GB
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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 Ψ_{ij}.

First study: Entanglement entropy

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

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

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

- 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 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

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

- 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?

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

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 Ψ_{ij} distributions

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

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

- Proton-neutron entanglement entropy

$$S_{pn} = -\sum_i \gamma_i^2 \ln \gamma_i^2 \tag{24}$$

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

$d_\pi \leq d_\nu$.

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

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

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

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

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

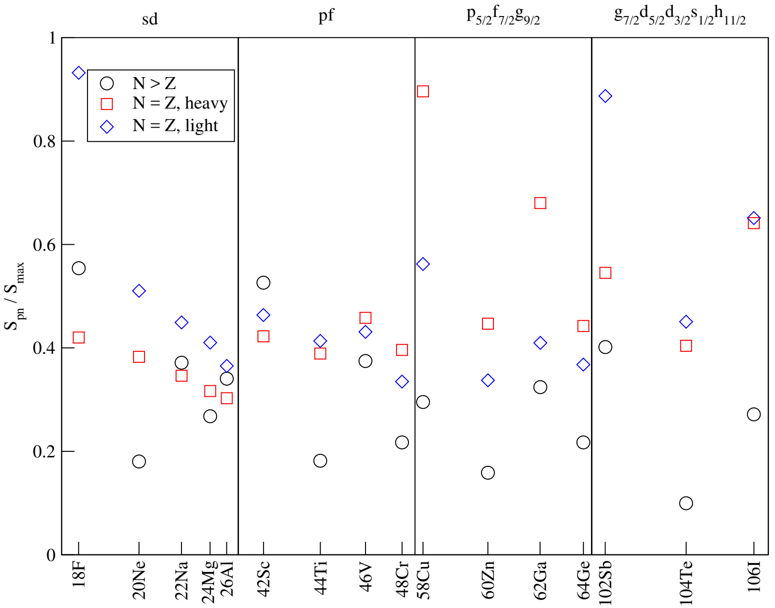

Figure 1: Proton-neutron entanglement entropy for particle-hole conjugate nuclei

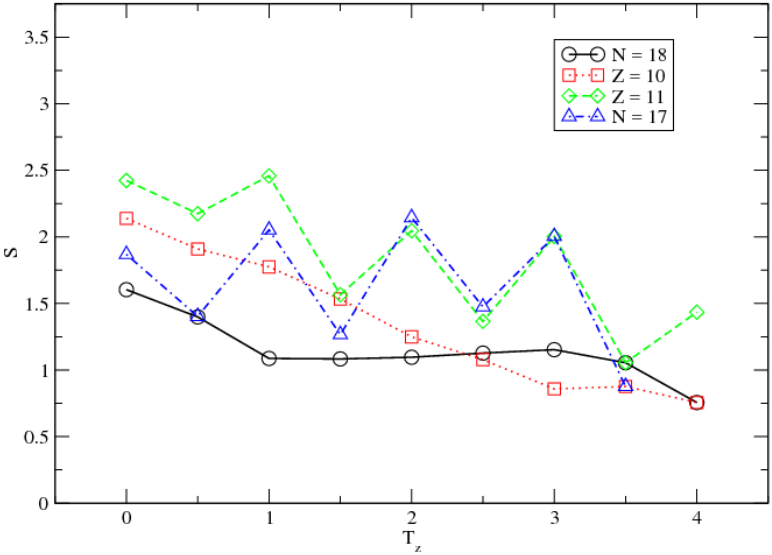

Figure 2: Proton-neutron entanglement entropy versus isospin in the sd-shell

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 λ affect S_{pn}?

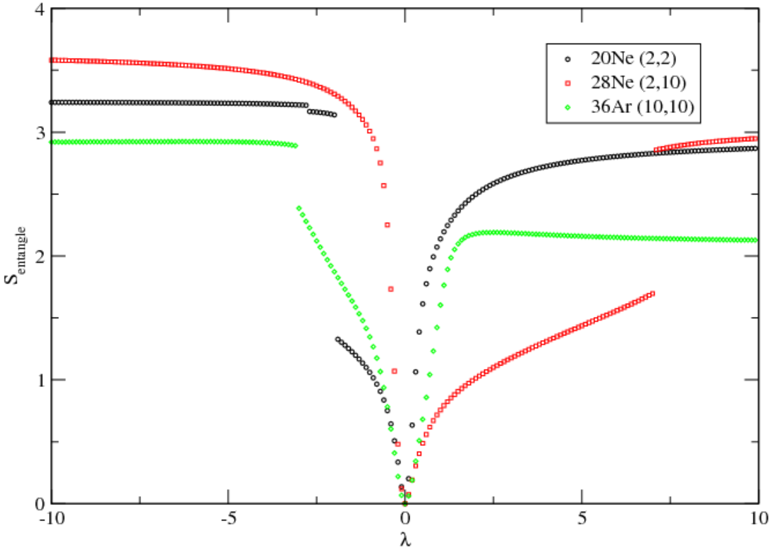

Figure 3: Proton-neutron entanglement entropy versus proton-neutron interaction strength

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

Toy model Hamiltonian:

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

with random interactions. Will this exhibit the same behavior?

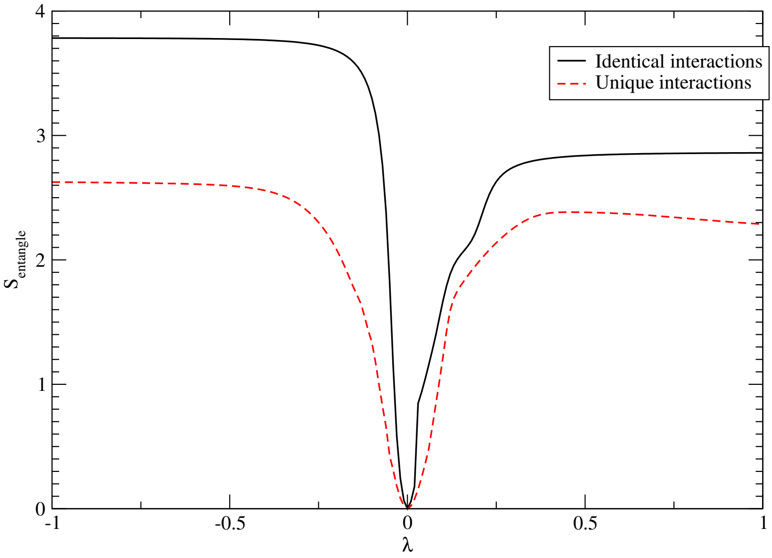

Figure 4: Toy model

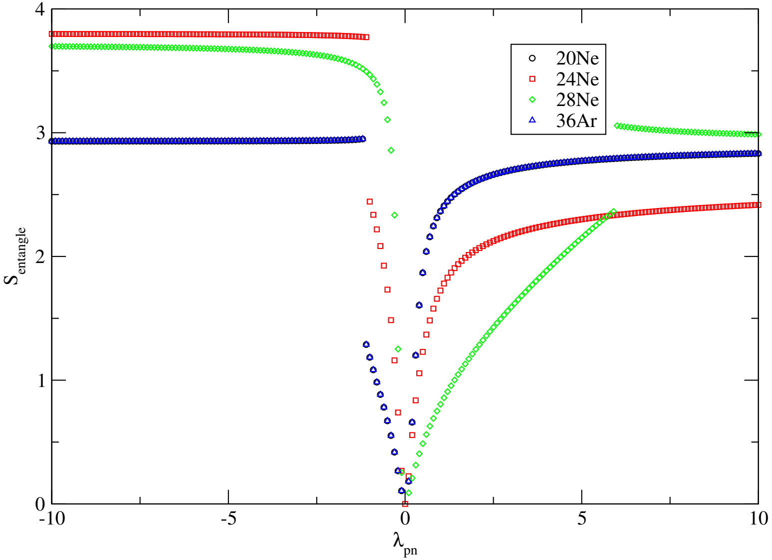

Figure 5: Proton-neutron entanglement entropy versus proton-neutron interaction strength with monopole terms removed (responsible for shell structure)

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_α^2.

Method: Strength function decomposition

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

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

Plot the strength function coefficients:

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

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

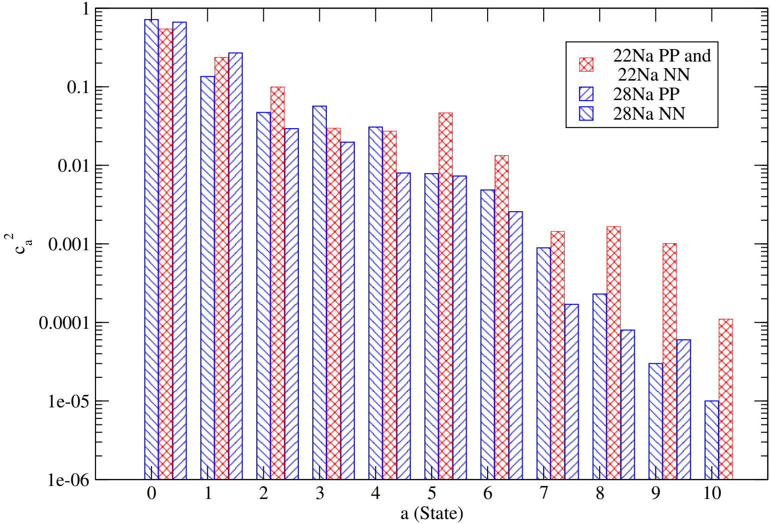

Figure 6: Proton-proton and neutron-neutron strength decomposition of nuclear wavefunctions

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

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

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

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.

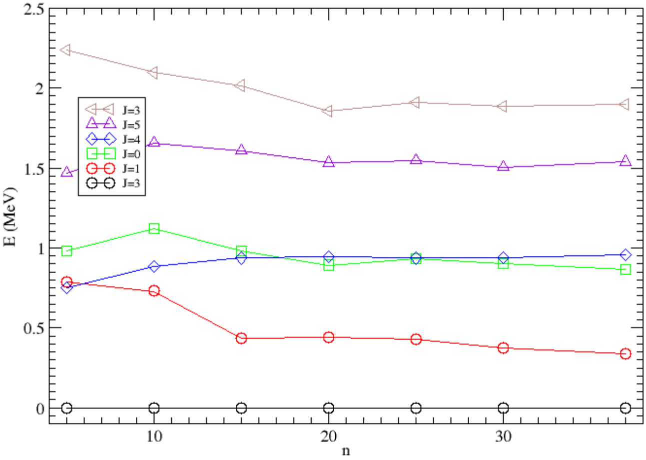

Figure 7: Excitation spectra for ^{22}Na

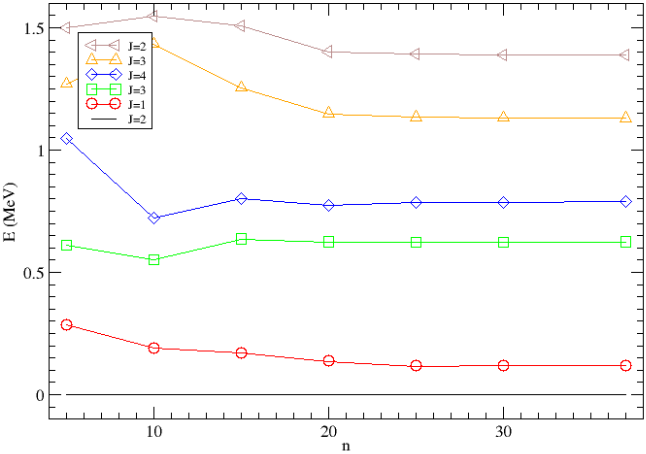

Figure 8: Excitation spectra for ^{28}Na

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

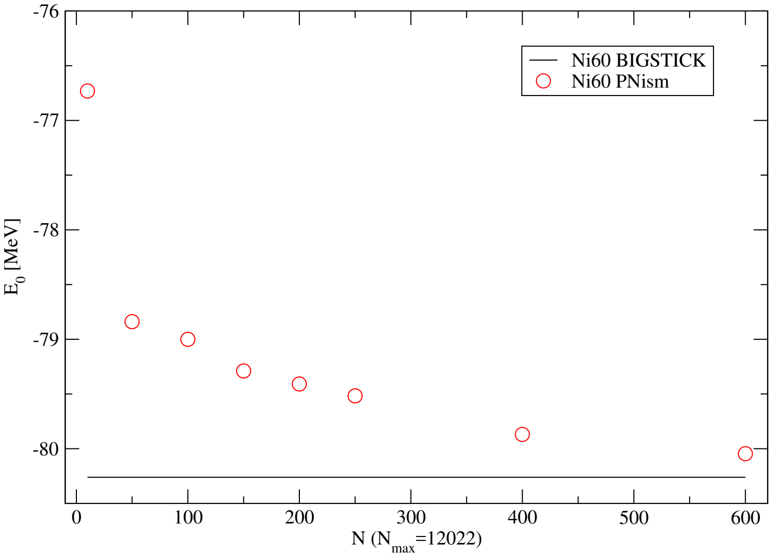

Figure 9: Ground state energy for ^{60}Ni

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.

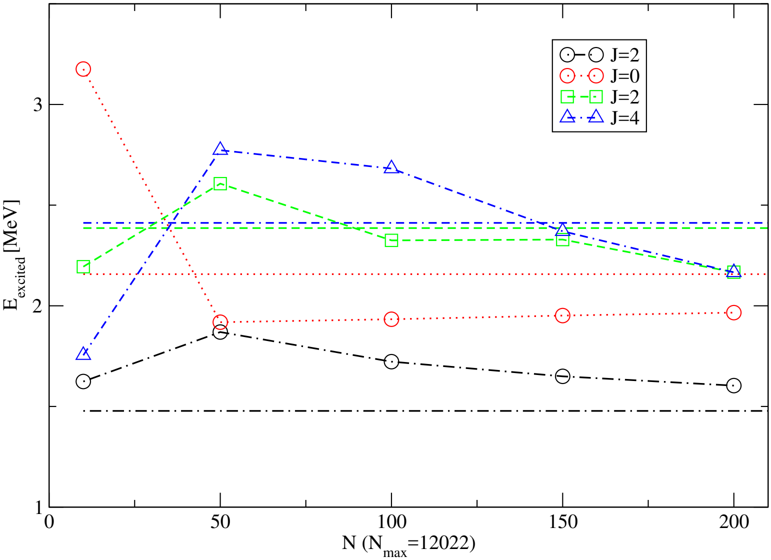

Figure 10: Excitation spectra for ^{60}Ni

Summary

- 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 λ.)
- 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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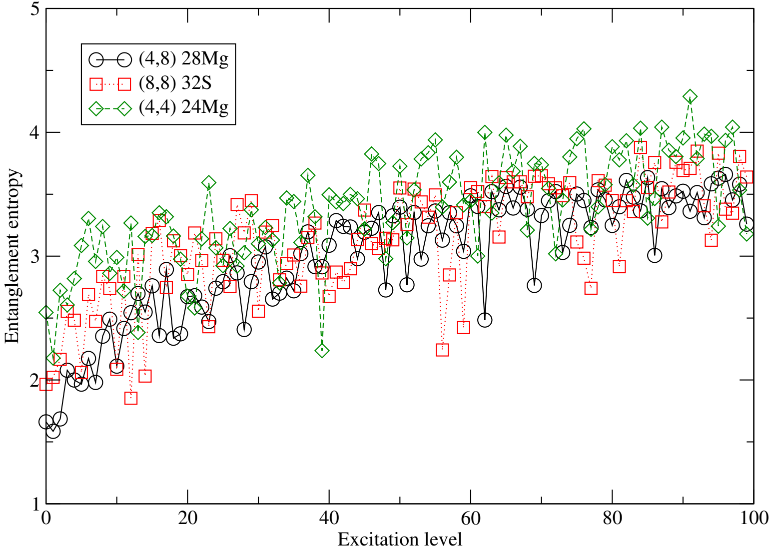

Figure 11: Proton-neutron entanglement entropy versus isospin in the sd-shell

Method: Entanglement entropy: A measure of 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

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

  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

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- Diagonal elements of D, γ_i, tell us about

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

- We can compute the eigenvalues of

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

to find γ_i^2.