A weak entanglement approximation for nuclear structure

Proton And Neutron Approximate Shell model (PANASh)

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Shell Model Symposium

Celebrating 75 Years of the Nuclear Shell Model and Maria Goeppert-Mayer

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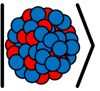
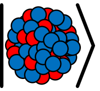
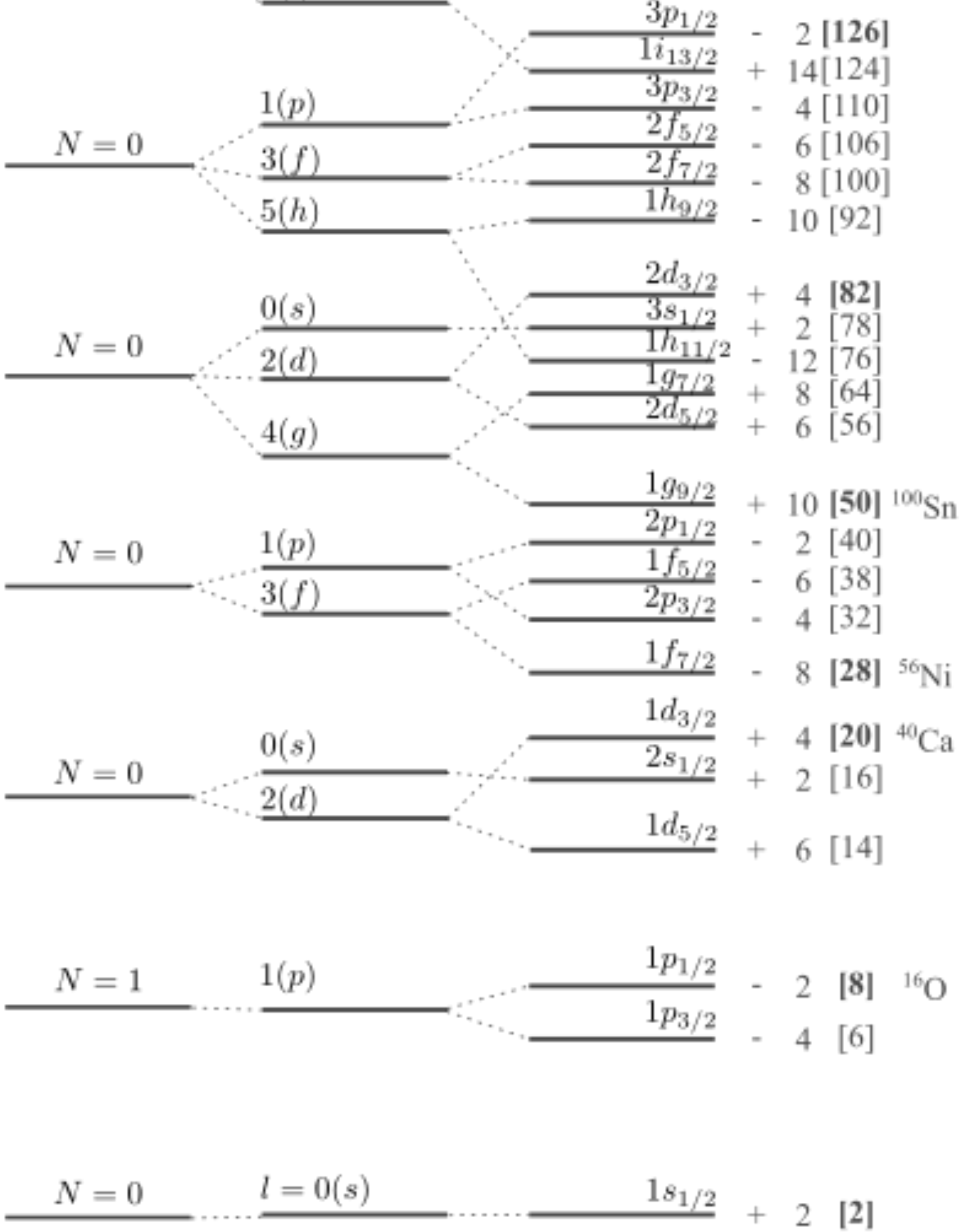
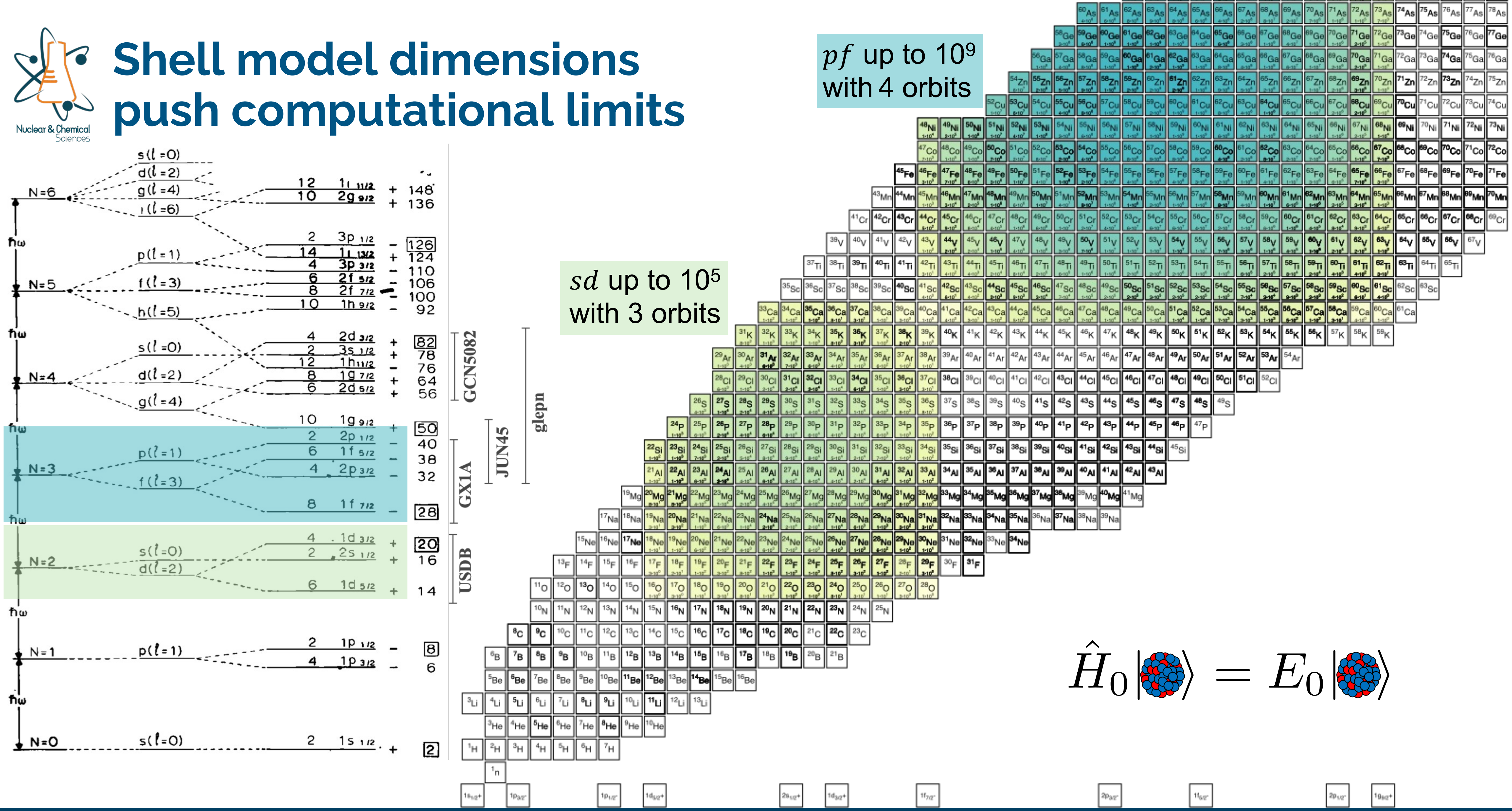
Shell model dimensions push computational limits

$\hat{H}_0|$  $\rangle = E_0|$  $\rangle$

Matrix diagonalization



Shell model dimensions push computational limits

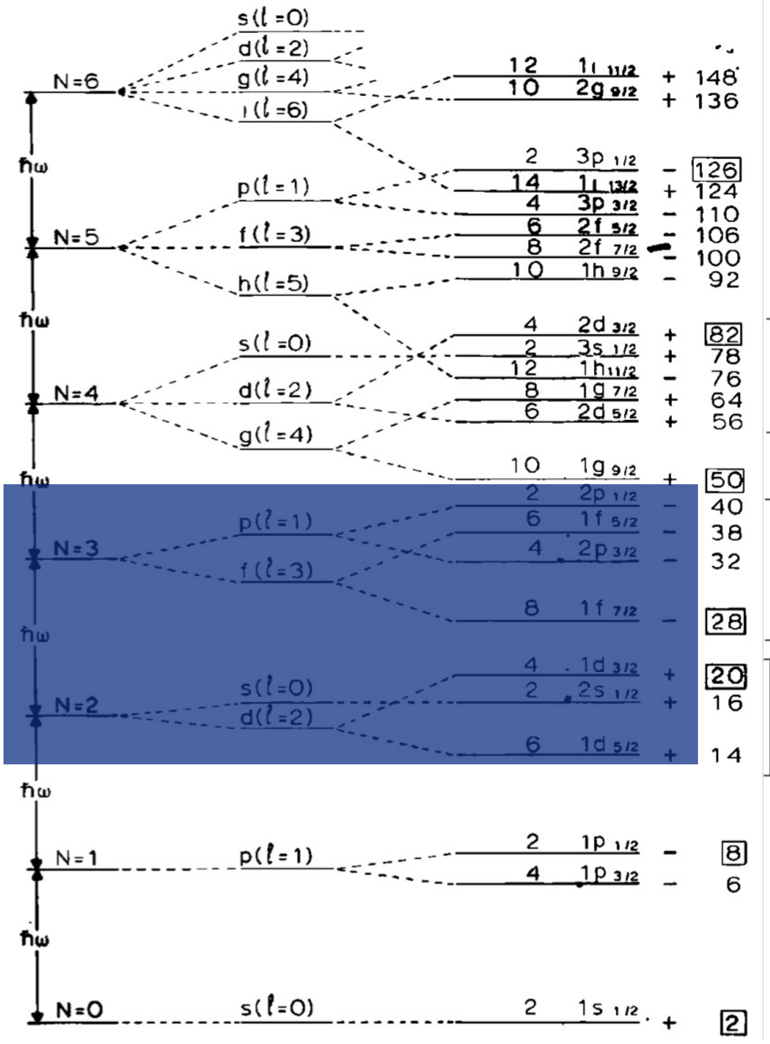


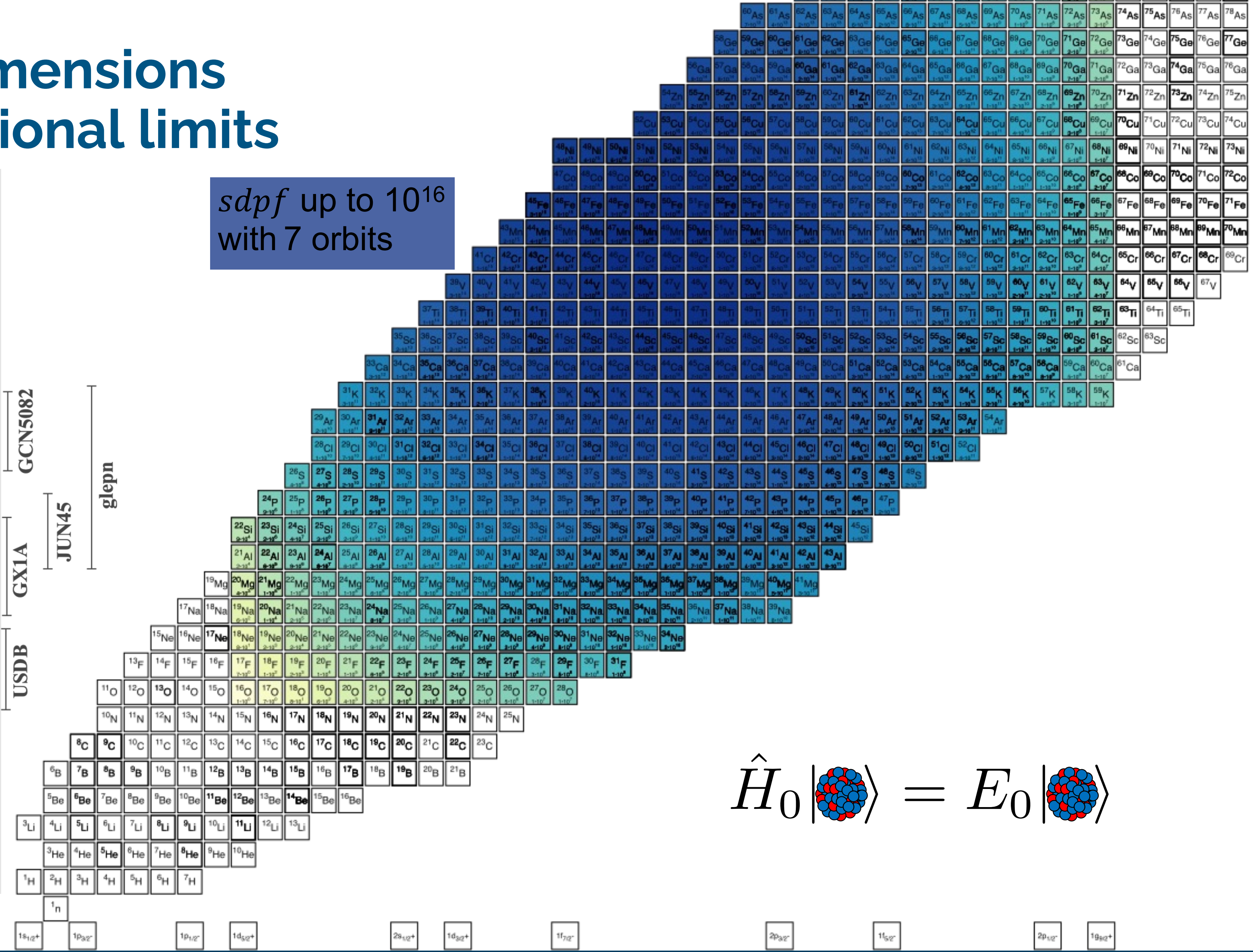
pf up to 10^9
with 4 orbits

sd up to 10^5
with 3 orbits

$$\hat{H}_0 | \rangle = E_0 | \rangle$$

Shell model dimensions push computational limits

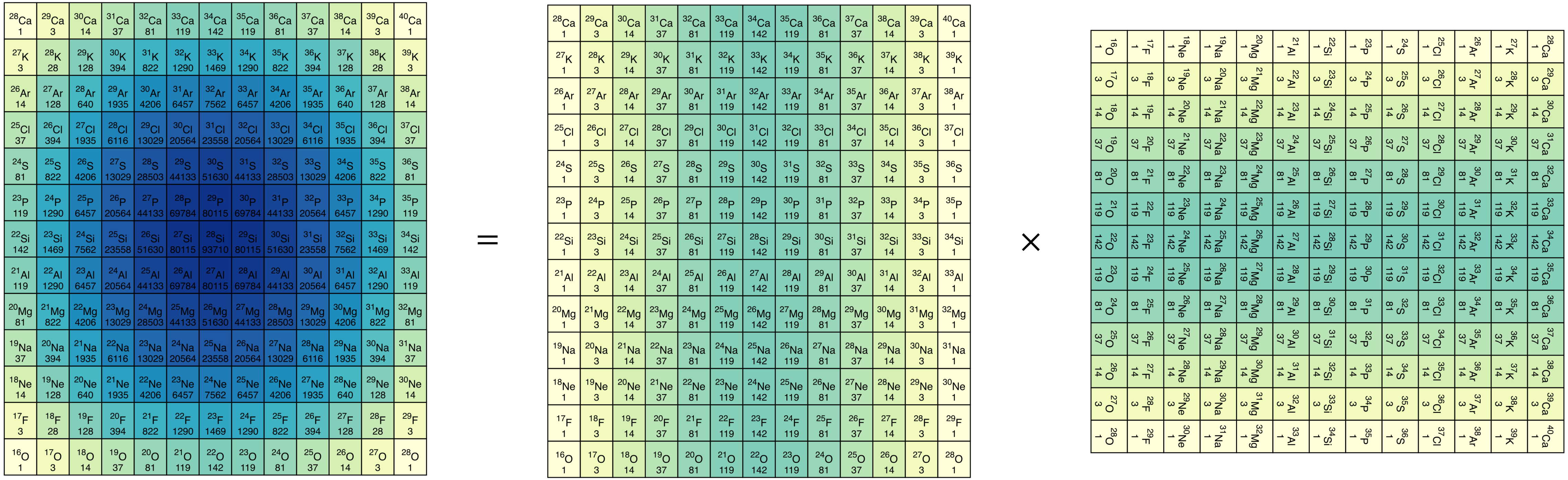




sdpf up to 10^{16} with 7 orbits

$$\hat{H}_0 | \rangle = E_0 | \rangle$$

Proton neutron factorization is a standard trick



^{28}Ca 1	^{29}Ca 3	^{30}Ca 14	^{31}Ca 37	^{32}Ca 81	^{33}Ca 119	^{34}Ca 142	^{35}Ca 119	^{36}Ca 81	^{37}Ca 37	^{38}Ca 14	^{39}Ca 3	^{40}Ca 1
^{27}K 3	^{28}K 28	^{29}K 128	^{30}K 394	^{31}K 822	^{32}K 1290	^{33}K 1469	^{34}K 1290	^{35}K 822	^{36}K 394	^{37}K 128	^{38}K 28	^{39}K 3
^{26}Ar 14	^{27}Ar 128	^{28}Ar 640	^{29}Ar 1935	^{30}Ar 4206	^{31}Ar 6457	^{32}Ar 7562	^{33}Ar 6457	^{34}Ar 4206	^{35}Ar 1935	^{36}Ar 640	^{37}Ar 128	^{38}Ar 14
^{25}Cl 37	^{26}Cl 394	^{27}Cl 1935	^{28}Cl 6116	^{29}Cl 13029	^{30}Cl 20564	^{31}Cl 23558	^{32}Cl 20564	^{33}Cl 13029	^{34}Cl 6116	^{35}Cl 1935	^{36}Cl 394	^{37}Cl 37
^{24}S 81	^{25}S 822	^{26}S 4206	^{27}S 13029	^{28}S 28503	^{29}S 44133	^{30}S 51630	^{31}S 44133	^{32}S 28503	^{33}S 13029	^{34}S 4206	^{35}S 822	^{36}S 81
^{23}P 119	^{24}P 1290	^{25}P 6457	^{26}P 20564	^{27}P 44133	^{28}P 69784	^{29}P 80115	^{30}P 69784	^{31}P 44133	^{32}P 20564	^{33}P 6457	^{34}P 1290	^{35}P 119
^{22}Si 142	^{23}Si 1469	^{24}Si 7562	^{25}Si 23558	^{26}Si 51630	^{27}Si 80115	^{28}Si 93710	^{29}Si 80115	^{30}Si 51630	^{31}Si 23558	^{32}Si 7562	^{33}Si 1469	^{34}Si 142
^{21}Al 119	^{22}Al 1290	^{23}Al 6457	^{24}Al 20564	^{25}Al 44133	^{26}Al 69784	^{27}Al 80115	^{28}Al 69784	^{29}Al 44133	^{30}Al 20564	^{31}Al 6457	^{32}Al 1290	^{33}Al 119
^{20}Mg 81	^{21}Mg 822	^{22}Mg 4206	^{23}Mg 13029	^{24}Mg 28503	^{25}Mg 44133	^{26}Mg 51630	^{27}Mg 44133	^{28}Mg 28503	^{29}Mg 13029	^{30}Mg 4206	^{31}Mg 822	^{32}Mg 81
^{19}Na 37	^{20}Na 394	^{21}Na 1935	^{22}Na 6116	^{23}Na 13029	^{24}Na 20564	^{25}Na 23558	^{26}Na 20564	^{27}Na 13029	^{28}Na 6116	^{29}Na 1935	^{30}Na 394	^{31}Na 37
^{18}Ne 14	^{19}Ne 128	^{20}Ne 640	^{21}Ne 1935	^{22}Ne 4206	^{23}Ne 6457	^{24}Ne 7562	^{25}Ne 6457	^{26}Ne 4206	^{27}Ne 1935	^{28}Ne 640	^{29}Ne 128	^{30}Ne 14
^{17}F 3	^{18}F 28	^{19}F 128	^{20}F 394	^{21}F 822	^{22}F 1290	^{23}F 1469	^{24}F 1290	^{25}F 822	^{26}F 394	^{27}F 128	^{28}F 28	^{29}F 3
^{16}O 1	^{17}O 3	^{18}O 14	^{19}O 37	^{20}O 81	^{21}O 119	^{22}O 142	^{23}O 119	^{24}O 81	^{25}O 37	^{26}O 14	^{27}O 3	^{28}O 1

=

^{28}Ca 1	^{29}Ca 3	^{30}Ca 14	^{31}Ca 37	^{32}Ca 81	^{33}Ca 119	^{34}Ca 142	^{35}Ca 119	^{36}Ca 81	^{37}Ca 37	^{38}Ca 14	^{39}Ca 3	^{40}Ca 1
^{27}K 1	^{28}K 3	^{29}K 14	^{30}K 37	^{31}K 81	^{32}K 119	^{33}K 142	^{34}K 119	^{35}K 81	^{36}K 37	^{37}K 14	^{38}K 3	^{39}K 1
^{26}Ar 1	^{27}Ar 3	^{28}Ar 14	^{29}Ar 37	^{30}Ar 81	^{31}Ar 119	^{32}Ar 142	^{33}Ar 119	^{34}Ar 81	^{35}Ar 37	^{36}Ar 14	^{37}Ar 3	^{38}Ar 1
^{25}Cl 1	^{26}Cl 3	^{27}Cl 14	^{28}Cl 37	^{29}Cl 81	^{30}Cl 119	^{31}Cl 142	^{32}Cl 119	^{33}Cl 81	^{34}Cl 37	^{35}Cl 14	^{36}Cl 3	^{37}Cl 1
^{24}S 1	^{25}S 3	^{26}S 14	^{27}S 37	^{28}S 81	^{29}S 119	^{30}S 142	^{31}S 119	^{32}S 81	^{33}S 37	^{34}S 14	^{35}S 3	^{36}S 1
^{23}P 1	^{24}P 3	^{25}P 14	^{26}P 37	^{27}P 81	^{28}P 119	^{29}P 142	^{30}P 119	^{31}P 81	^{32}P 37	^{33}P 14	^{34}P 3	^{35}P 1
^{22}Si 1	^{23}Si 3	^{24}Si 14	^{25}Si 37	^{26}Si 81	^{27}Si 119	^{28}Si 142	^{29}Si 119	^{30}Si 81	^{31}Si 37	^{32}Si 14	^{33}Si 3	^{34}Si 1
^{21}Al 1	^{22}Al 3	^{23}Al 14	^{24}Al 37	^{25}Al 81	^{26}Al 119	^{27}Al 142	^{28}Al 119	^{29}Al 81	^{30}Al 37	^{31}Al 14	^{32}Al 3	^{33}Al 1
^{20}Mg 1	^{21}Mg 3	^{22}Mg 14	^{23}Mg 37	^{24}Mg 81	^{25}Mg 119	^{26}Mg 142	^{27}Mg 119	^{28}Mg 81	^{29}Mg 37	^{30}Mg 14	^{31}Mg 3	^{32}Mg 1
^{19}Na 1	^{20}Na 3	^{21}Na 14	^{22}Na 37	^{23}Na 81	^{24}Na 119	^{25}Na 142	^{26}Na 119	^{27}Na 81	^{28}Na 37	^{29}Na 14	^{30}Na 3	^{31}Na 1
^{18}Ne 1	^{19}Ne 3	^{20}Ne 14	^{21}Ne 37	^{22}Ne 81	^{23}Ne 119	^{24}Ne 142	^{25}Ne 119	^{26}Ne 81	^{27}Ne 37	^{28}Ne 14	^{29}Ne 3	^{30}Ne 1
^{17}F 1	^{18}F 3	^{19}F 14	^{20}F 37	^{21}F 81	^{22}F 119	^{23}F 142	^{24}F 119	^{25}F 81	^{26}F 37	^{27}F 14	^{28}F 3	^{29}F 1
^{16}O 1	^{17}O 3	^{18}O 14	^{19}O 37	^{20}O 81	^{21}O 119	^{22}O 142	^{23}O 119	^{24}O 81	^{25}O 37	^{26}O 14	^{27}O 3	^{28}O 1

×

^{16}O 1	^{17}F 1	^{18}Ne 1	^{19}Na 1	^{20}Mg 1	^{21}Al 1	^{22}Si 1	^{23}P 1	^{24}S 1	^{25}Cl 1	^{26}Ar 1	^{27}K 1	^{28}Ca 1
^{17}O 3	^{18}F 3	^{19}Ne 3	^{20}Na 3	^{21}Mg 3	^{22}Al 3	^{23}Si 3	^{24}P 3	^{25}S 3	^{26}Cl 3	^{27}Ar 3	^{28}K 3	^{29}Ca 3
^{18}O 14	^{19}F 14	^{20}Ne 14	^{21}Na 14	^{22}Mg 14	^{23}Al 14	^{24}Si 14	^{25}P 14	^{26}S 14	^{27}Cl 14	^{28}Ar 14	^{29}K 14	^{30}Ca 14
^{19}O 37	^{20}F 37	^{21}Ne 37	^{22}Na 37	^{23}Mg 37	^{24}Al 37	^{25}Si 37	^{26}P 37	^{27}S 37	^{28}Cl 37	^{29}Ar 37	^{30}K 37	^{31}Ca 37
^{20}O 81	^{21}F 81	^{22}Ne 81	^{23}Na 81	^{24}Mg 81	^{25}Al 81	^{26}Si 81	^{27}P 81	^{28}S 81	^{29}Cl 81	^{30}Ar 81	^{31}K 81	^{32}Ca 81
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^{22}O 142	^{23}F 142	^{24}Ne 142	^{25}Na 142	^{26}Mg 142	^{27}Al 142	^{28}Si 142	^{29}P 142	^{30}S 142	^{31}Cl 142	^{32}Ar 142	^{33}K 142	^{34}Ca 142
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^{24}O 81	^{25}F 81	^{26}Ne 81	^{27}Na 81	^{28}Mg 81	^{29}Al 81	^{30}Si 81	^{31}P 81	^{32}S 81	^{33}Cl 81	^{34}Ar 81	^{35}K 81	^{36}Ca 81
^{25}O 37	^{26}F 37	^{27}Ne 37	^{28}Na 37	^{29}Mg 37	^{30}Al 37	^{31}Si 37	^{32}P 37	^{33}S 37	^{34}Cl 37	^{35}Ar 37	^{36}K 37	^{37}Ca 37
^{26}O 14	^{27}F 14	^{28}Ne 14	^{29}Na 14	^{30}Mg 14	^{31}Al 14	^{32}Si 14	^{33}P 14	^{34}S 14	^{35}Cl 14	^{36}Ar 14	^{37}K 14	^{38}Ca 14
^{27}O 3	^{28}F 3	^{29}Ne 3	^{30}Na 3	^{31}Mg 3	^{32}Al 3	^{33}Si 3	^{34}P 3	^{35}S 3	^{36}Cl 3	^{37}Ar 3	^{38}K 3	^{39}Ca 3
^{28}O 1	^{29}F 1	^{30}Ne 1	^{31}Na 1	^{32}Mg 1	^{33}Al 1	^{34}Si 1	^{35}P 1	^{36}S 1	^{37}Cl 1	^{38}Ar 1	^{39}K 1	^{40}Ca 1

$$|\Psi\rangle = \sum_{pn} \psi_{pn} |p\rangle \otimes |n\rangle \longleftrightarrow H = P + N + H_{pn}$$

Factorization improves efficiency of on-the-fly matrix element calculation

See BIGSTICK (https://github.com/cwjsdsu/BigstickPublick)

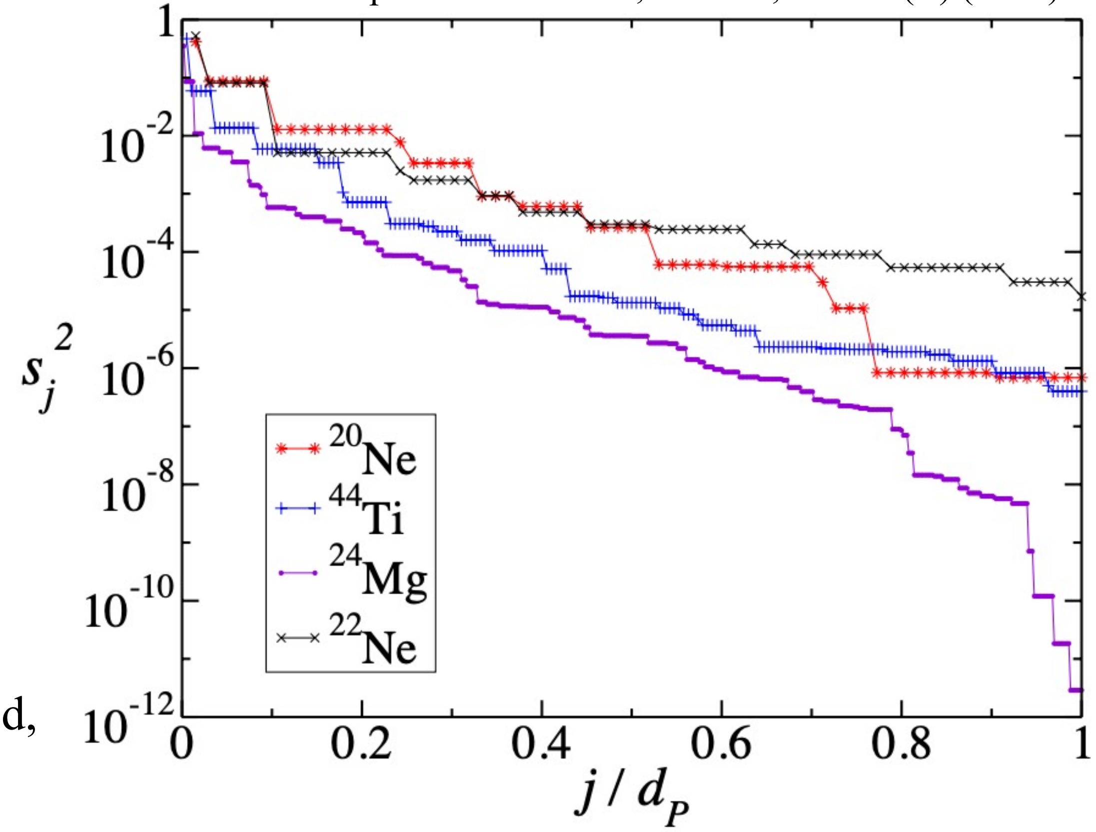
PN factorization also enables singular value methods

$$|\Psi\rangle = \sum_{pn} \psi_{pn} |p\rangle \otimes |n\rangle$$

$$\boldsymbol{\psi} = \boldsymbol{U}\,\boldsymbol{S}\,\boldsymbol{V}^{\boldsymbol{T}}$$

There are "optimal" factors, $|p\rangle$ and $|n\rangle$, where wave function is diagonal

From Papenbrock & Dean, PRC 67, 051303(R) (2003)



Exponential decay of components ⇒ truncation can be performed, ***if optimal basis factors can be found***:

- DMRG (S. White)
- Variational wave function factorization (T. Papenbrock)

Both iterative approaches starting from random ansatz

Desired approach: approximate SVD to avoid iteration

Goal: find the optimal basis factors $|p\rangle$ and $|n\rangle$.

$$|\Psi\rangle = \sum_{pn} \psi_{pn} |p\rangle \otimes |n\rangle$$

There is an "optimal" basis
where wave function is diagonal

Can we guess a "good-enough" set of $|p\rangle$ and $|n\rangle$, *a priori,* where ψ has components that decay exponentially?

Hint: SVD equivalent to diagonalization of both P, N reduced density matrices:

- Proton factors: $\rho^p = US^2U^T$
- Neutron factors: $\rho^n = VS^2V^T$

$$\rho^p = \mathrm{Tr}_n |\Psi\rangle\langle\Psi|$$

Quantum information: entanglement

Two spin ½ particles:

Two systems are **entangled** if joint wave function cannot be written as a **product**

$$|\uparrow_a\rangle|\downarrow_b\rangle$$

Effective dimension additive

$$\frac{1}{\sqrt{2}}\left(|\uparrow_a\rangle|\downarrow_b\rangle + |\downarrow_a\rangle|\uparrow_b\rangle\right)$$

Effective dimension multiplicative

Entanglement “entropy”:
$S_{entangle} = -\mathrm{Tr}(\rho^p \, ln\rho^p)$

$$|\Psi\rangle = \sum_{pn} \psi_{pn}|p\rangle \otimes |n\rangle$$

P, N reduced density matrices

- Proton factors: $\rho^p = US^2U^T$
- Neutron factors: $\rho^n = VS^2V^T$

$$\rho^p = \mathrm{Tr}_n|\Psi\rangle\langle\Psi|$$

Proton-neutron entanglement in the nuclear shell model

C. Johnson and O. Gorton, J. Phys. G 50, 045110 (2023)

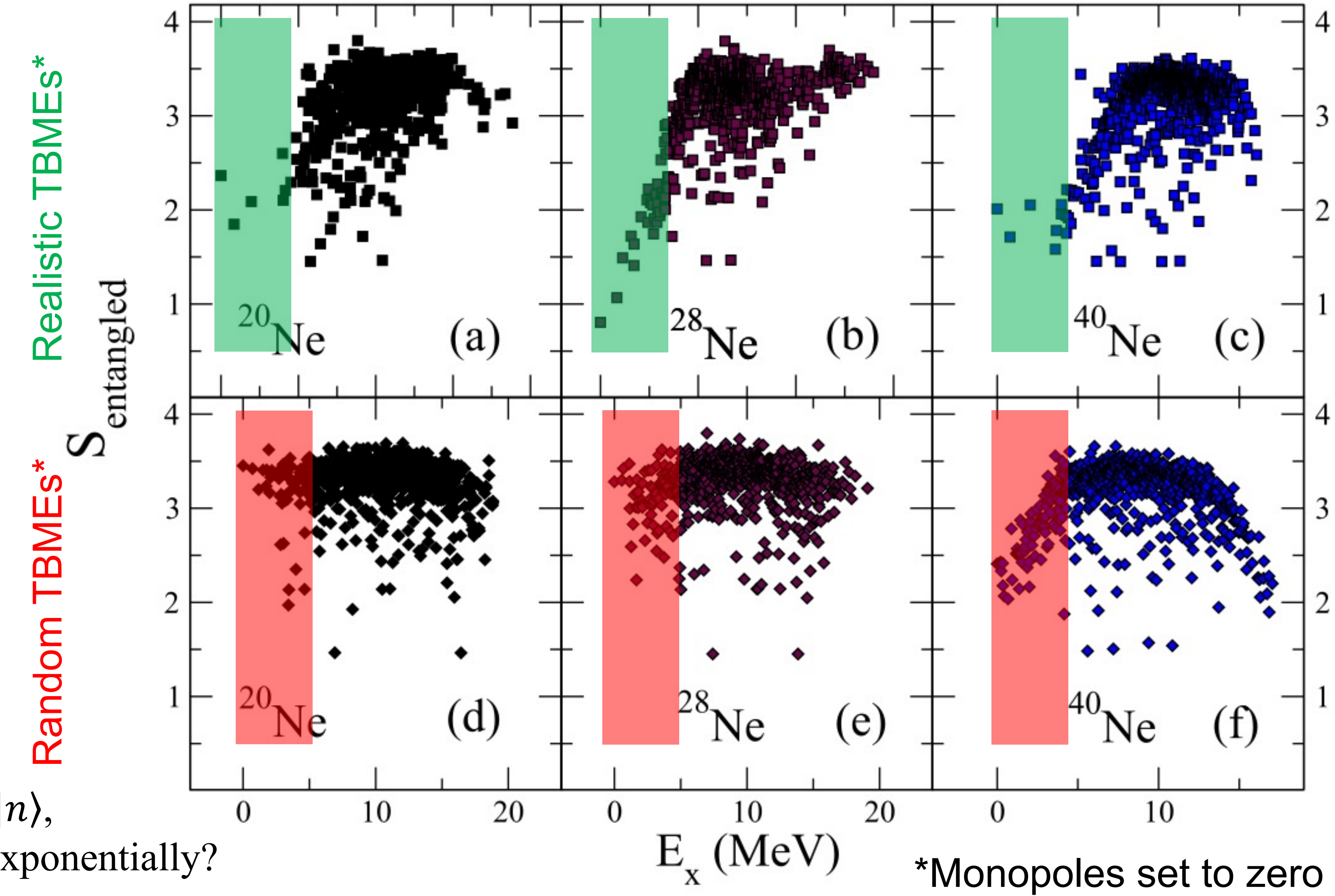
Compute entanglement “entropy”:
$S_{entangle} = -\mathrm{Tr}(\rho^p ln \rho^p)$

Lesson: low-lying shell model wave functions have low PN entanglement

$\Rightarrow$

A small number of SVD eigenvalues dominate (already known)

In $S = 0$ limit, $H_{pn} \rightarrow 0$.



*Monopoles set to zero

Can we guess a “good-enough” set of $|p\rangle$ and $|n\rangle$, *a priori,* where ψ has components that decay exponentially?

Other reasons this might be a good idea

Protons and neutrons have weak entanglement, and *lower when N>Z*.

Among orbital equipartitions, the proton-neutron bipartition has *weakest* entanglement.

Gorton MS thesis, San Diego State University, 2018.

Johnson and **Gorton:** J. Phys. G 50 (4) 045110 (2023)

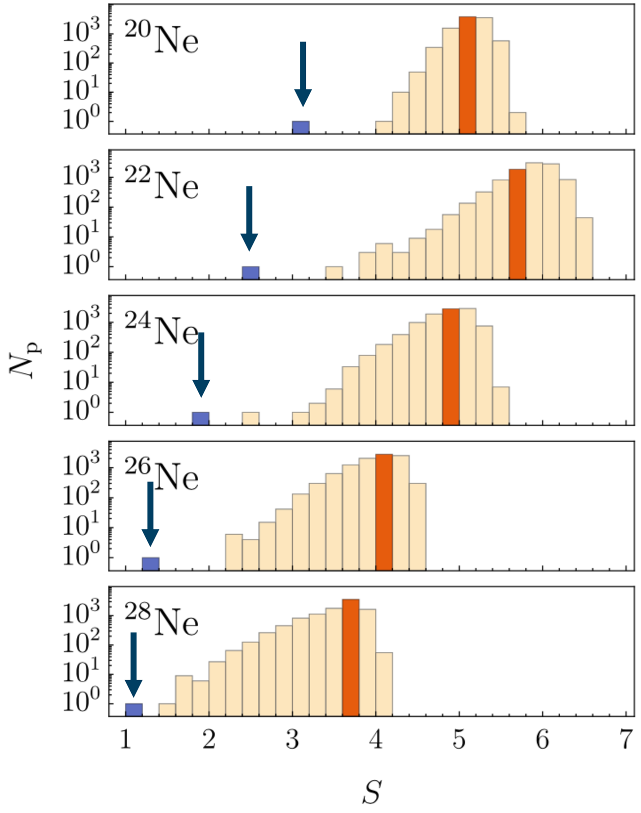
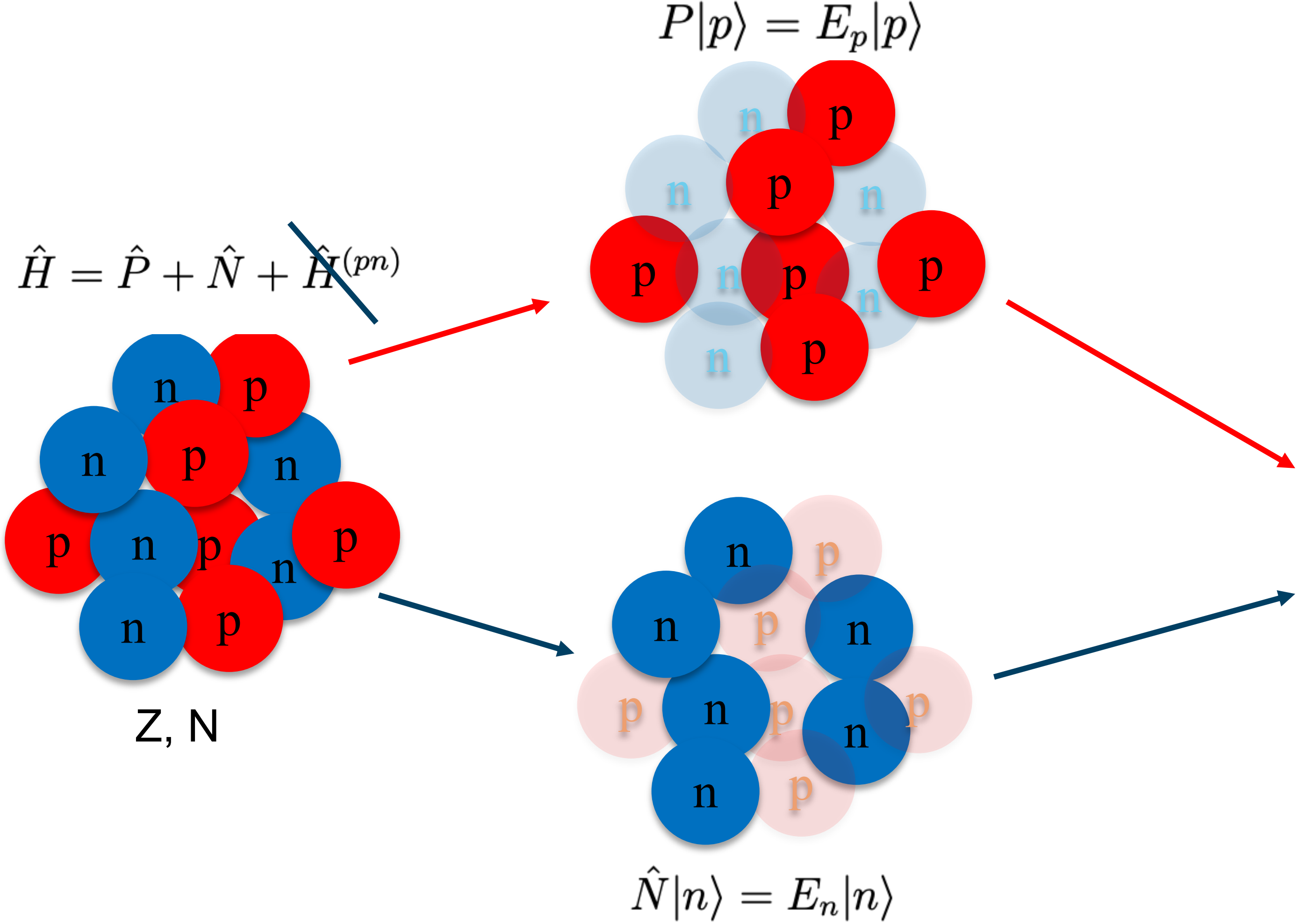


Fig. 8 Same as in Fig. 6, for $^{20-28}$Ne. Here 1% samples of all equipartitions have been calculated

Pérez-Obiol et al., Eur. Phys. J. A **59**, 240 (2023).

Let's take this "weak coupling" to its limit: $H^{pn} \rightarrow 0$



$$\hat{P}|p\rangle = E_p|p\rangle$$

$$\hat{H} = \hat{P} + \hat{N} + \cancel{\hat{H}^{(pn)}}$$

Z, N

$$\hat{N}|n\rangle = E_n|n\rangle$$

Instead of slater determinants, these are complex many-body wave functions

$$|\phi_{pn}\rangle \equiv |p\rangle|n\rangle$$

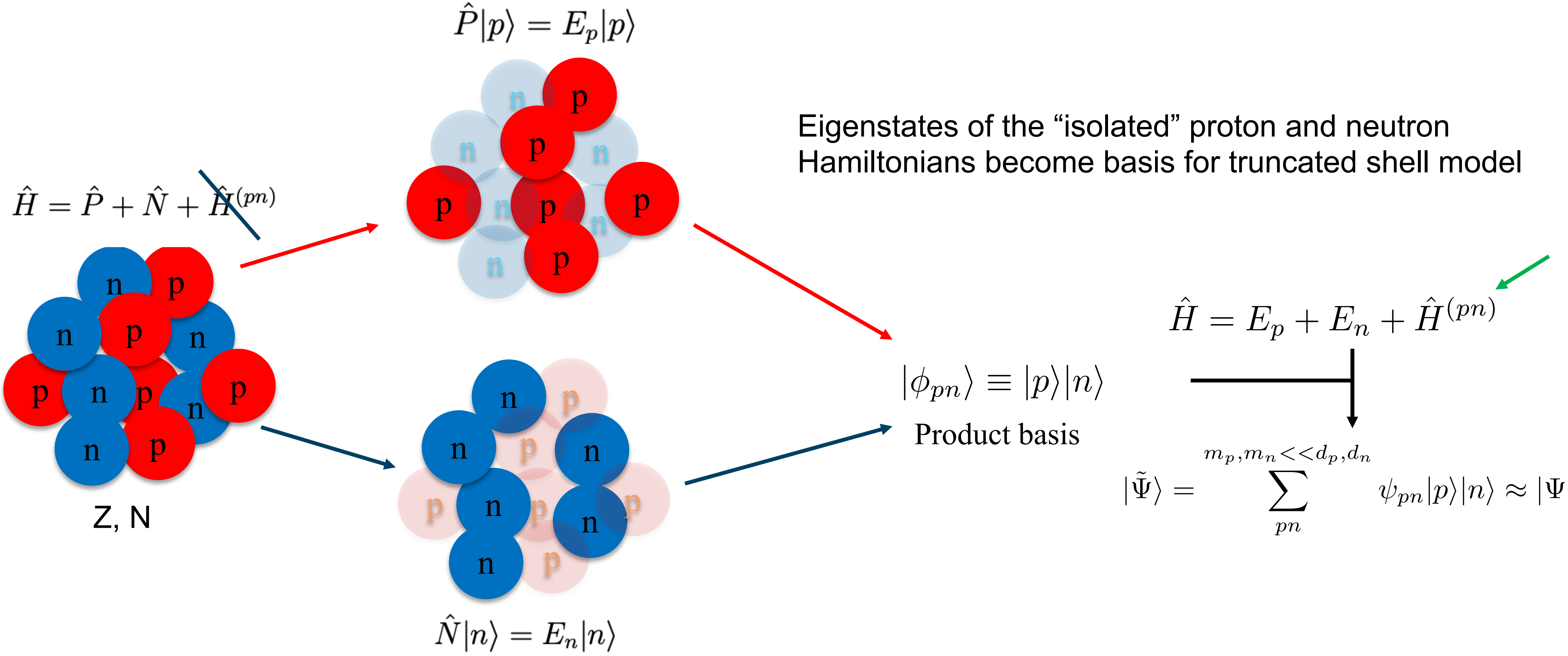
Product basis

In the weak entanglement limit, this is the "optimal" basis (SVD sense)

In the weak entanglement limit, SVD basis factors reduce to eigenstates of $\hat{P}$ and $\hat{N}$

Nuclear & Chemical Sciences

Proton and Neutron Approximate Shell model (PANASh)



$$\hat{H} = \hat{P} + \hat{N} + \cancel{\hat{H}^{(pn)}}$$

Z, N

$$\hat{P}|p\rangle = E_p|p\rangle$$

$$\hat{N}|n\rangle = E_n|n\rangle$$

Eigenstates of the “isolated” proton and neutron Hamiltonians become basis for truncated shell model

$$|\phi_{pn}\rangle \equiv |p\rangle|n\rangle$$

Product basis

$$\hat{H} = E_p + E_n + \hat{H}^{(pn)}$$

$$|\tilde{\Psi}\rangle = \sum_{pn}^{m_p,m_n<<d_p,d_n} \psi_{pn}|p\rangle|n\rangle \approx |\Psi\rangle$$

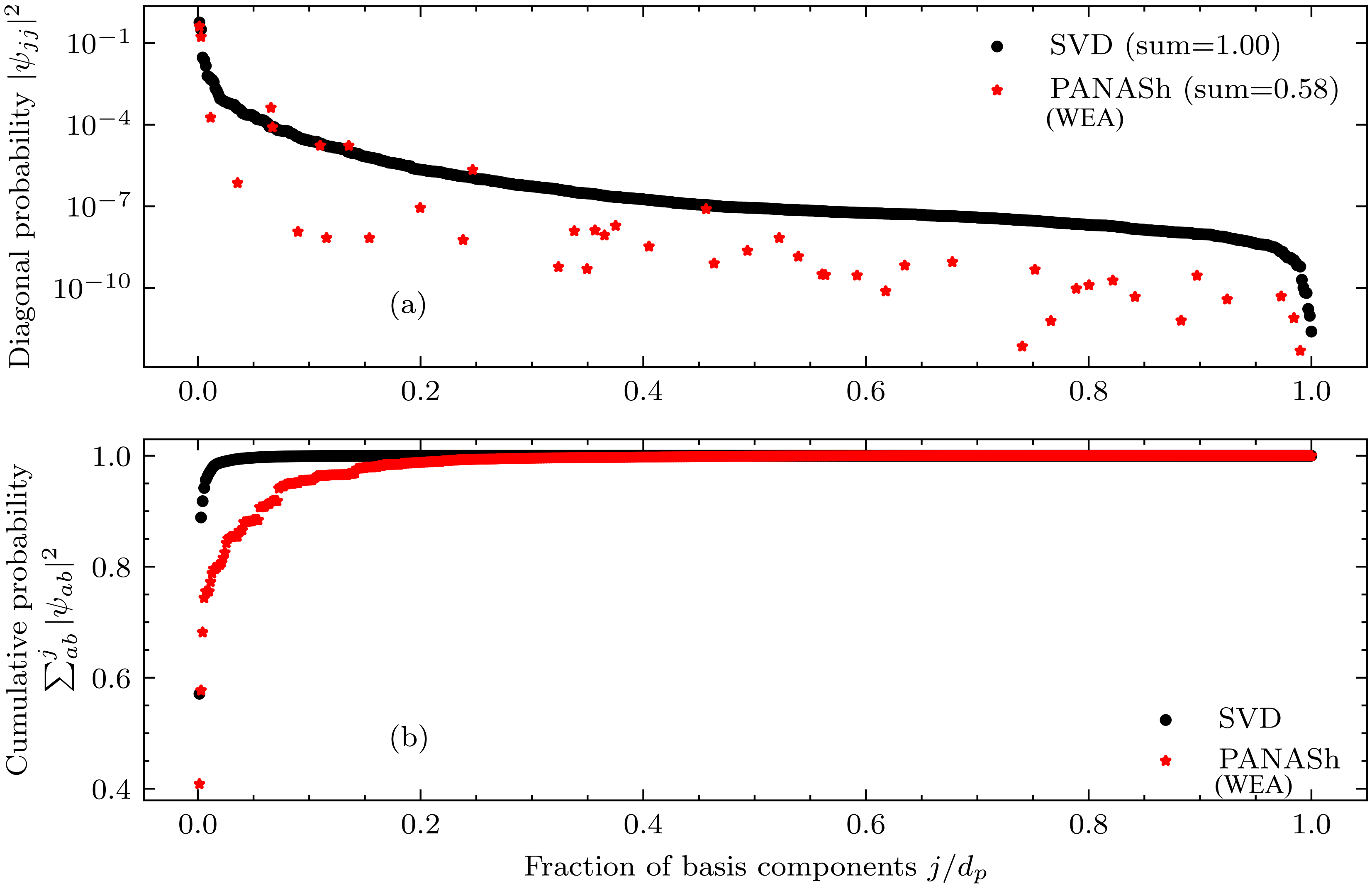
How does our PN WEA compare to SVD?

$$|\Psi\rangle = \sum_j \psi_j |p_{SVD}\rangle \otimes |n_{SVD}\rangle$$

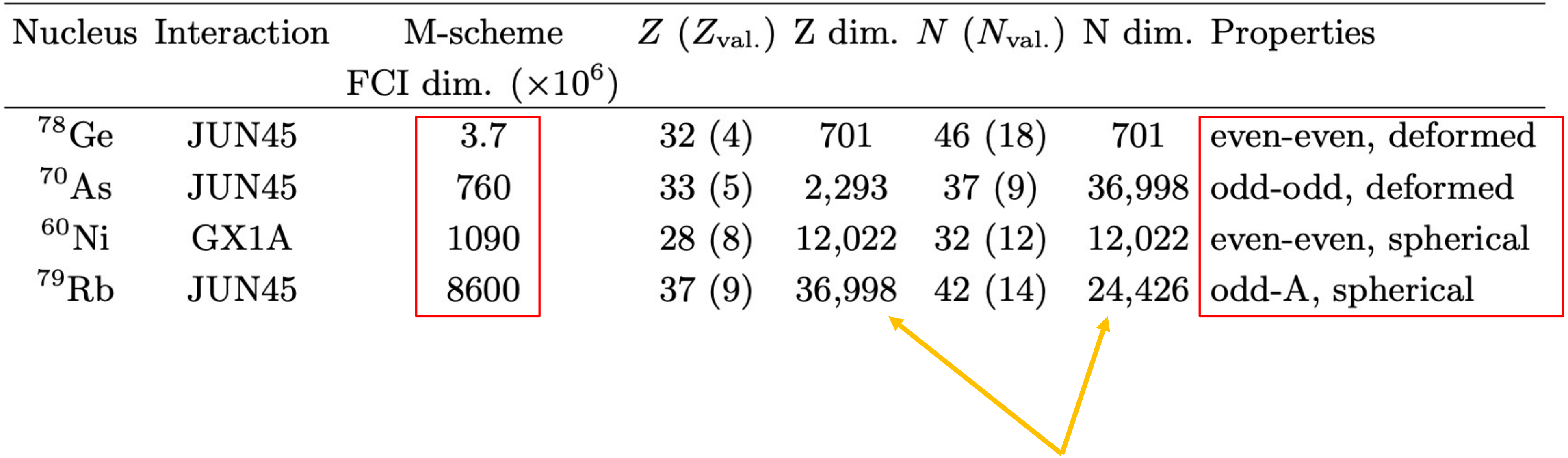
SVD (optimal, diagonal)

$$= \sum_{pn} \tilde{\psi}_{pn} |p_{WEA}\rangle \otimes |n_{WEA}\rangle$$

PANASh/WEA



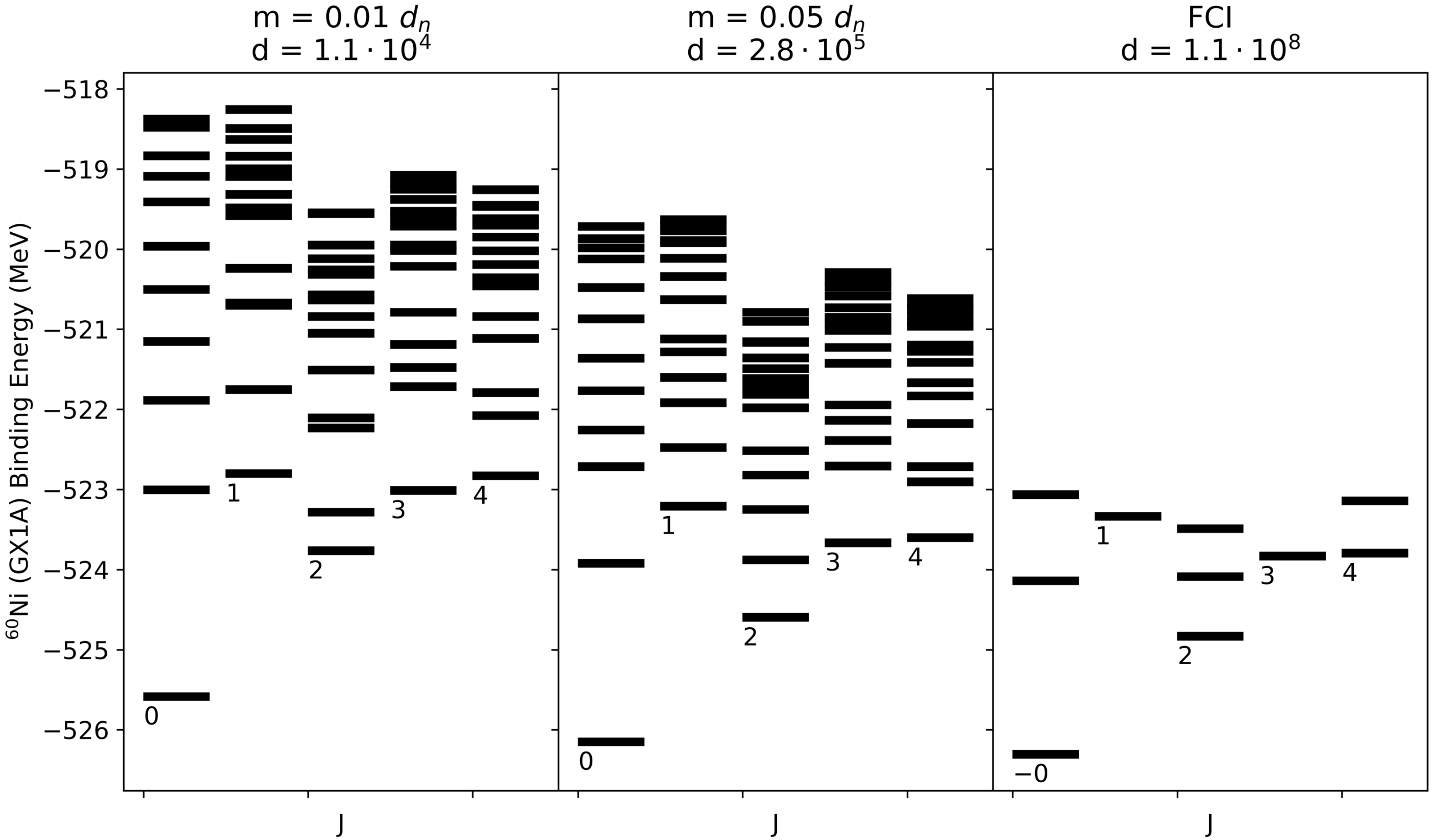
Benchmark cases



Nucleus	Interaction	M-scheme FCI dim. ($\times 10^6$)	Z ($Z_{\text{val.}}$)	Z dim.	N ($N_{\text{val.}}$)	N dim.	Properties
^{78}Ge	JUN45	3.7	32 (4)	701	46 (18)	701	even-even, deformed
^{70}As	JUN45	760	33 (5)	2,293	37 (9)	36,998	odd-odd, deformed
^{60}Ni	GX1A	1090	28 (8)	12,022	32 (12)	12,022	even-even, spherical
^{79}Rb	JUN45	8600	37 (9)	36,998	42 (14)	24,426	odd-A, spherical

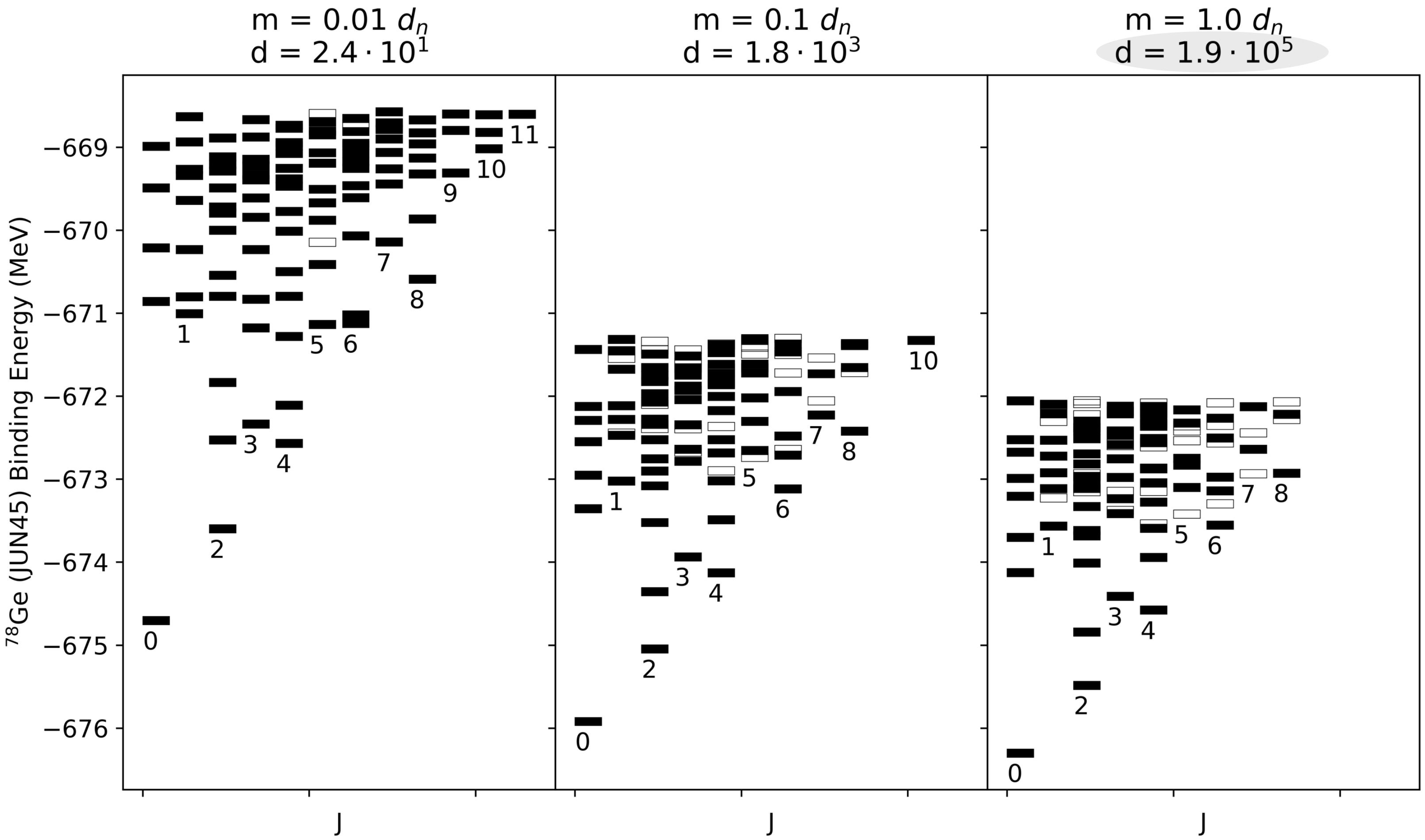
Prerequisite for p/n basis factors

Even-even, spherical: ^{56}Ni in the lower *pf* shell with GX1A



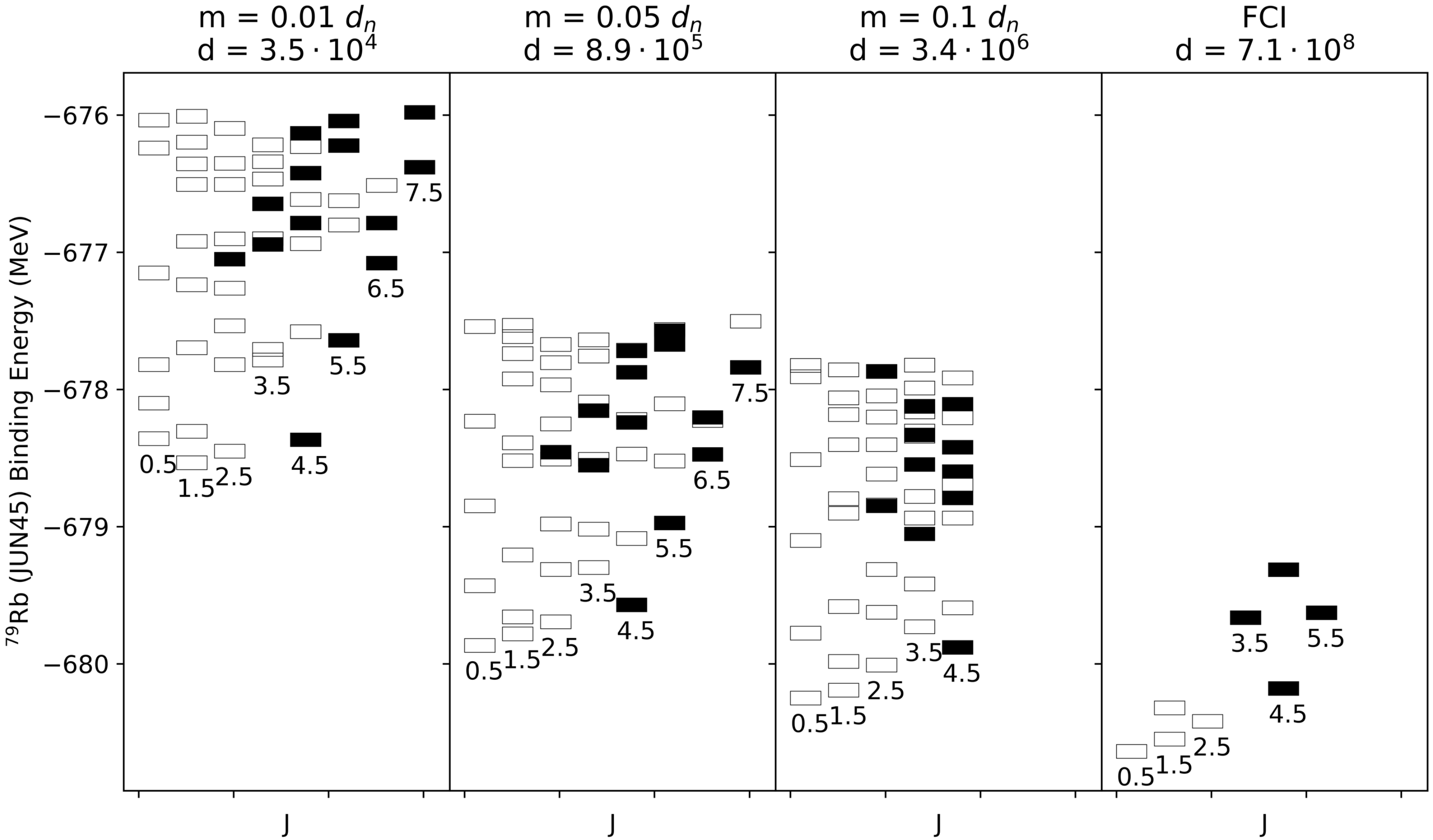
Excellent agreement with 3-4 orders of magnitude reduction

Even-even, deformed: ^{78}Ge in the upper *pf* shell with JUN45

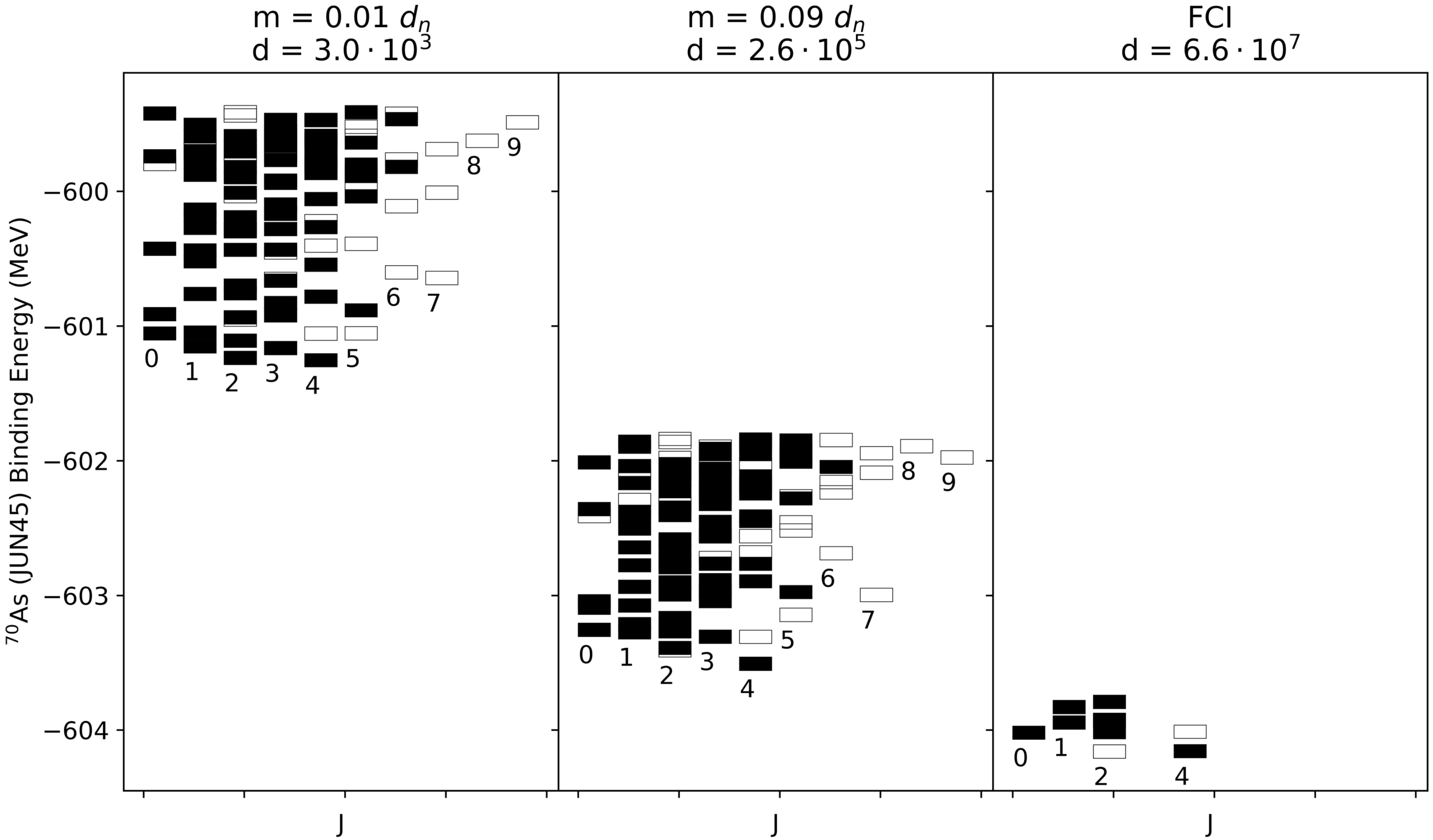


Convergence is slower for deformed system

Odd-A, spherical: ^{79}Rb in the upper *pf* shell with JUN45

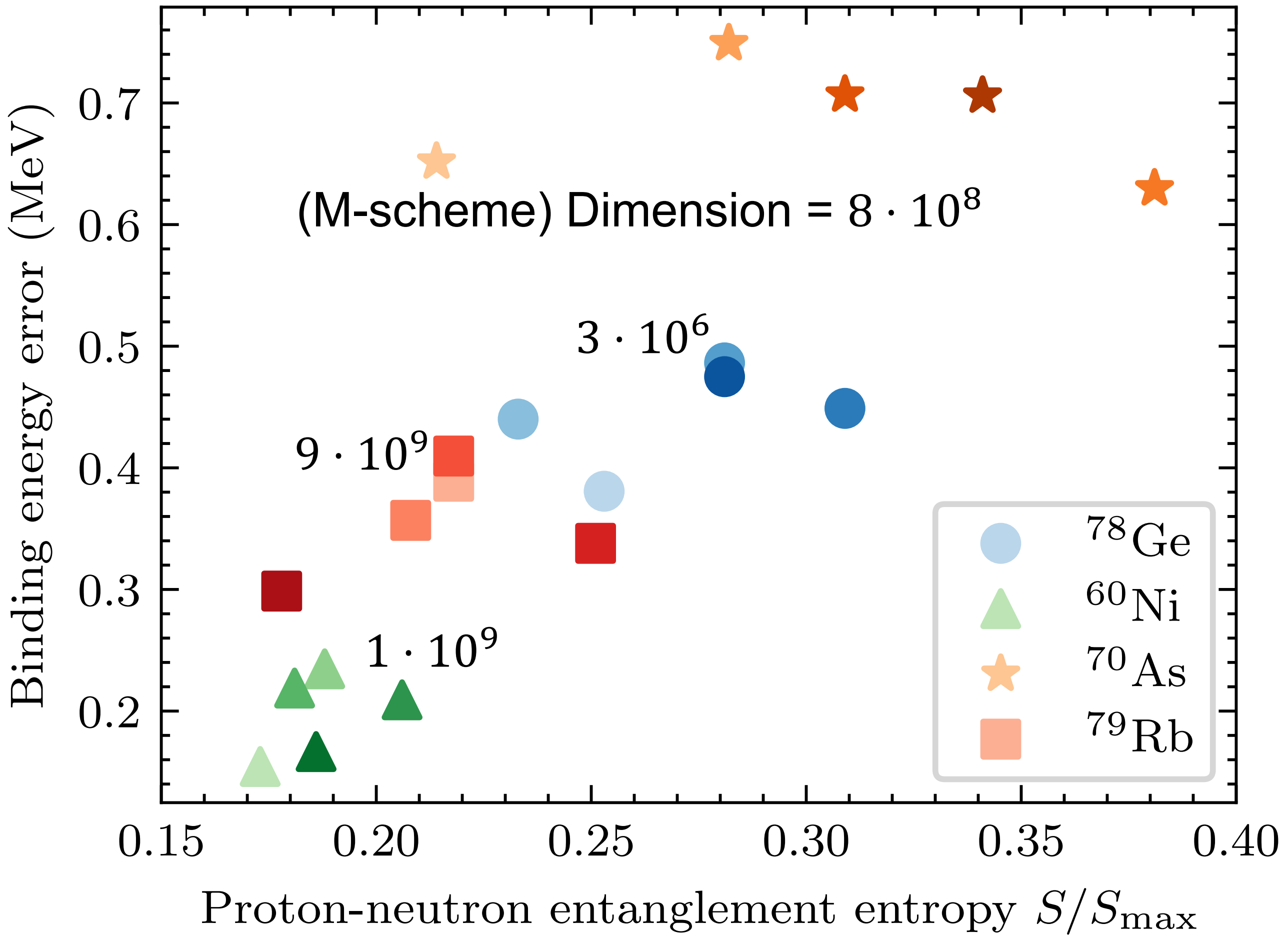


Odd-odd, deformed: ^{70}As in the upper *pf* shell with JUN45

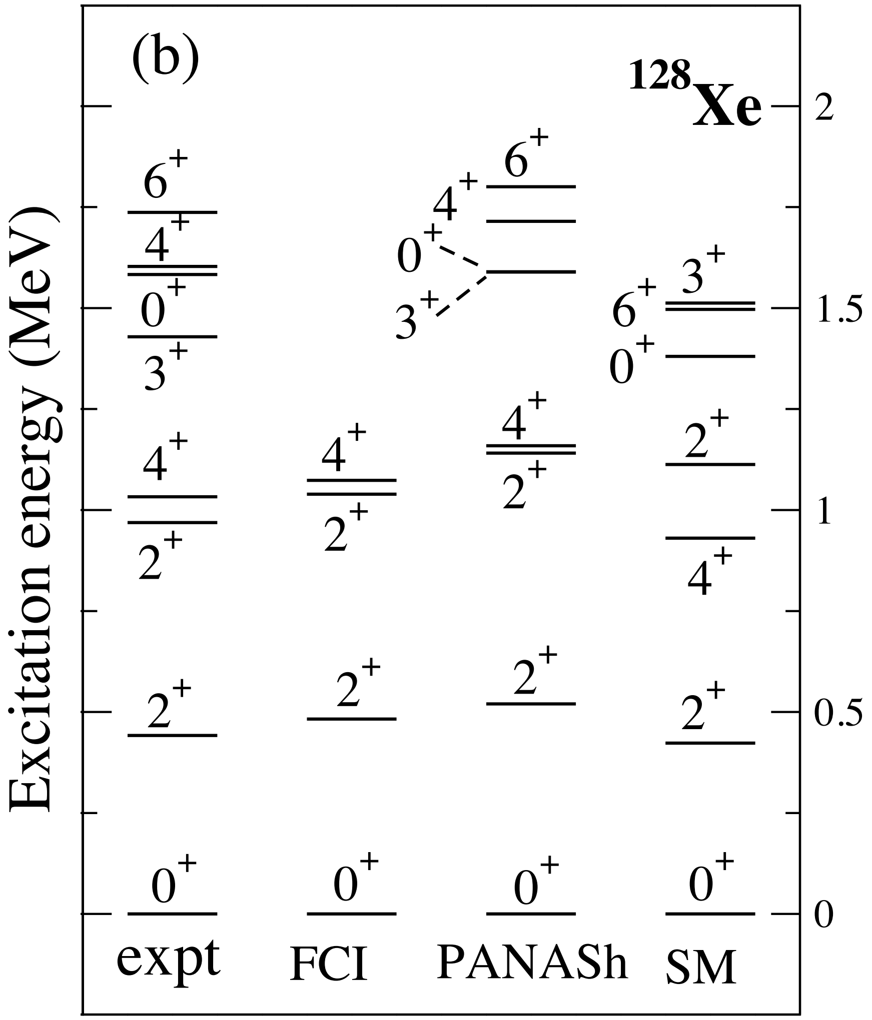


Dimension 200 times smaller (compute cost: $\mathrm{dimension}^3$)

Rate of convergence correlated with proton-neutron entanglement



Beyond current limits in 50-82 shell

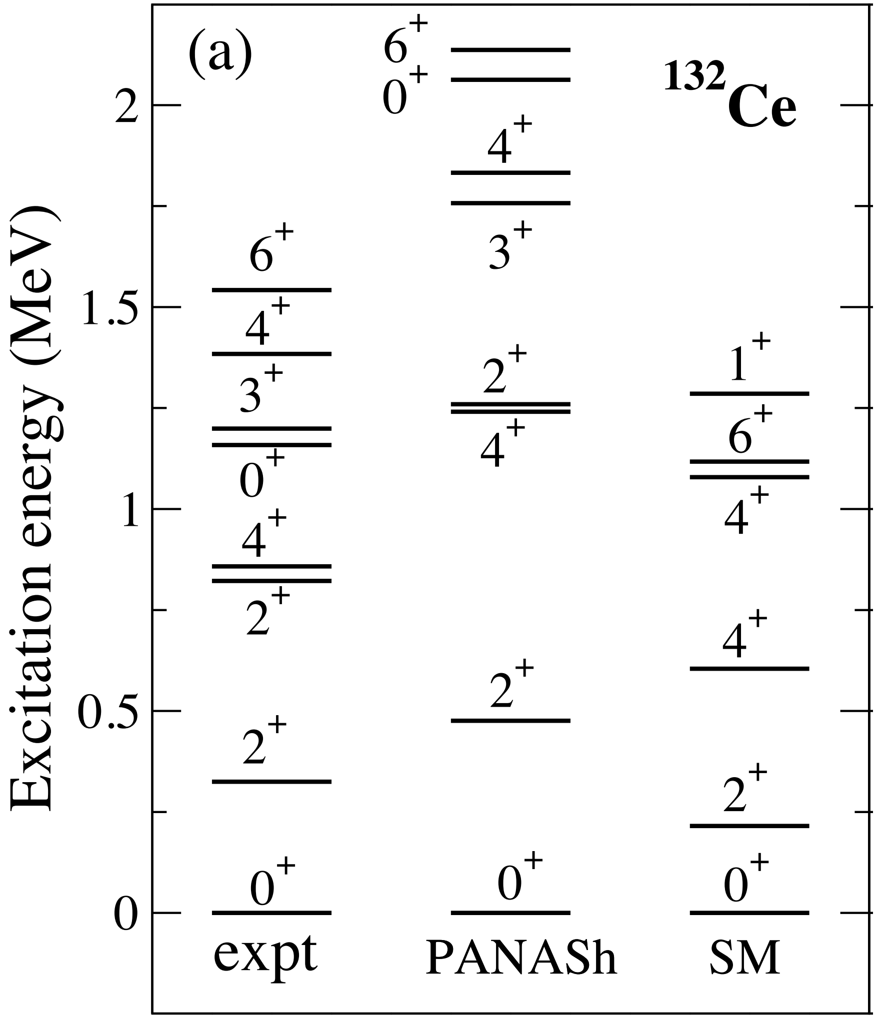


GCN5082 interaction
Model dimensions used

Method	^{128}Xe	^{132}Ce
FCI	$9 \cdot 10^9$	$2 \cdot 10^{12}$
SM	$5 \cdot 10^8$	$1 \cdot 10^9$
PANASh (WEA)	$4 \cdot 10^5$	$4 \cdot 10^5$

SM = truncated shell model restricting configurations approx. by orbital centroid energy

Beyond current limits in 50-82 shell



GCN5082 interaction
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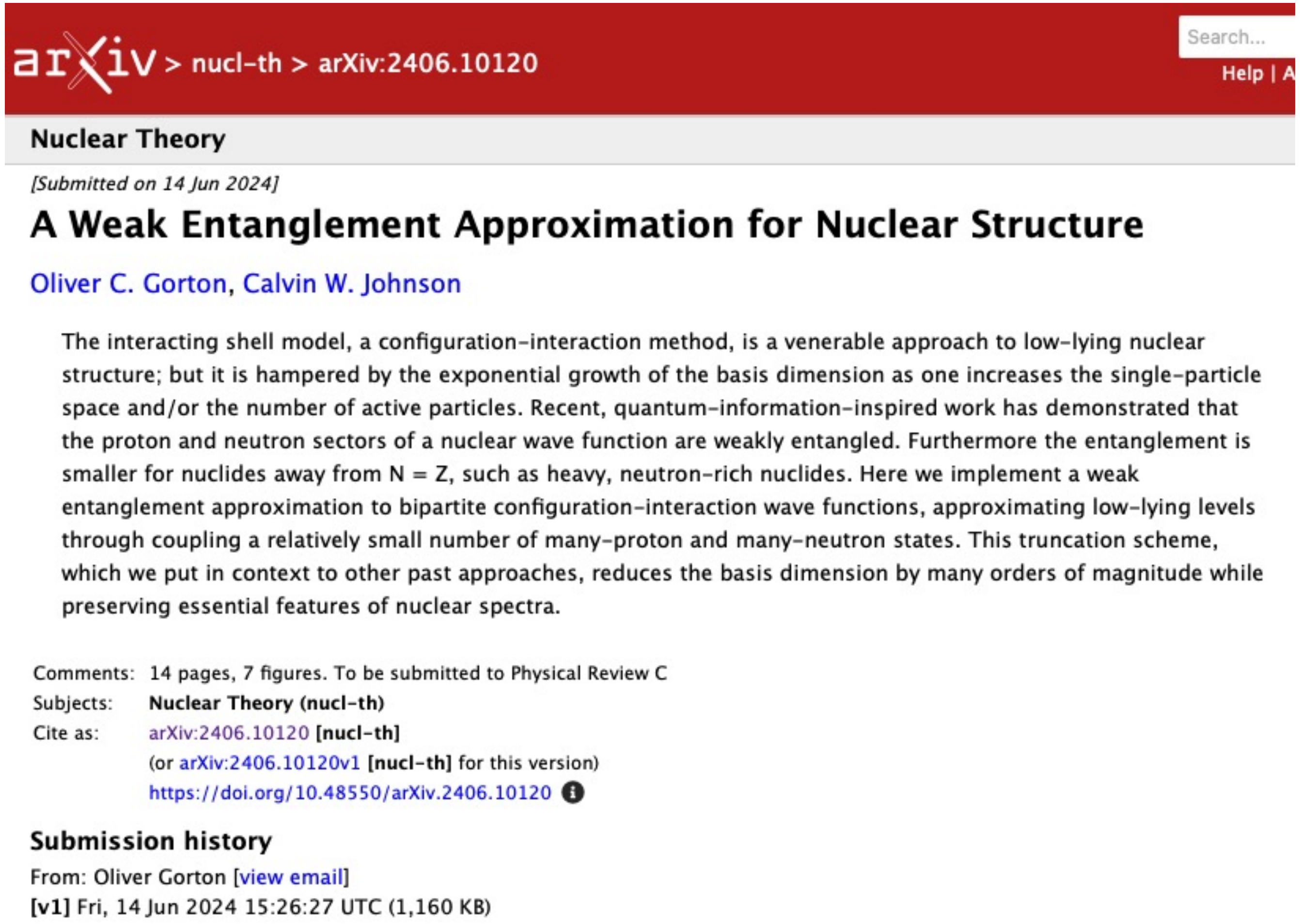
Get the details

arXiv 2406.10120



Nuclear Theory

[Submitted on 14 Jun 2024]

A Weak Entanglement Approximation for Nuclear Structure

Oliver C. Gorton, Calvin W. Johnson

The interacting shell model, a configuration-interaction method, is a venerable approach to low-lying nuclear structure; but it is hampered by the exponential growth of the basis dimension as one increases the single-particle space and/or the number of active particles. Recent, quantum-information-inspired work has demonstrated that the proton and neutron sectors of a nuclear wave function are weakly entangled. Furthermore the entanglement is smaller for nuclides away from N = Z, such as heavy, neutron-rich nuclides. Here we implement a weak entanglement approximation to bipartite configuration-interaction wave functions, approximating low-lying levels through coupling a relatively small number of many-proton and many-neutron states. This truncation scheme, which we put in context to other past approaches, reduces the basis dimension by many orders of magnitude while preserving essential features of nuclear spectra.

Comments:	14 pages, 7 figures. To be submitted to Physical Review C
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