SAN DIEGO STATE UNIVERSITY

A weak entanglement approximation for nuclear structure

Calvin W. Johnson

Oliver Gorton & Hayden Frye

CWJ & OG, Phys. Rev. C **110**, 034305 (2024)

“This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics, under Award Number DE-FG02-96ER40985,
and by the Office of High Energy Physics, under Award No.~DE-SC0019465, and
by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, with support from the ACT-UP award”

Ischia, May 22, 2025

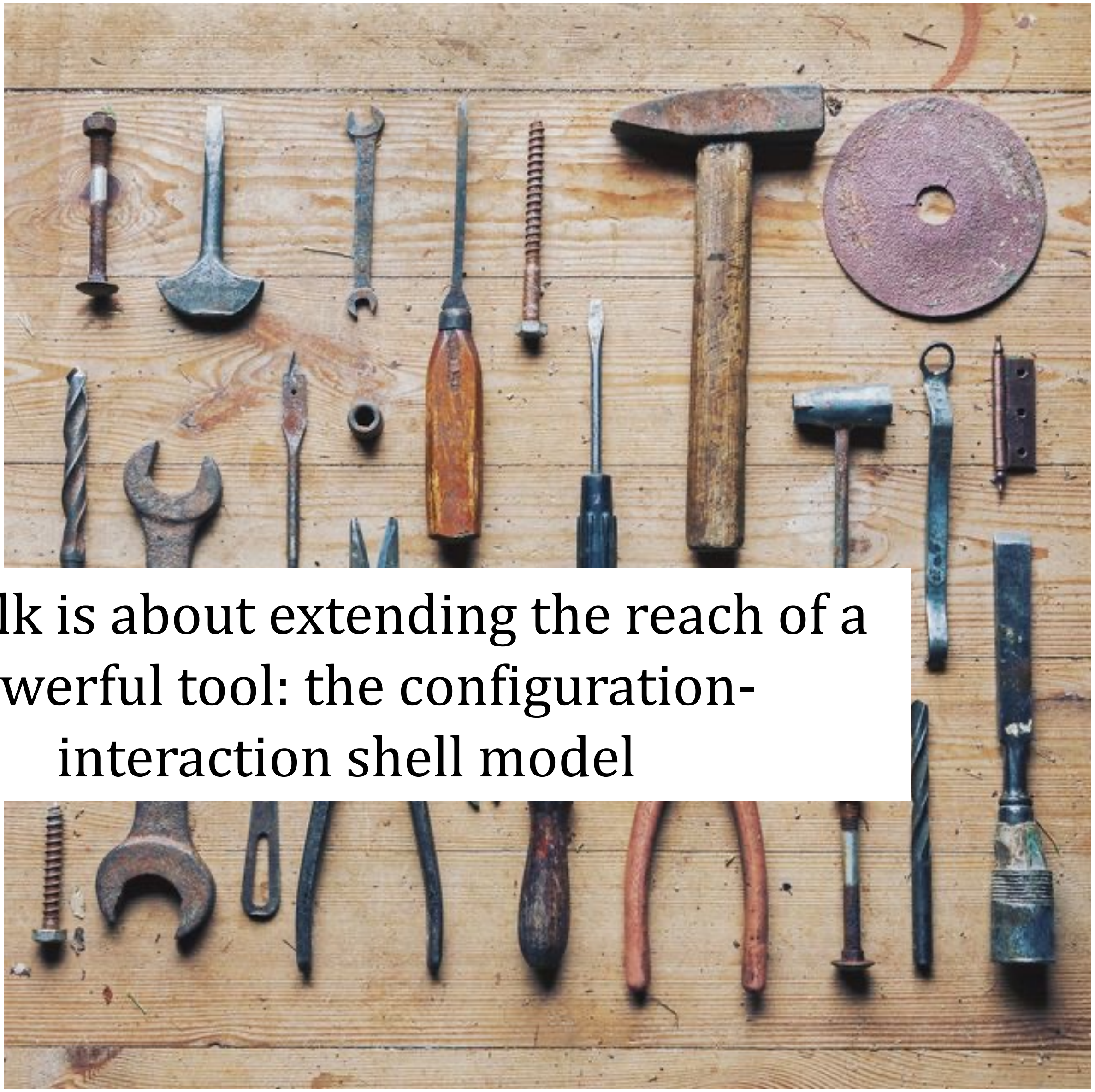
San Diego State University

Topic of the school:

"Cutting-edge developments in nuclear physics"

Ischia, May 22, 2025

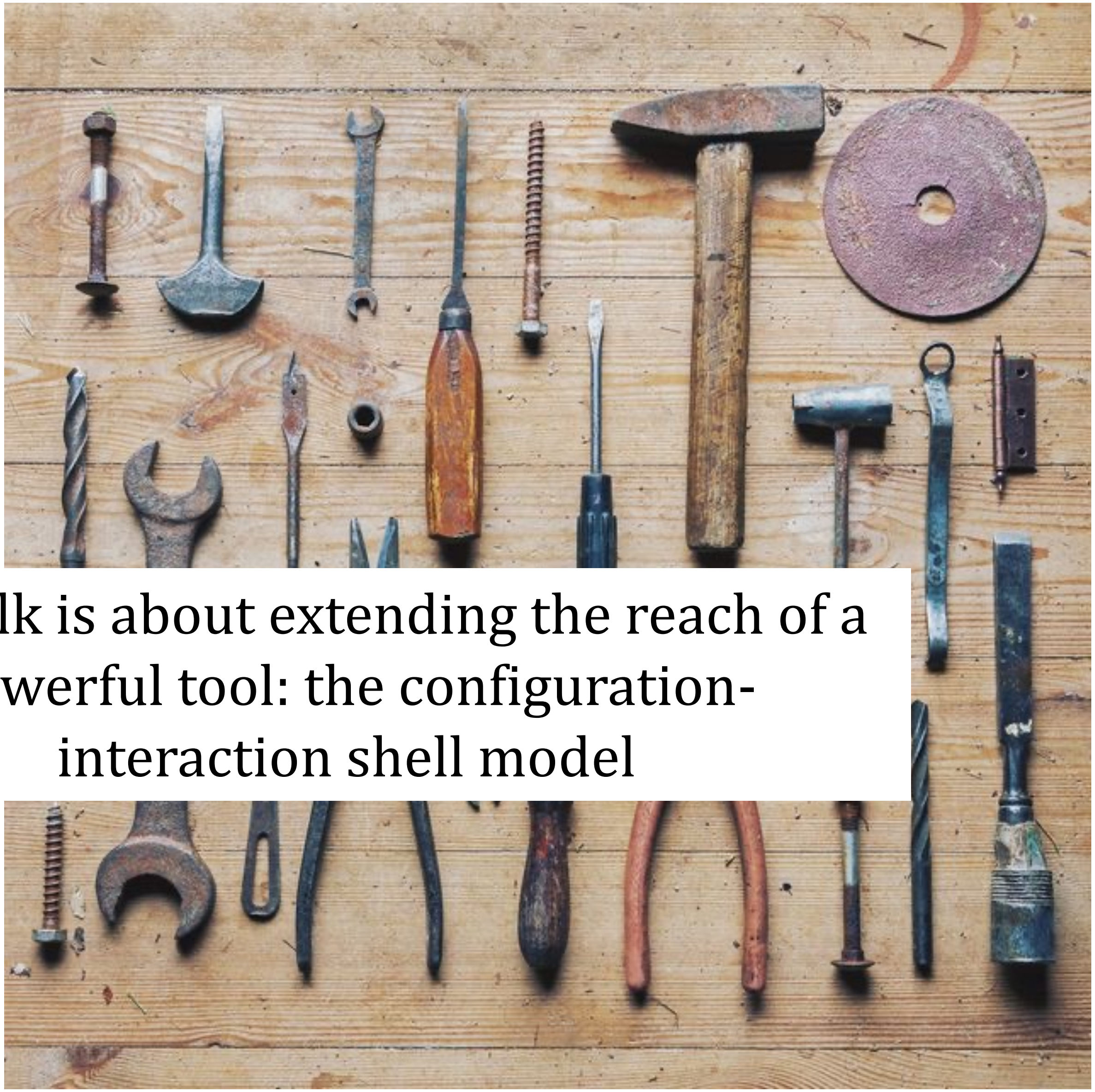
The theme of this Talk…



This talk is about extending the reach of a powerful tool: the configuration-interaction shell model

San Diego State University

The theme of this Talk…



This talk is about extending the reach of a powerful tool: the configuration-interaction shell model

See also talks by Miyagi, Otsuka, Dao, Nowacki, etc.

THE THEME OF THIS TALK…

The configuration-interaction shell model is a powerful tool:

- Transparent formalism
- Flexible with respect to interactions
- Excited states with similar cost to ground state
- **Explicit wave function makes analysis (e.g. group decomposition) straightforward**

SAN DIEGO STATE UNIVERSITY

THE THEME OF THIS TALK…

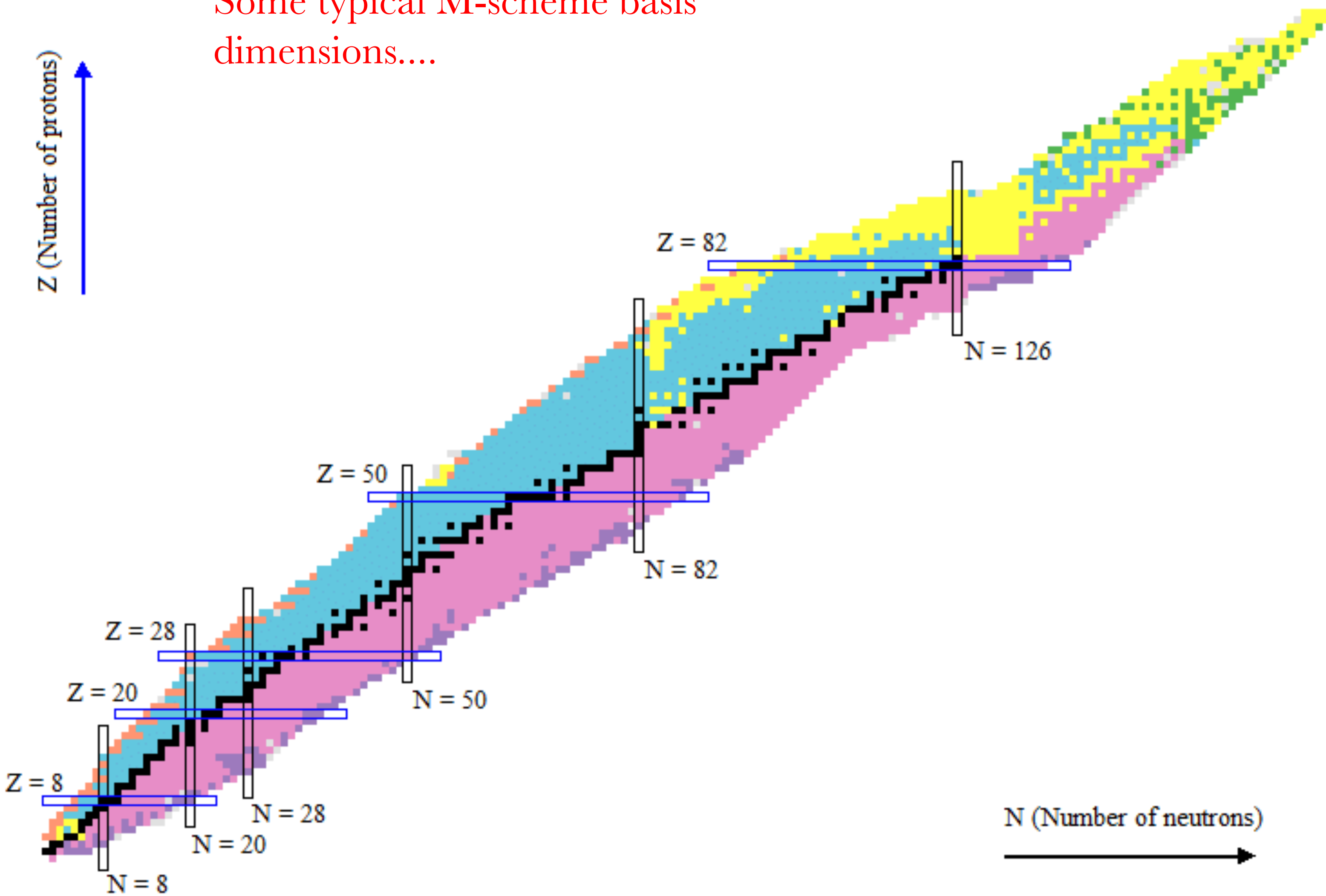
SAN DIEGO STATE UNIVERSITY

The configuration-interaction shell model is a powerful tool:

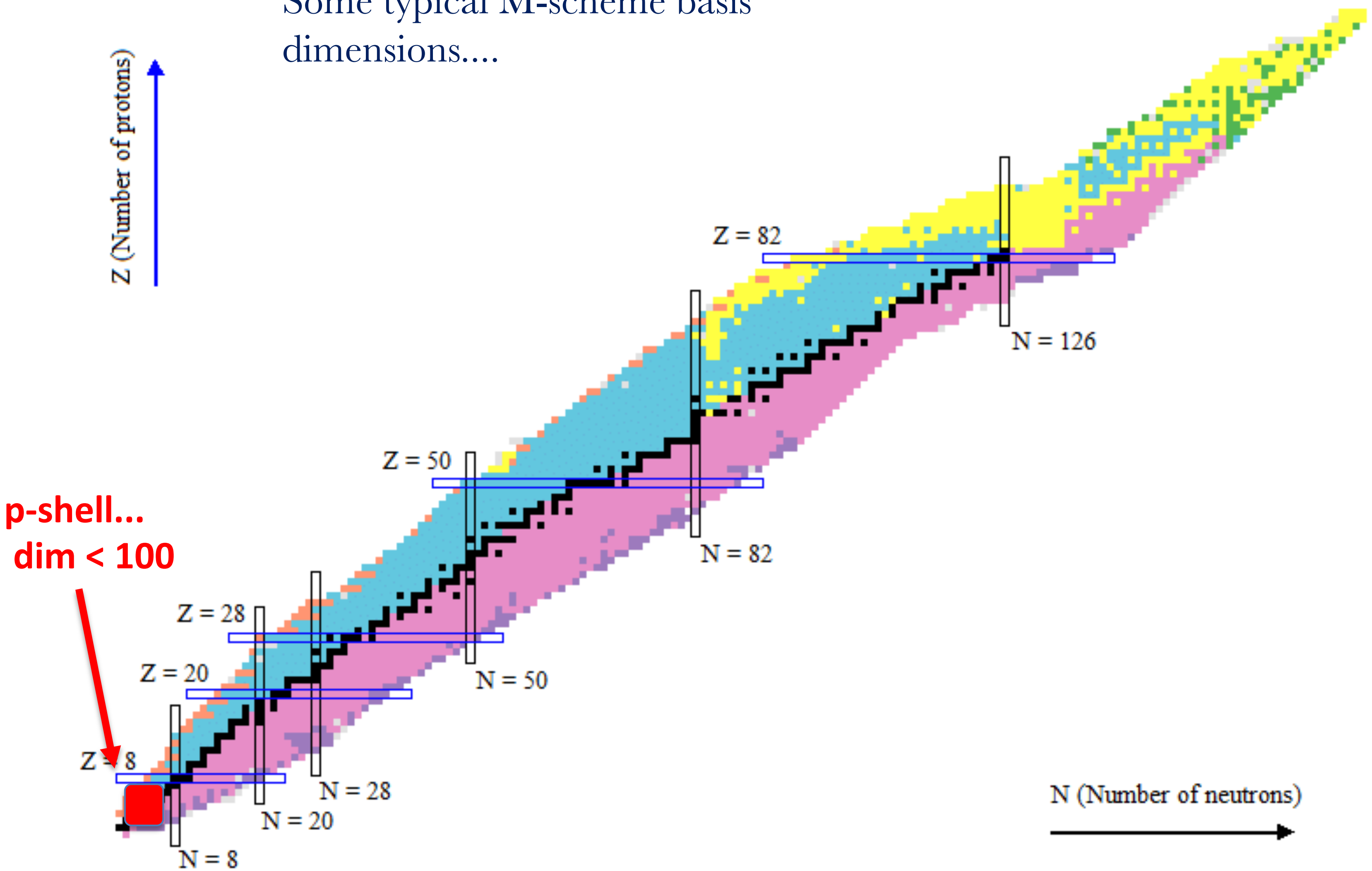
- Transparent formalism
- Flexible with respect to interactions
- Excited states with similar cost to ground state
- Explicit wave function makes analysis (e.g. group decomposition) straightforward

Drawback: the exponential growth in the basis dimension

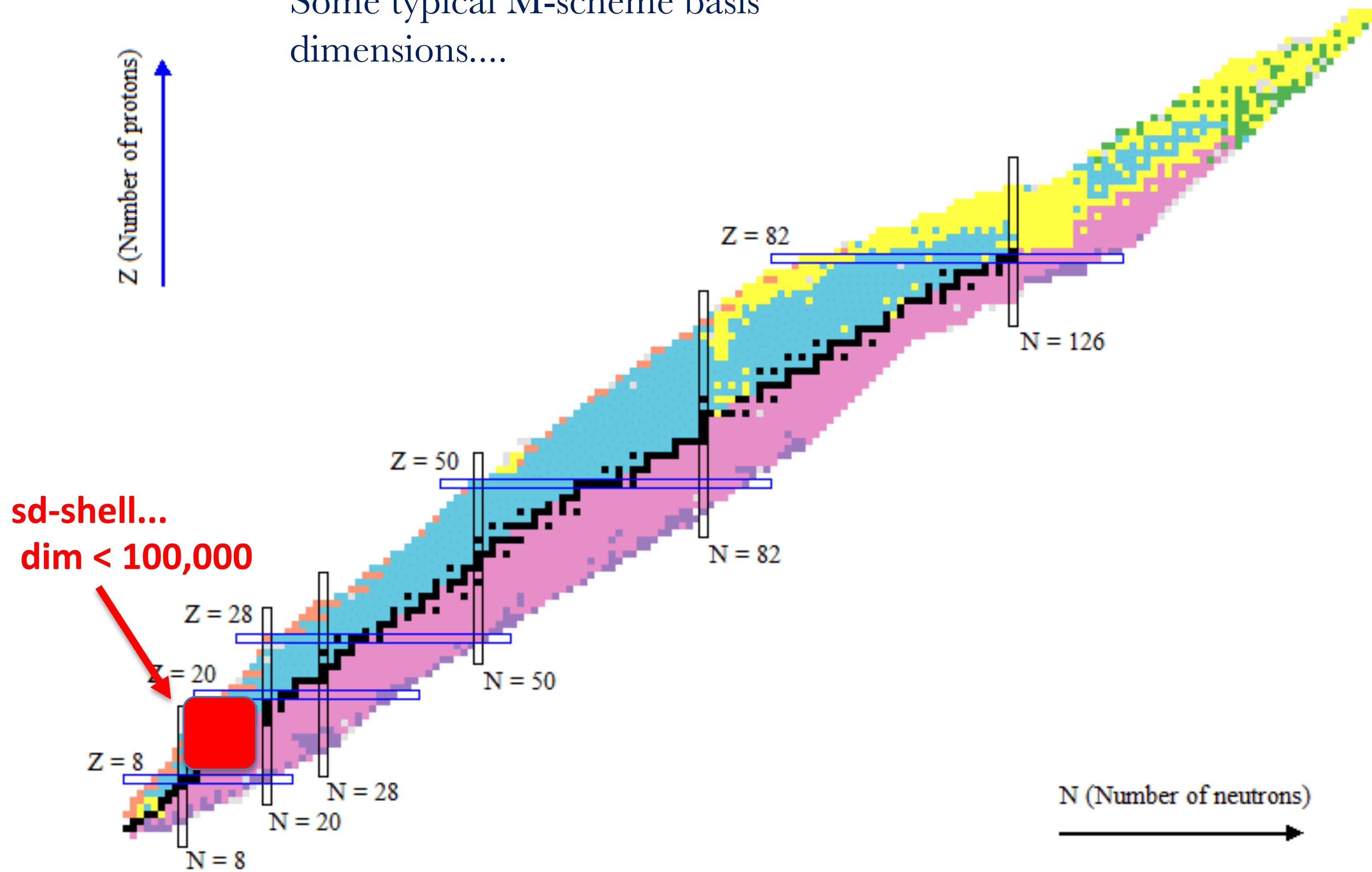
Some typical M-scheme basis dimensions....



Some typical M-scheme basis dimensions....

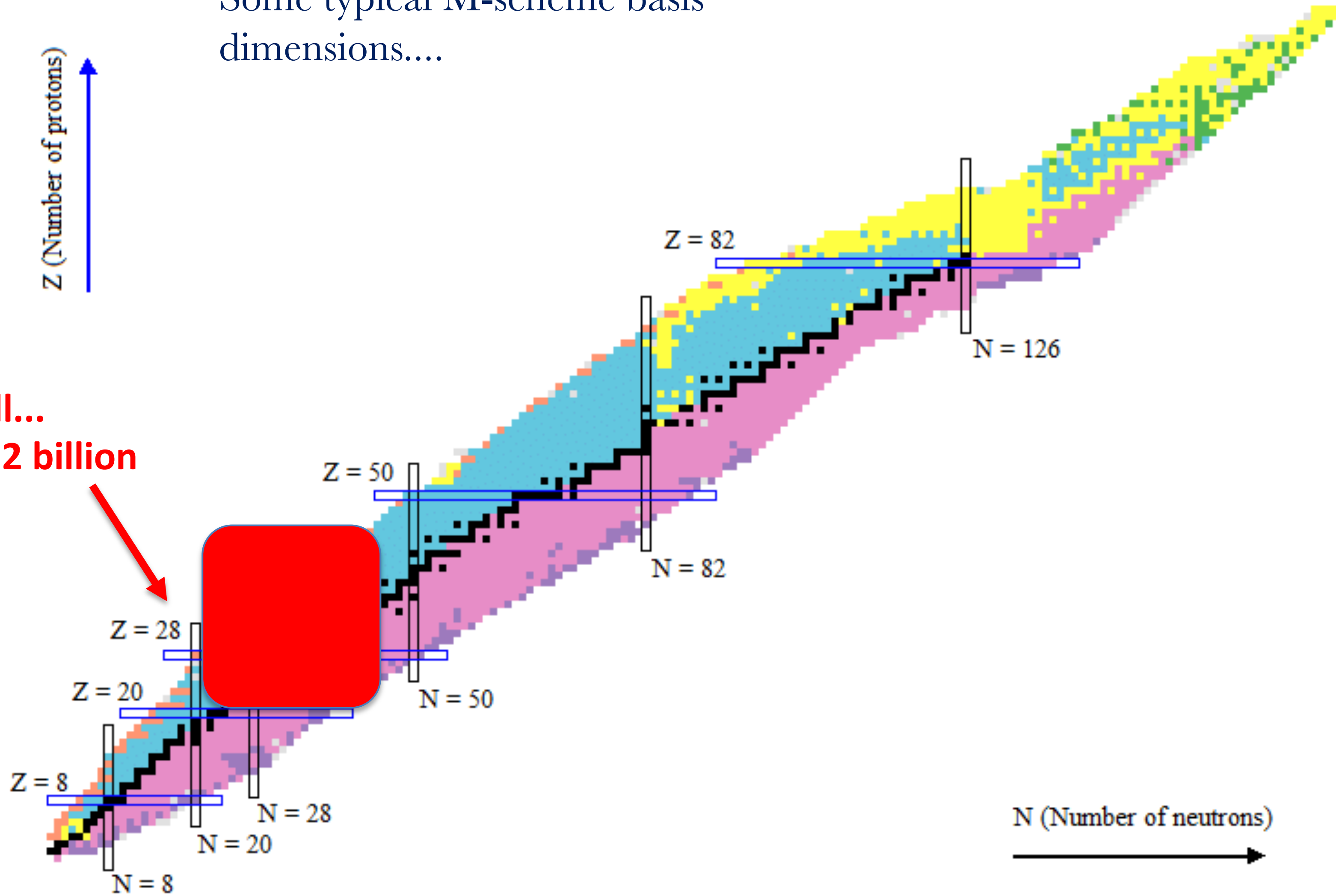


Some typical M-scheme basis dimensions....



Some typical M-scheme basis dimensions....

pf-shell...
dim < 2 billion

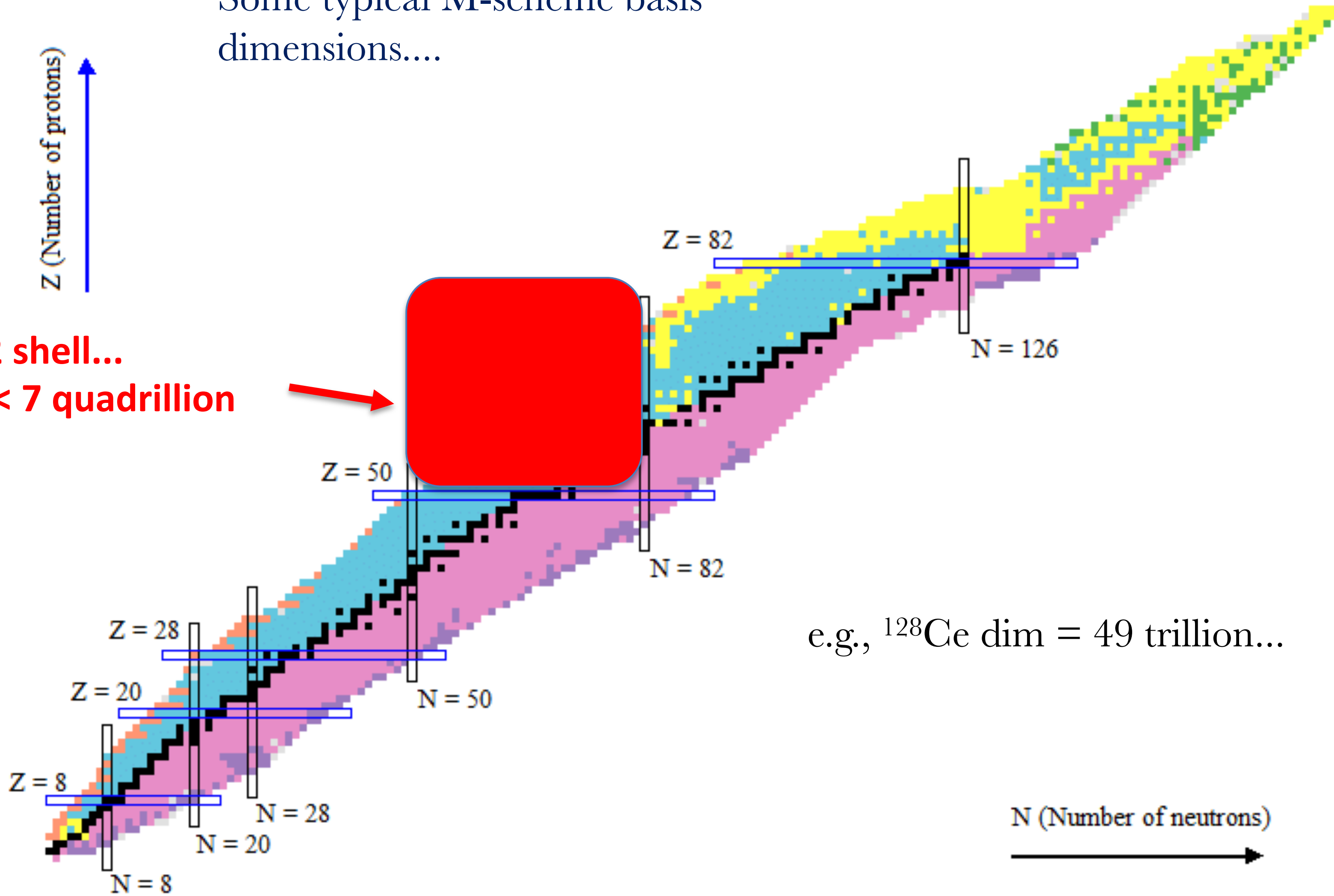


Ischia, May 22, 2025

d

SAN DIEGO STATE UNIVERSITY

Some typical M-scheme basis dimensions....



50-82 shell...
dim < 7 quadrillion

e.g., ^{128}Ce dim = 49 trillion...

How do we fight the monster of dimensionality?

See polynomial methods, e.g. talk by Forssen, Scalesi, etc.

SAN DIEGO STATE UNIVERSITY

How most shell-model codes represent the basis: Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

SAN DIEGO STATE UNIVERSITY

For fast calculation these are typically bit strings, or "*occupation representation of Slater determinants*"

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

$$\left|01101000...\right\rangle \left|10010100...\right\rangle$$

For fast calculation these are typically bit strings, or "*occupation representation of Slater determinants*"

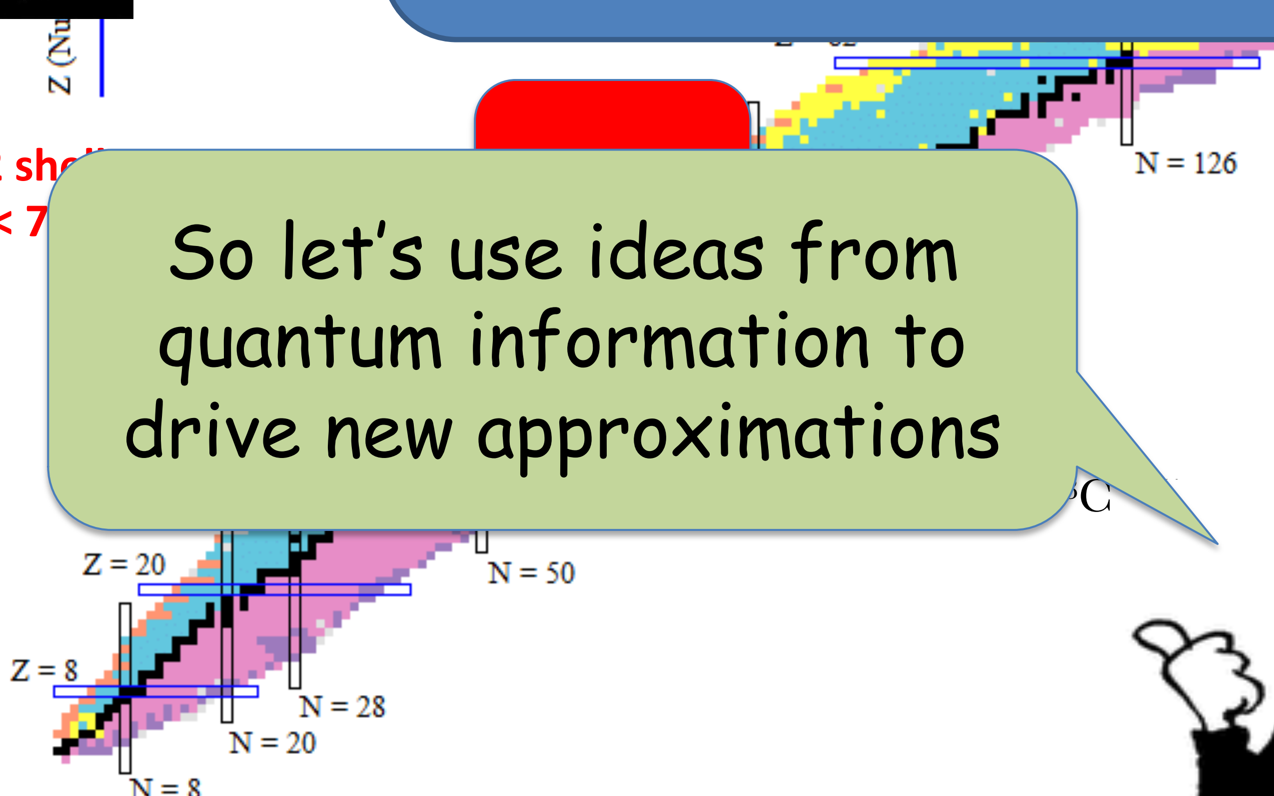
$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

$$\left|01101000...\right\rangle \left|10010100...\right\rangle$$

Even with the efficiencies of modern codes, the dimension can be too large to handle d

Some t
dimens

Even with the efficiencies of modern codes, the dimension can be too large to handle



50-82 sh
dim < 7

So let’s use ideas from quantum information to drive new approximations

SAN DIEGO STATE UNIVERSITY

Alternate approach for medium/heavy nuclei:
Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

Can we truncate to just a few components?

Alternate approach for medium/heavy nuclei:
Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

$$\left(a_1\left|010110...\right\rangle + a_2\left|110010...\right\rangle + a_3\left|001011...\right\rangle + ...\right)$$

No longer single "Slater determinants" but linear combinations…

SAN DIEGO STATE UNIVERSITY

Alternate approach for medium/heavy nuclei: Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

Can we truncate to just a few components?

Priori work by Papenbrock, Juodagalvis, Dean, Phys. Rev. C **69**, 024312 (2004), **focused on N =Z**

similar to DMRG (density-matrix renormalization group) (but not exactly)

SAN DIEGO STATE UNIVERSITY

Alternate approach for medium/heavy nuclei: Proton-neutron factorization

This work was 'proof of principle' but never put into practical applications

Priori work by Papenbrock, Juodagalvis, Dean, Phys. Rev. C **69**, 024312 (2004), **focused on N =Z**

similar to DMRG (density-matrix renormalization group) (but not exactly)

Key steps :

- Numerical experiments show *weak entanglement* between the proton and neutron partitions of shell-model wavefunctions

- This is especially so for $N \neq Z$

- Furthermore, low-energy many-proton/many-neutron components dominate

- This leads to a *practical* approximation in the shell-model for large-dimension calculations

San Diego State University

How most shell-model codes represent the basis:
Proton-neutron factorization

$$\left| \Psi \right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left| p_\mu \right\rangle \left| n_\nu \right\rangle$$

San Diego State University

How most shell-model codes represent the basis: Proton-neutron factorization

$$|\Psi\rangle = \sum_{\mu\nu} c_{\mu\nu} |p_\mu\rangle |n_\nu\rangle$$

can be extracted easily from `Bigstick` shell model code

How most shell-model codes represent the basis: Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

can be extracted easily from `Bigstick` shell model code

We can compute the *entanglement* between the proton and neutron components

This is formally equivalent to doing **singular-value decomposition** (or "Schmidt decomposition") of $c_{\mu\nu}$

SAN DIEGO STATE UNIVERSITY

How most shell-model codes represent the basis:
Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

can be extracted easily from `Bigstick` shell model code

We can compute the *entanglement* between the proton and neutron components

This is formally equivalent to doing **singular-value decomposition** (or “Schmidt decomposition”) of $c_{\mu\nu}$

O. Gorton MS thesis, 2018; CWJ and O. C. Gorton, J. Phys. G **50**, 045110 (2023)

SAN DIEGO STATE UNIVERSITY

How most shell-model codes represent the basis:
Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

can be extracted easily from `Bigstick` shell model code

Steps:

Find SVD eigenvalues λ_n of $c_{\mu\nu}$

How most shell-model codes represent the basis: Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

can be extracted easily from `Bigstick` shell model code

Steps:

Find SVD eigenvalues λ_n of $c_{\mu\nu}$

this is equivalent to finding eigenvalues of the *reduced density matrix*

SAN DIEGO STATE UNIVERSITY

How most shell-model codes represent the basis: Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

can be extracted easily from `Bigstick` shell model code

Steps:

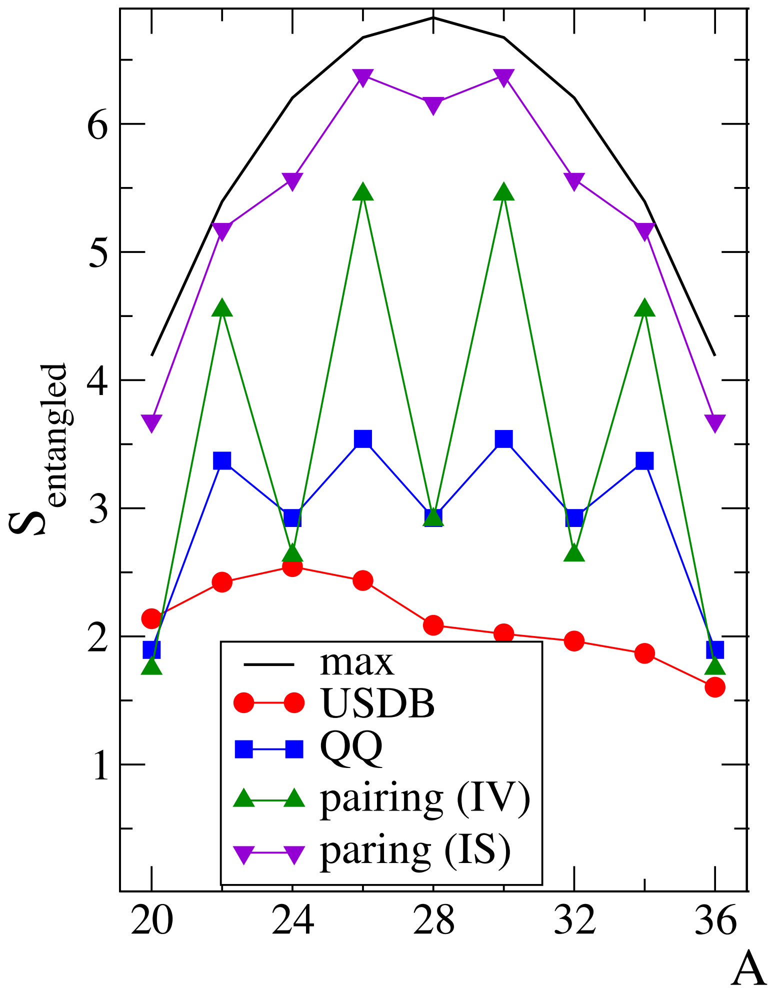
Find SVD eigenvalues λ_n of $c_{\mu\nu}$

this is equivalent to finding eigenvalues of the *reduced density matrix*

Compute the *entanglement entropy:* $S = -\sum_n \lambda_n \ln \lambda_n$

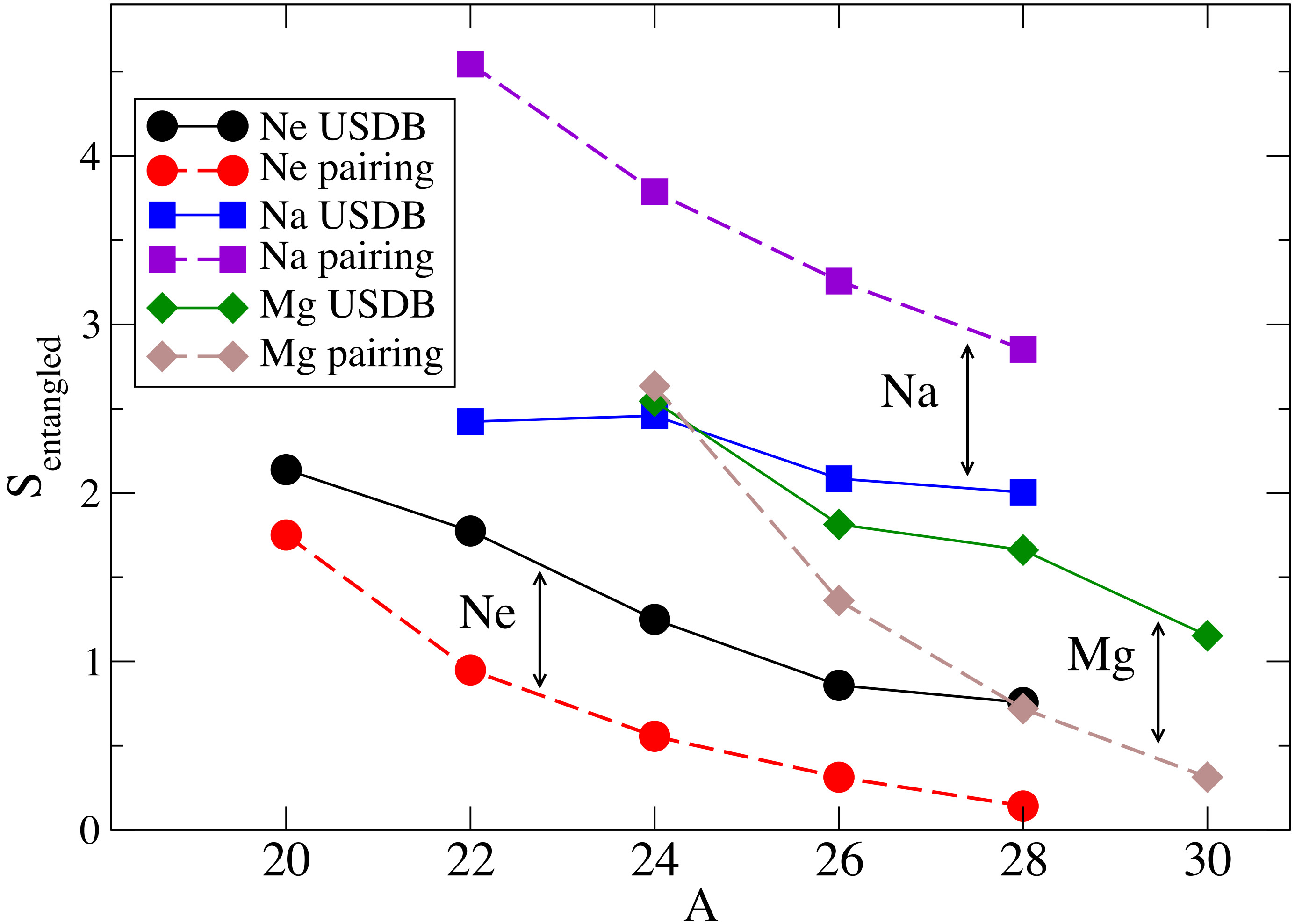
If the reduced density matrix has dimension N, then the maximum entropy is $S_{\max} = \ln N$.

Z = N nuclides in *sd* shell

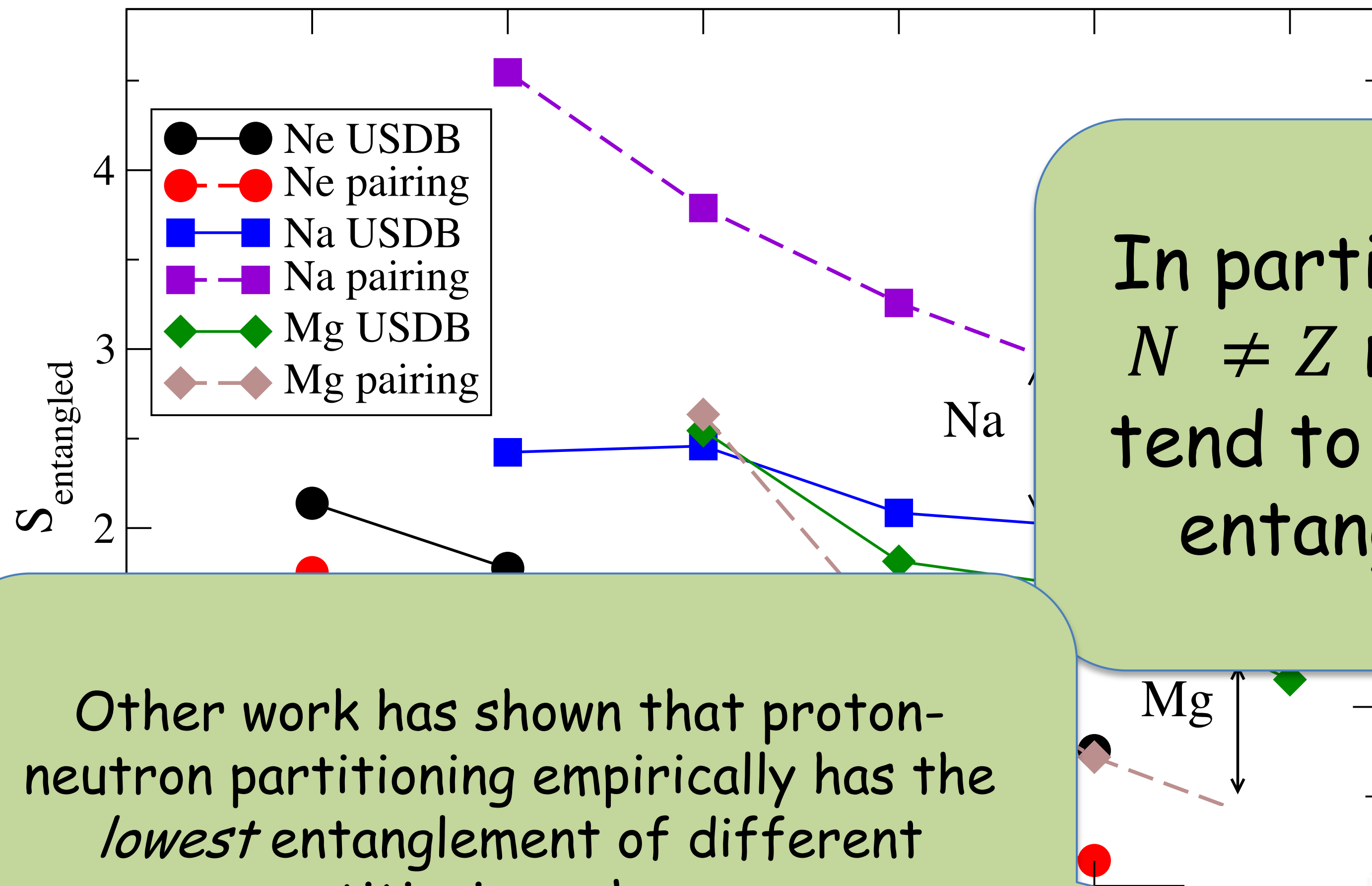


San Diego State University

For $N \neq Z$ we see interesting (but unexplained) patterns….



Ne USDB
Ne pairing
Na USDB
Na pairing
Mg USDB
Mg pairing
Na
Ne
Mg
$S_{entangled}$
A
0
1
2
3
4
20
22
24
26
28
30



In particular, for $N \neq Z$ nuclei, we tend to see lower entanglement

Other work has shown that proton-neutron partitioning empirically has the *lowest* entanglement of different partitioning schemes (Perez-Obiol *et al*, EPJA **59**, 240 (2023))

More evidence why this could work:
Decompose full wfn into proton, neutron components

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

$frac_\mu = \sum_\nu \left|c_{\mu\nu}\right|^2$ = fraction of full wave function with *proton* (eigen)state μ

$$\hat{H} = \hat{H}_{pp} + \hat{H}_{nn} + \hat{H}_{pn}$$

$$\hat{H}_{pp} | p_\mu \rangle = E_\mu | p_\mu \rangle$$

$$\hat{H}_{nn} | n_\nu \rangle = E_\upsilon | n_\nu \rangle$$

SAN DIEGO STATE UNIVERSITY

More evidence why this could work: Decompose full wfn into proton, neutron components

Eigenstate of proton part of H

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

Eigenstate of neutron part of H

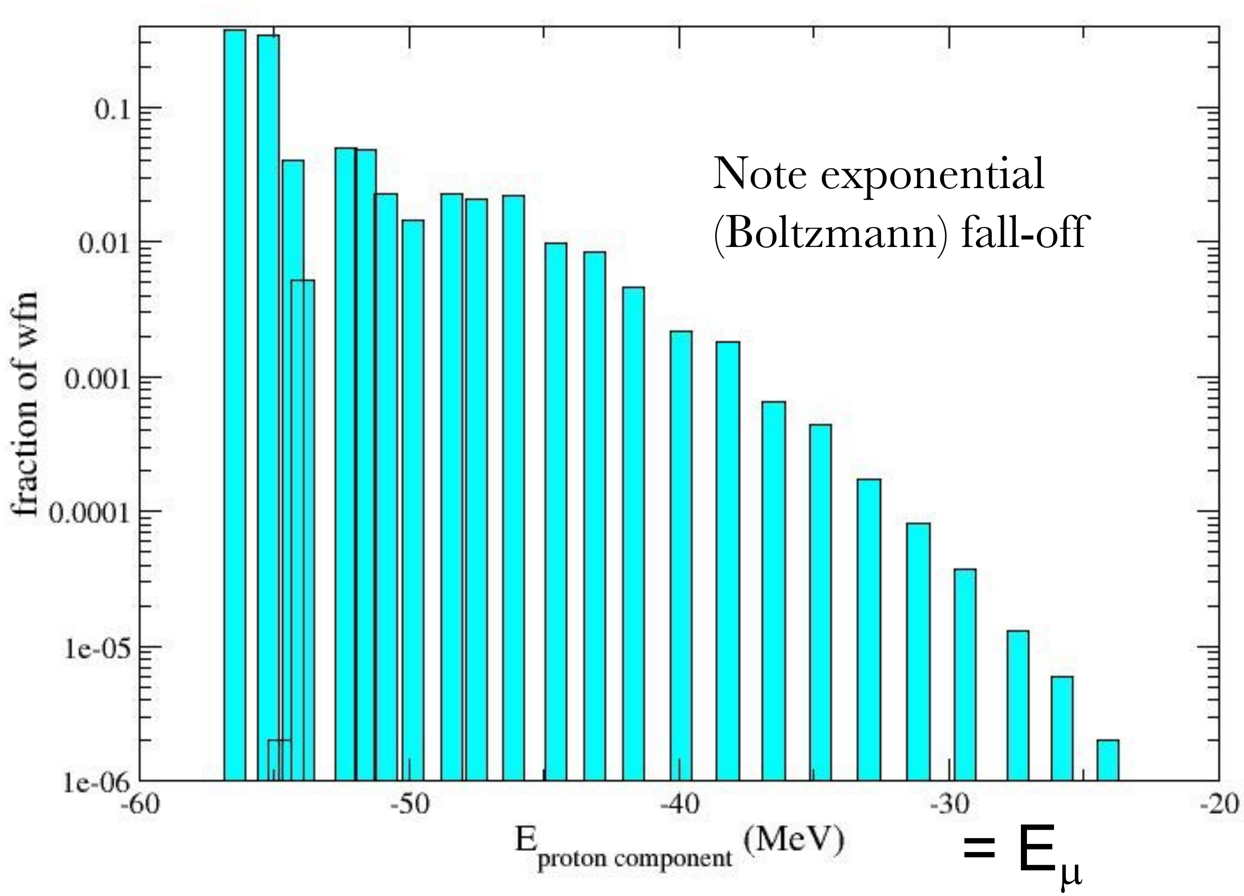
$$frac_\mu = \sum_\nu \left|c_{\mu\nu}\right|^2$$

= fraction of full wave function with *proton* (eigen)state μ and energy E_μ

(one can compute this very efficiently with the Lanczos algorithm)

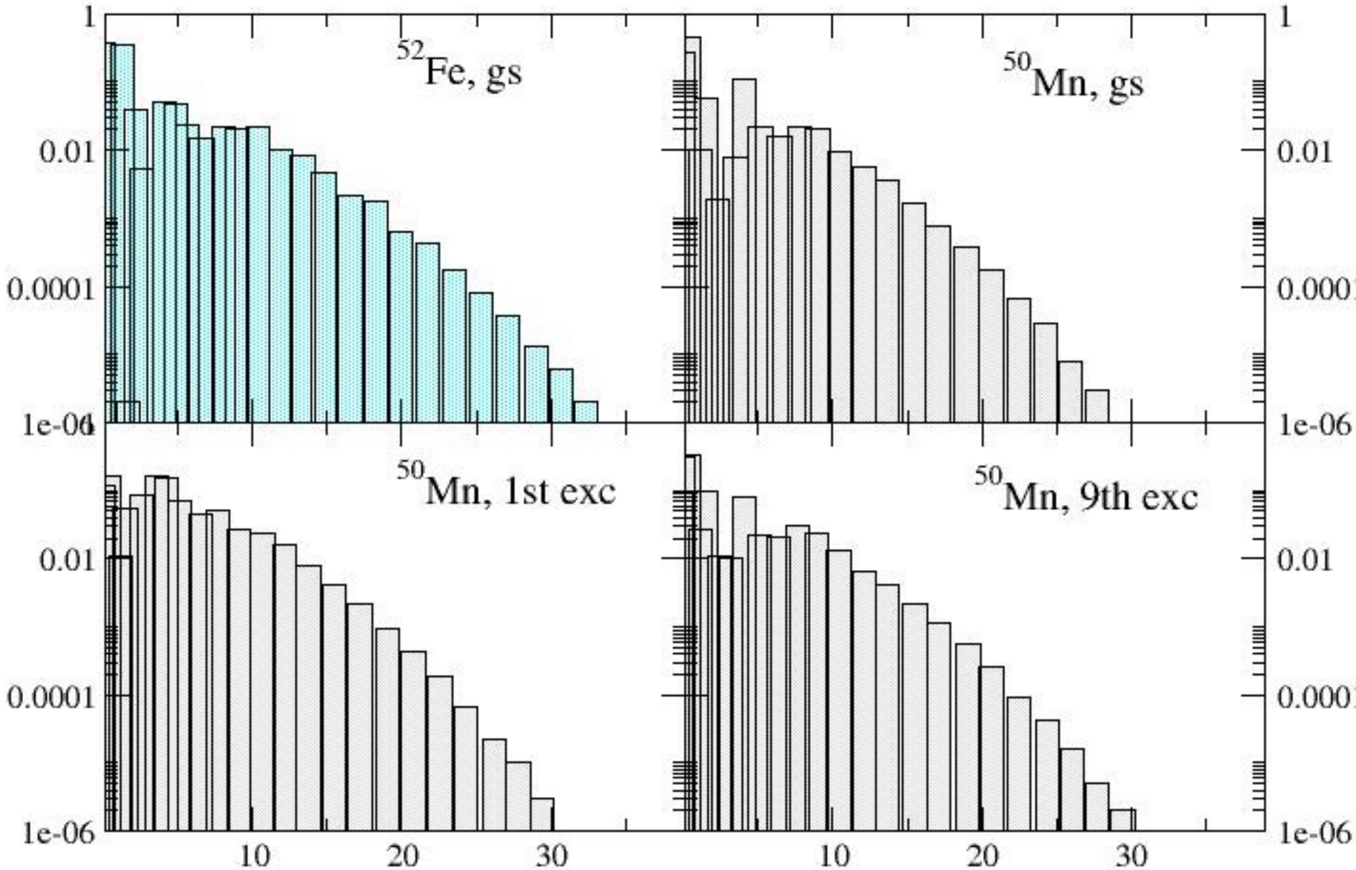
^{52}Fe in *pf*-shell with GX1A interaction

decomposition of g.s.

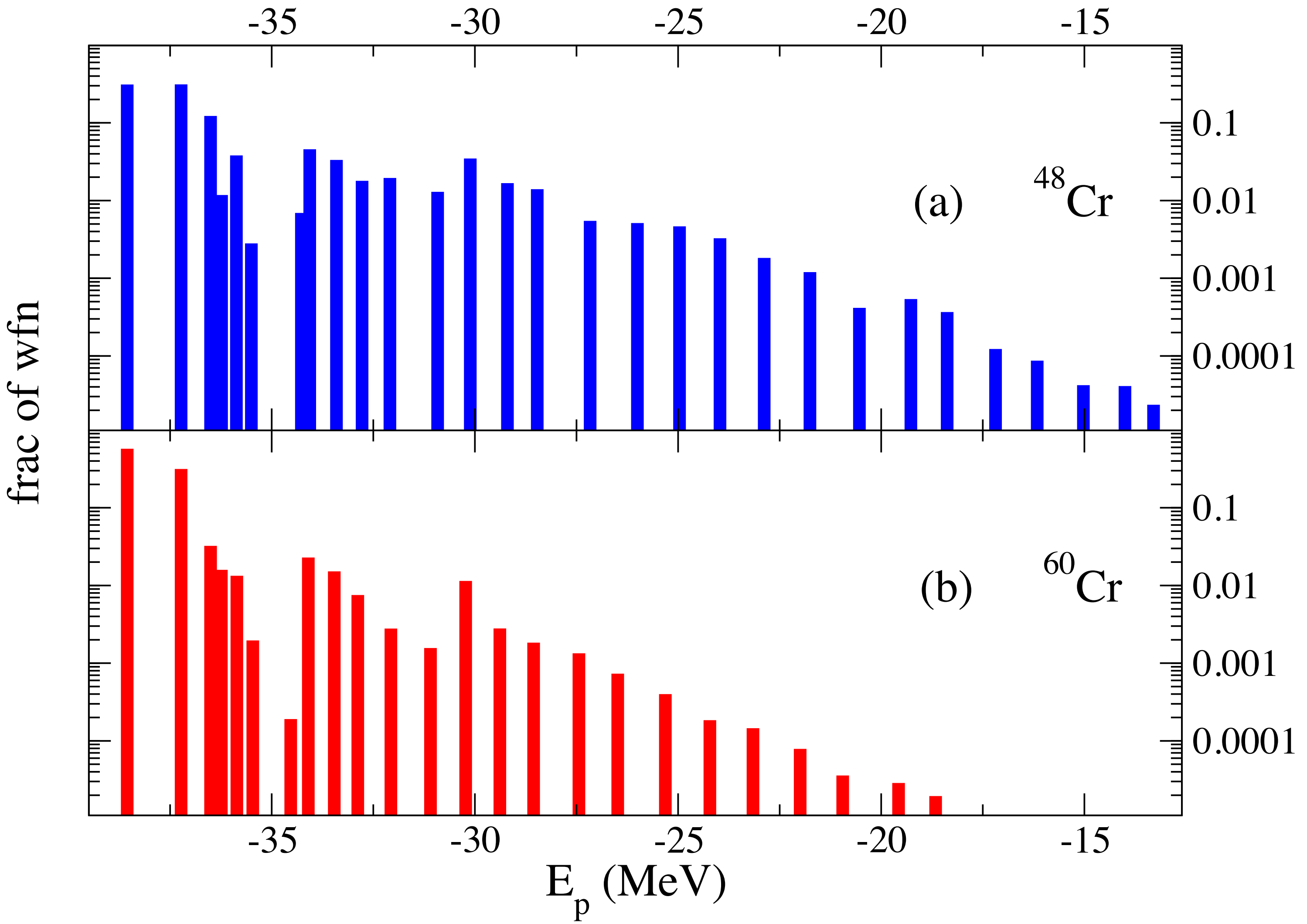


These energies are the eigenenergies of 6 valence protons in the *pf* shell *pf*-shell with GX1A interaction

decomposition into proton components



Note exponential
(Boltzmann) fall-off



frac of wfn
(a)
^{48}Cr
(b)
^{60}Cr
0.1
0.01
0.001
0.0001
-35
-30
-25
-20
-15
E_p (MeV)

SAN DIEGO STATE UNIVERSITY

Example of the utility of this approach:

shells between 50 and 82 ($0g_{7/2}$ 2s1d $0h_{11/2}$)

^{129}Cs: M-scheme dim 50 billion

Proton Slater determinant dimension: 14,677
Neutron Slater determinant dimension: 646,430

We have written a code (O. Gorton)

Proton And Neutron Approximate Shell model:

PANASh

We want to find solutions to

$$\hat{H}\left|\Psi\right\rangle = E\left|\Psi\right\rangle \quad \text{where} \quad \hat{H} = \hat{H}_{pp} + \hat{H}_{nn} + \hat{H}_{pn}$$

We solve $\hat{H}_{pp}\left|\Psi_p\right\rangle = E_p\left|\Psi_p\right\rangle \quad \hat{H}_{nn}\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle$

and choose certain $\left|\Psi_p\right\rangle\left|\Psi_n\right\rangle$ as basis for diagonalization;

SAN DIEGO STATE UNIVERSITY

Oliver Gorton

Using BIGSTICK we construct many-**proton** states of good J

$$\left|\Psi_p, J_p M\right\rangle = \sum_\mu c_\mu \left| p_\mu, M\right\rangle$$

and the same for many-**neutron** states; these we **couple** together in a *J-scheme* code with fixed *J* for basis:

$$\left|\Psi_J\right\rangle = \sum_{ab} c_{ab} \left[\left|\Psi_p a, J_p\right\rangle \otimes \left|\Psi_n b, J_n\right\rangle \right]_J$$

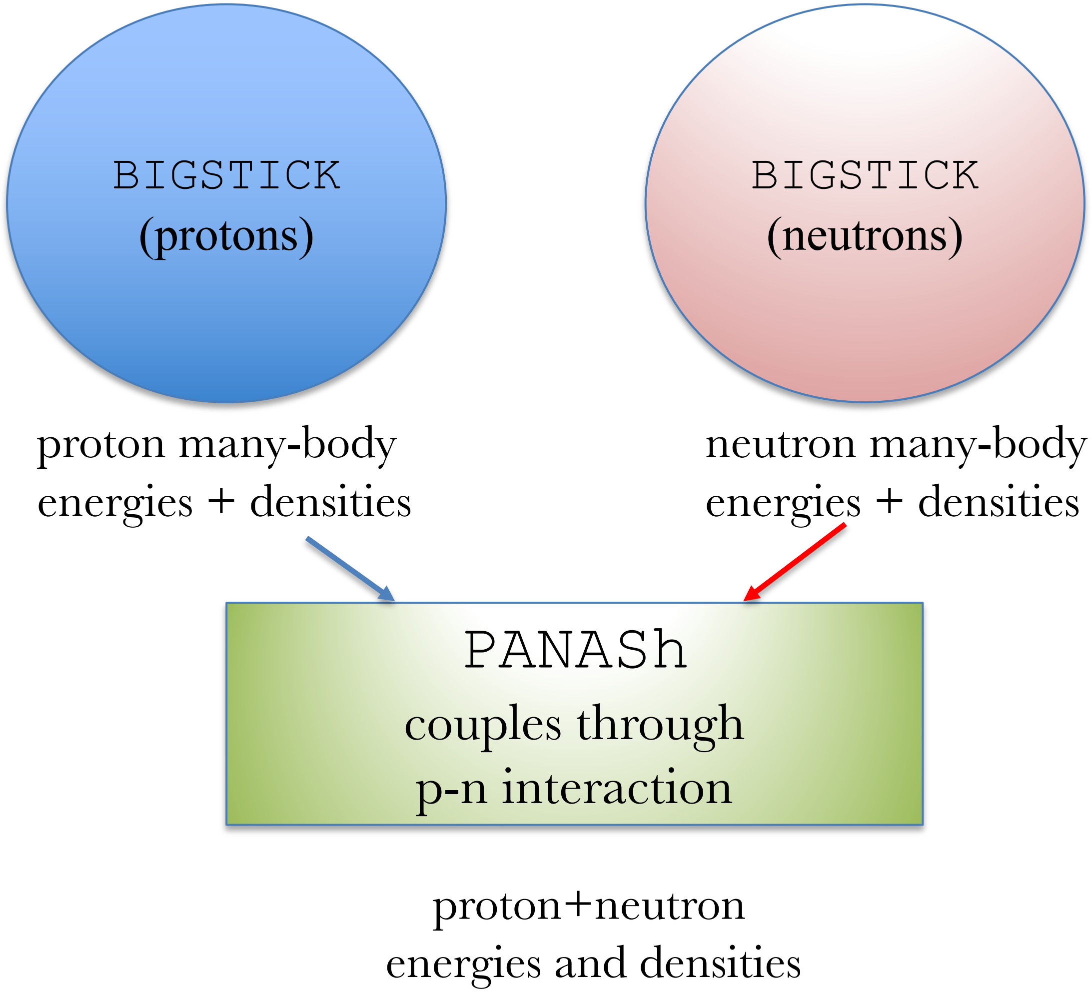
same here,
only for neutrons

We don't take all possible of these,
but choose those lowest in energy
when solving the proton-only system

Ischia, May 22, 2025

San Diego State University

Oliver Gorton



Ischia, May 22, 2025

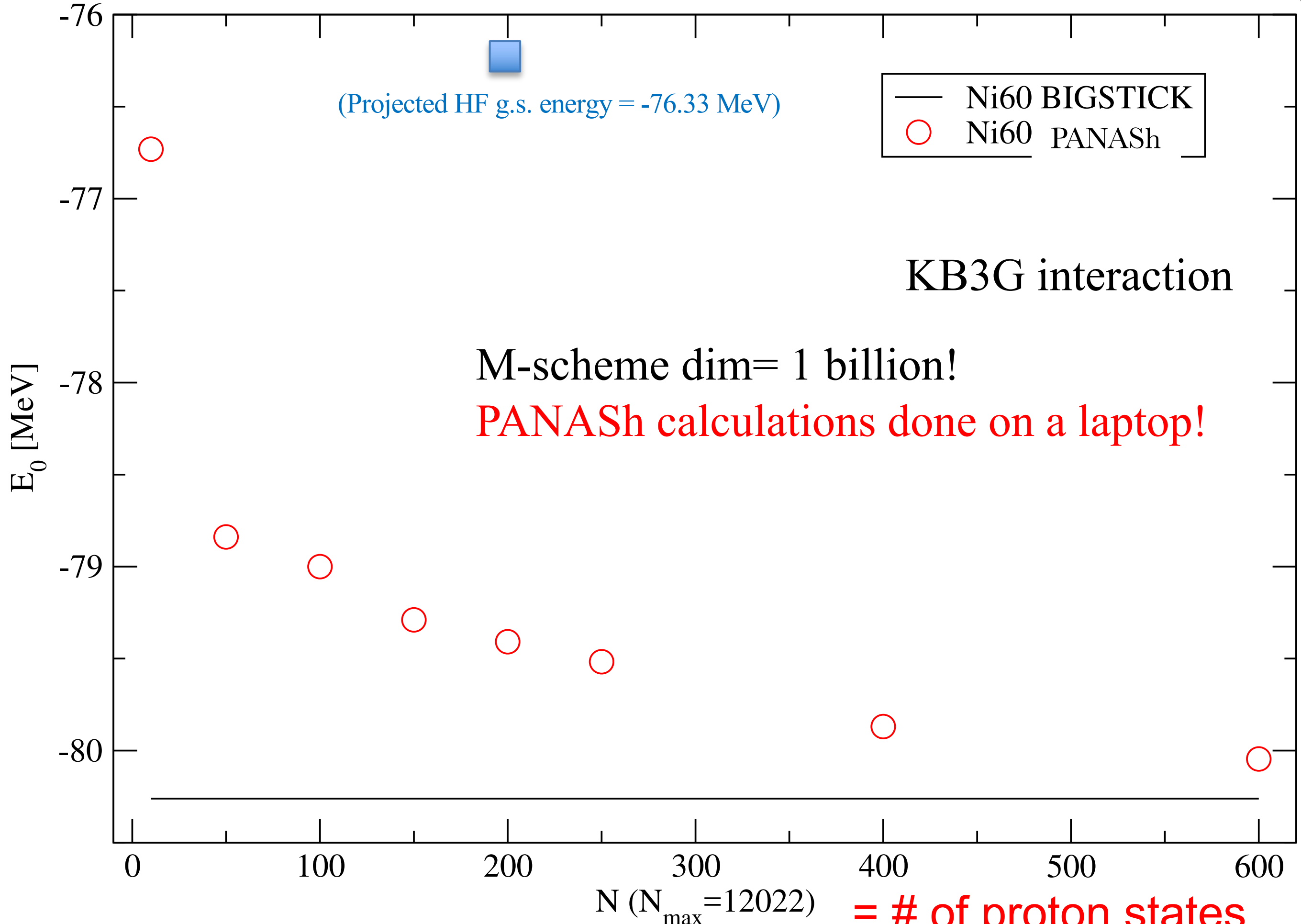
We have validated against full configuration-interaction, e.g. in the pf shell and in the 28-50, 50-82 spaces:

e.g., ^{60}Ni, ^{60}Zn, ^{70}As, ^{128}Xe (FCI dim: 9.3 billion!), ^{132}Ba, ^{129}Cs

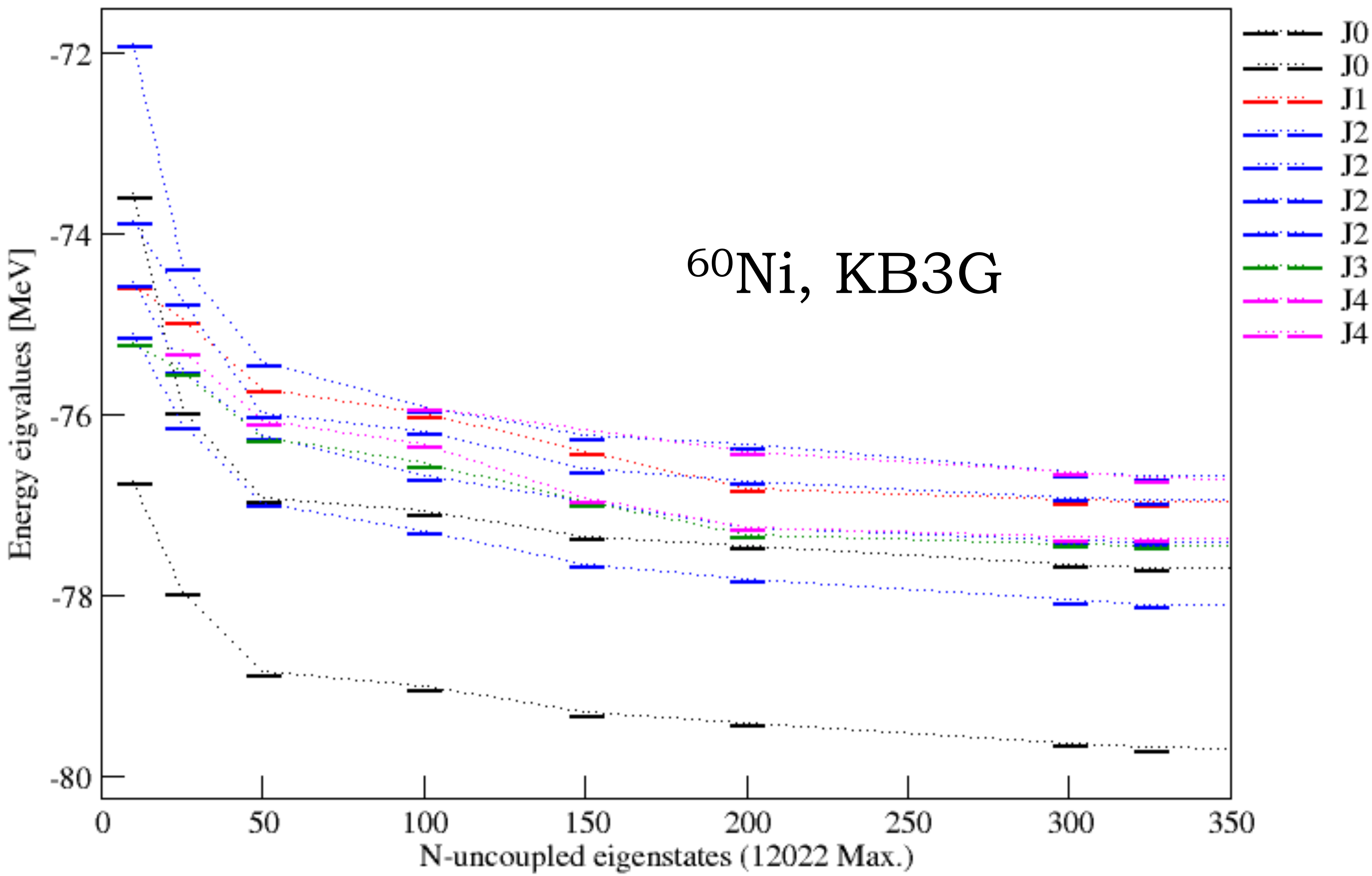
We have also demonstrated calculations for impossible FCI, e.g., ^{132}Ce (FCI dimension: 2.4 *trillion*!)

The PANASh calculations can be run on a laptop or on a workstation

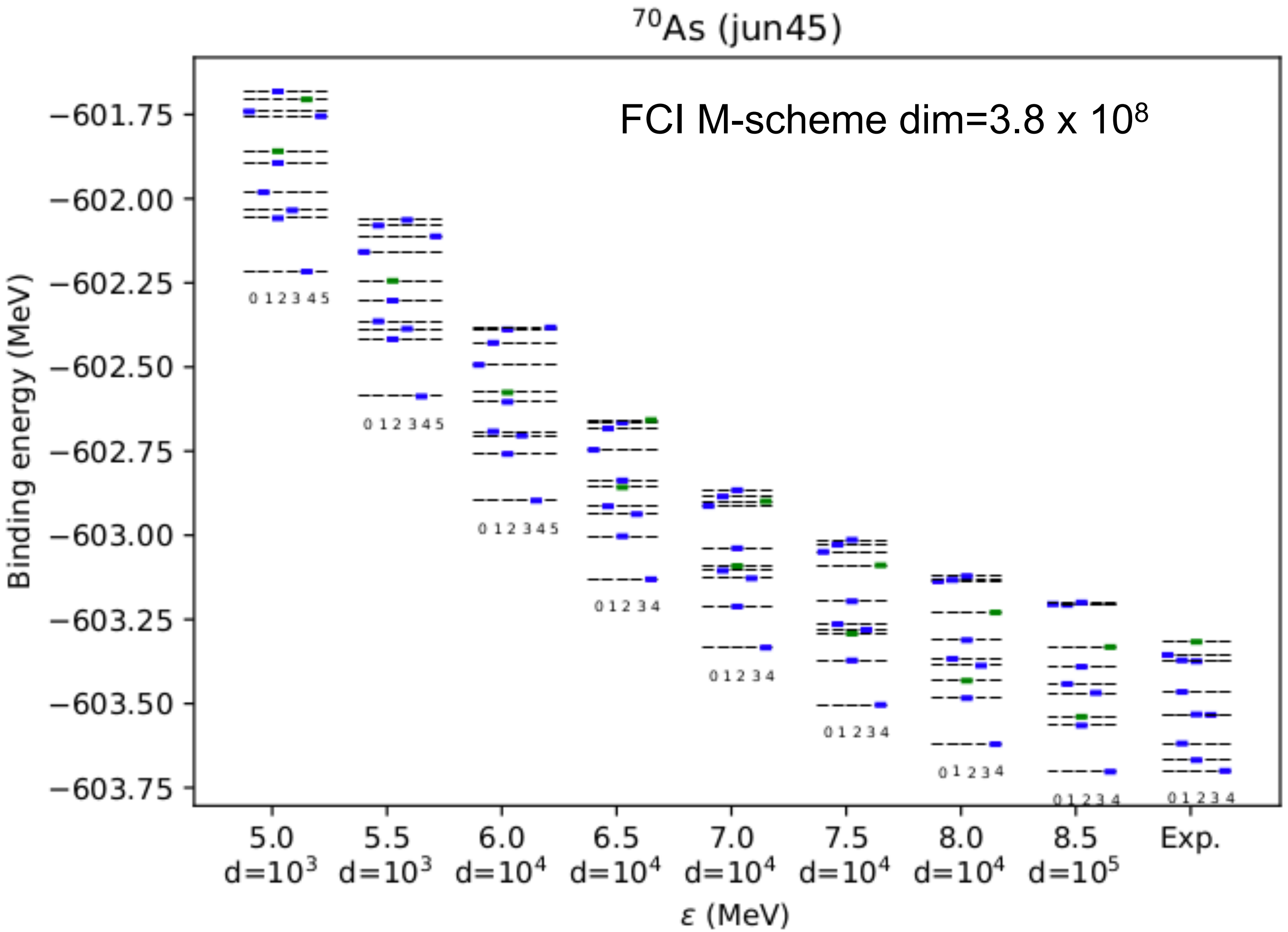
Example: ^{60}Ni in *pf* shell



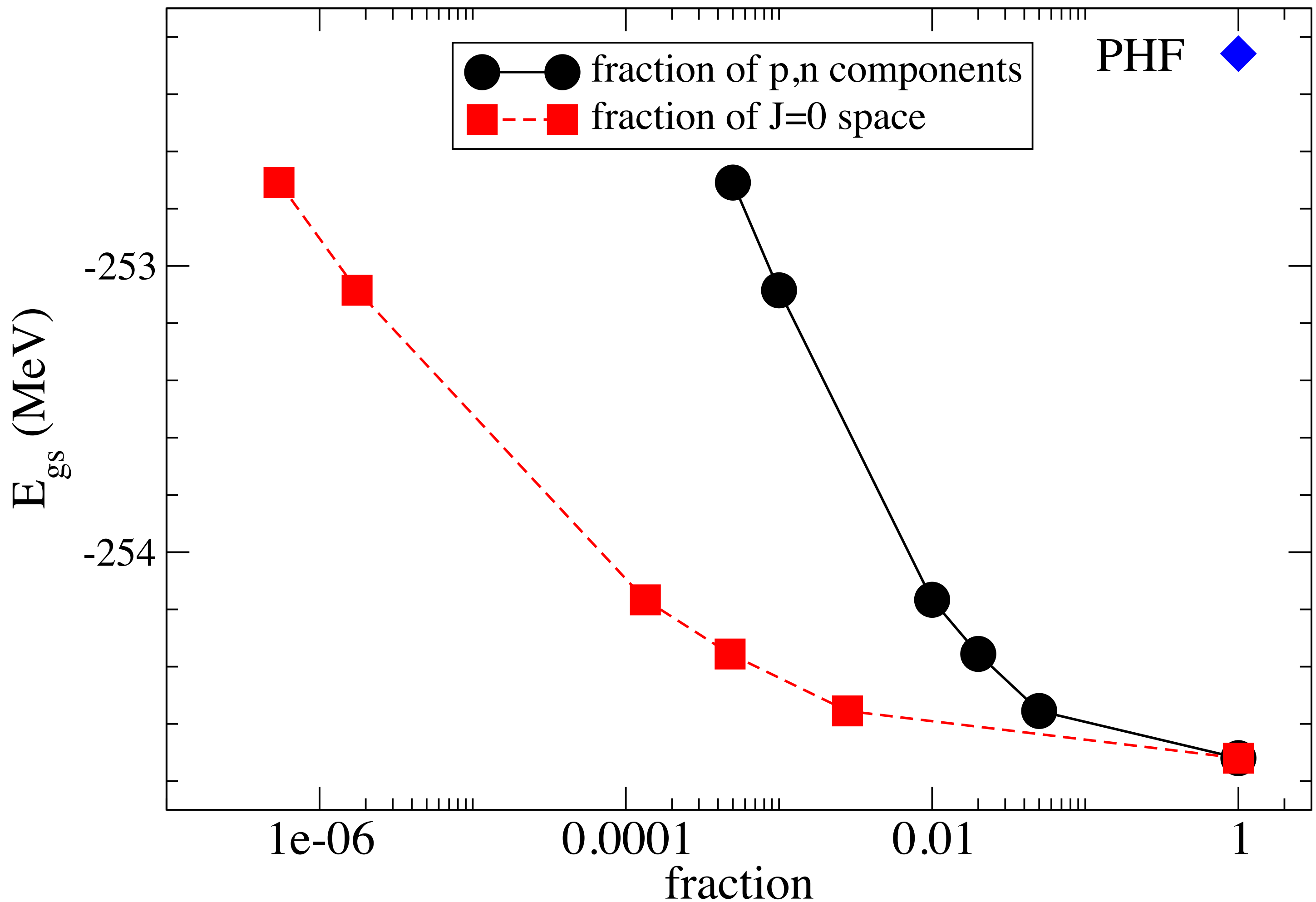
= # of proton states



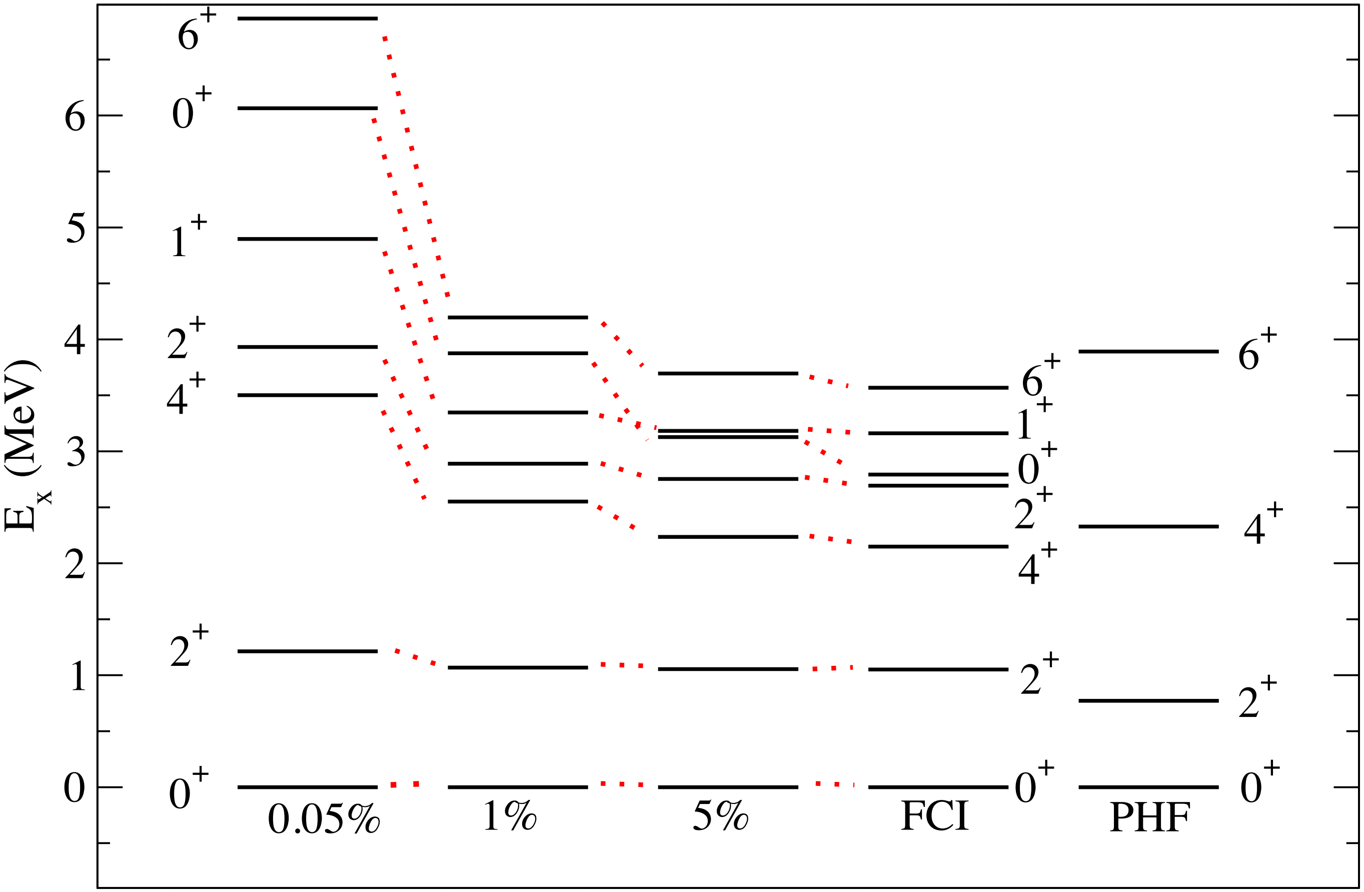
^{60}Ni, KB3G
Energy eigvalues [MeV]
N-uncoupled eigenstates (12022 Max.)
-72
-74
-76
-78
-80
0
50
100
150
200
250
300
350
J0
J0
J1
J2
J2
J2
J2
J3
J4
J4



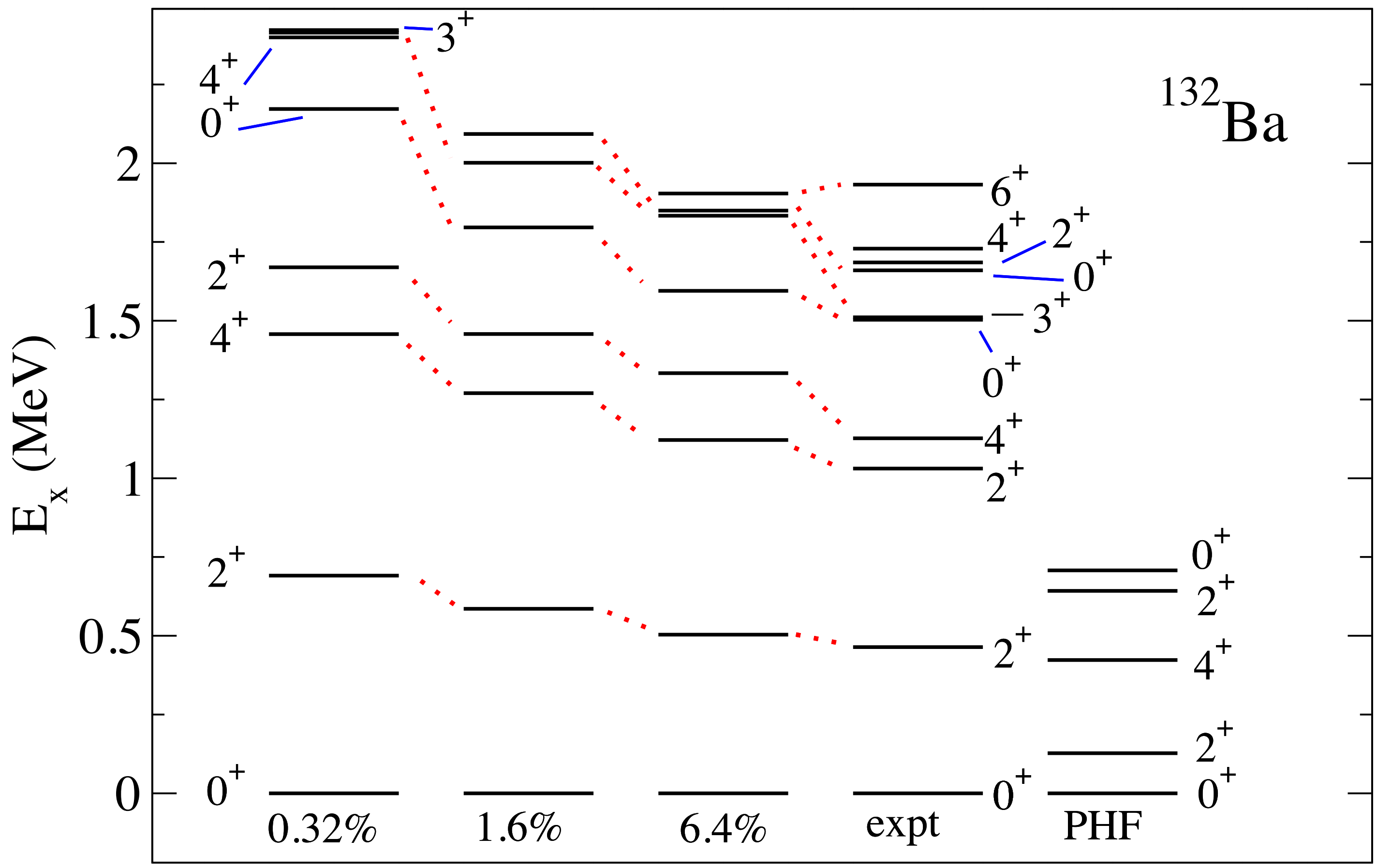
^{70}As (jun45)
FCI M-scheme dim=3.8 x 10^8
Binding energy (MeV)
−601.75
−602.00
−602.25
−602.50
−602.75
−603.00
−603.25
−603.50
−603.75
0 1 2 3 4 5
0 1 2 3 4
5.0 d=10^3
5.5 d=10^3
6.0 d=10^4
6.5 d=10^4
7.0 d=10^4
7.5 d=10^4
8.0 d=10^4
8.5 d=10^5
Exp.
ε (MeV)



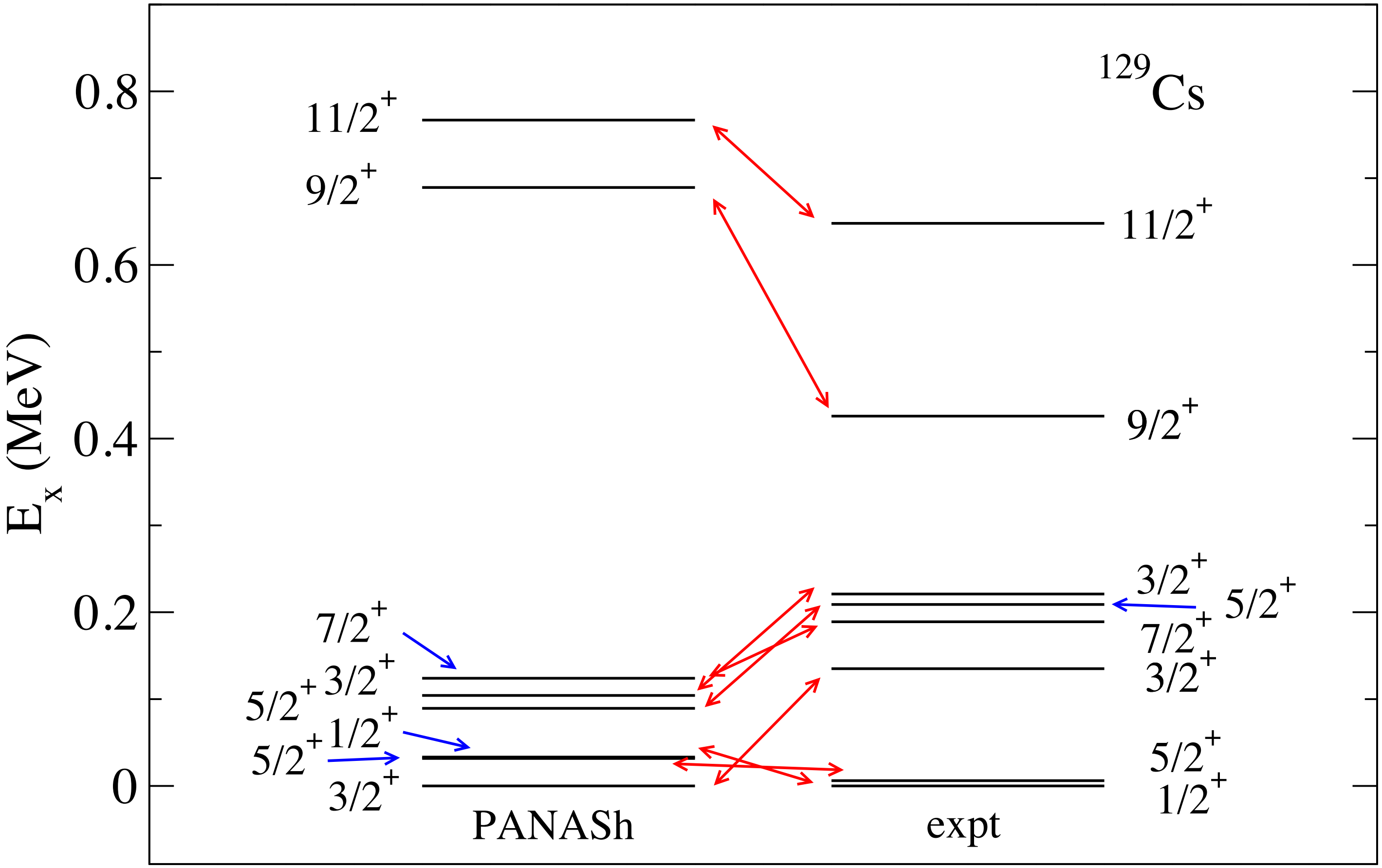
^{60}Zn
in pf shell
with GX1A



^{60}Zn
in pf shell
with GX1A



in 50-82 space (w/int from F. Nowacki)



in 50-82 space (w/int from F. Nowacki)

FCI dim= 2.4 trillion!

SAN DIEGO STATE UNIVERSITY

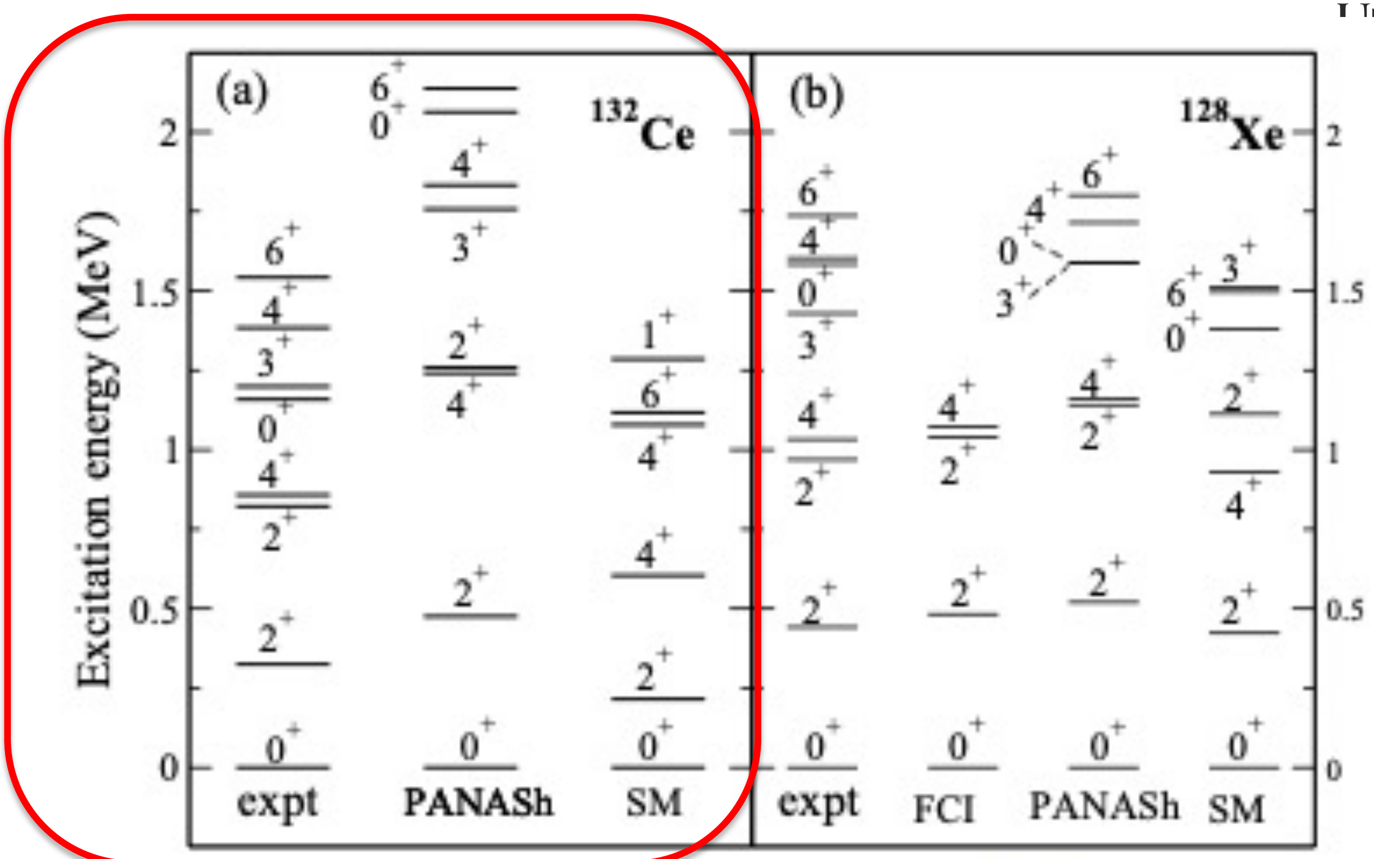


FIG. 6. Excitation spectra for (a) ^{132}Ce and (b) ^{128}Xe, including from experiment (Refs. [31,34], respectively). We assume a ^{100}Sn core and a valence space of the orbitals between magic numbers 50 and 82, and use the interaction in Ref. [32], including the recommended 0.9 reduction of neutron-neutron two-body matrix elements. Only for ^{128}Xe is a full configuration-interaction (FCI) calculation possible, with an M-scheme dimension of 9.3 billion; the FCI M-scheme dimension for ^{132}Ce would be 2.4 trillion. The PANASh calculations have neutron fractions $m = 0.015\, d_n$; the $J = 6$ PANASh dimensions are 377 000 for ^{128}Xe and 432 000 for ^{132}Ce. Also shown are truncated (see text for details) configuration-interaction shell-model (SM) levels, with M-scheme dimensions of 507 million for ^{128}Xe and 1.29 billion for ^{132}Ce.

Shape transitions in chromium isotopes

SAN DIEGO STATE UNIVERSITY

We currently generate the proton and neutron components independently.

Yet the proton-neutron interaction generates quadrupole collectivity.

Can the weak-entanglement approximation capture shape transitions?

Shape transitions in chromium isotopes

SAN DIEGO STATE UNIVERSITY

We currently generate the proton and neutron components independently.

Yet the proton-neutron interaction generates quadrupole collectivity.

Can the weak-entanglement approximation capture shape transitions?

We consider the chromium isotopes: at N = 28 (A=52) should be spherical, otherwise deformed

Shape transitions in chromium isotopes

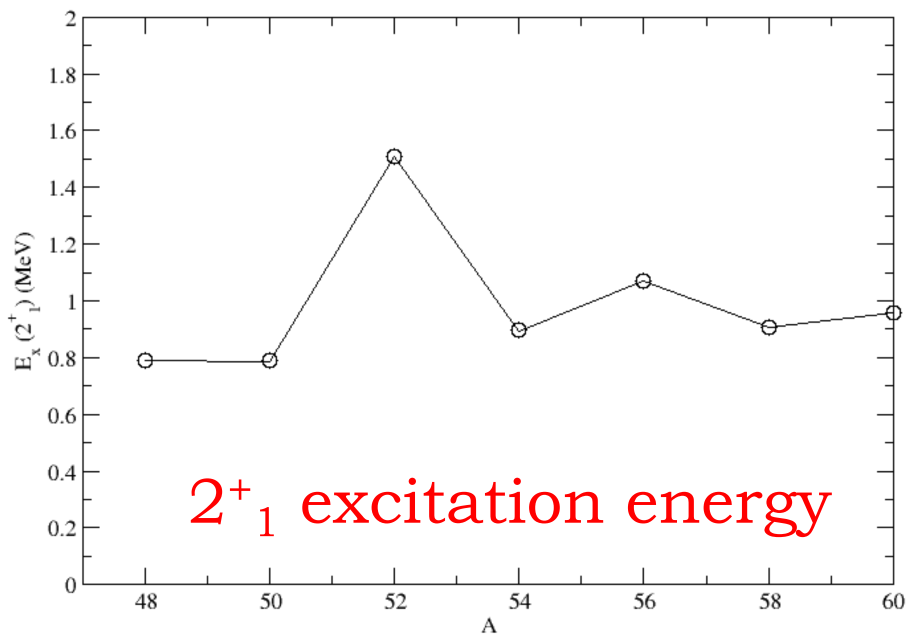
SAN DIEGO STATE UNIVERSITY

We currently generate the proton and neutron components independently.

Yet the proton-neutron interaction generates quadrupole collectivity.

Can the weak-entanglement approximation capture shape transitions?

We consider the chromium isotopes: at N = 28 (A=52) should be spherical, otherwise deformed



This is valence space, in *pf* shell (with GX1A)

Shape transitions in chromium isotopes

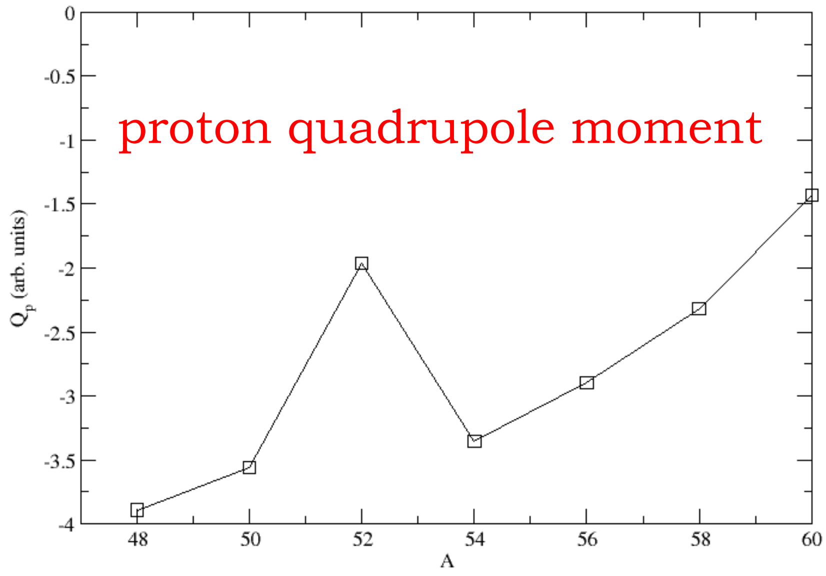
We currently generate the proton and neutron components independently.

Yet the proton-neutron interaction generates quadrupole collectivity.

Can the weak-entanglement approximation capture shape transitions?

We consider the chromium isotopes: at N = 28 (A=52) should be spherical, otherwise deformed

This is valence space, in *pf* shell (with GX1A)



Shape transitions in chromium isotopes

SAN DIEGO STATE UNIVERSITY

W rrently ge independently.

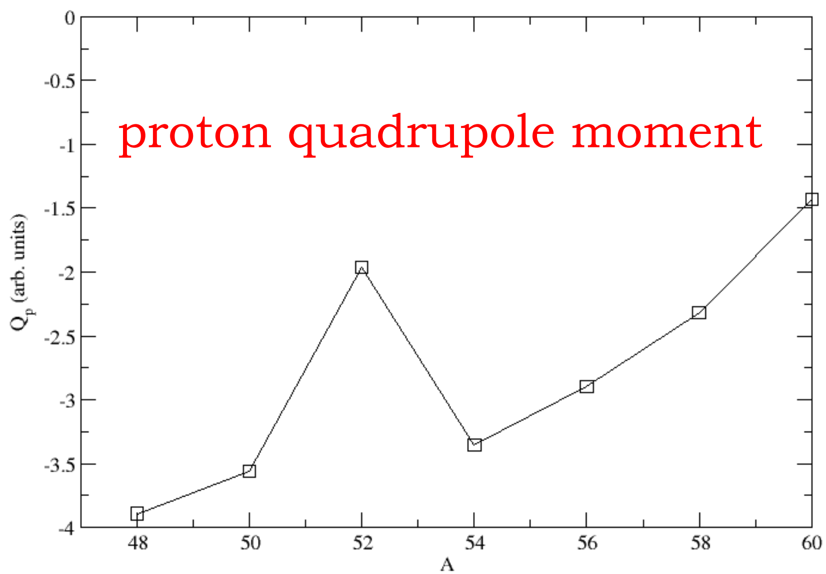
proton- lectivity.

Let's see what the **weak entanglement approximation** can do!

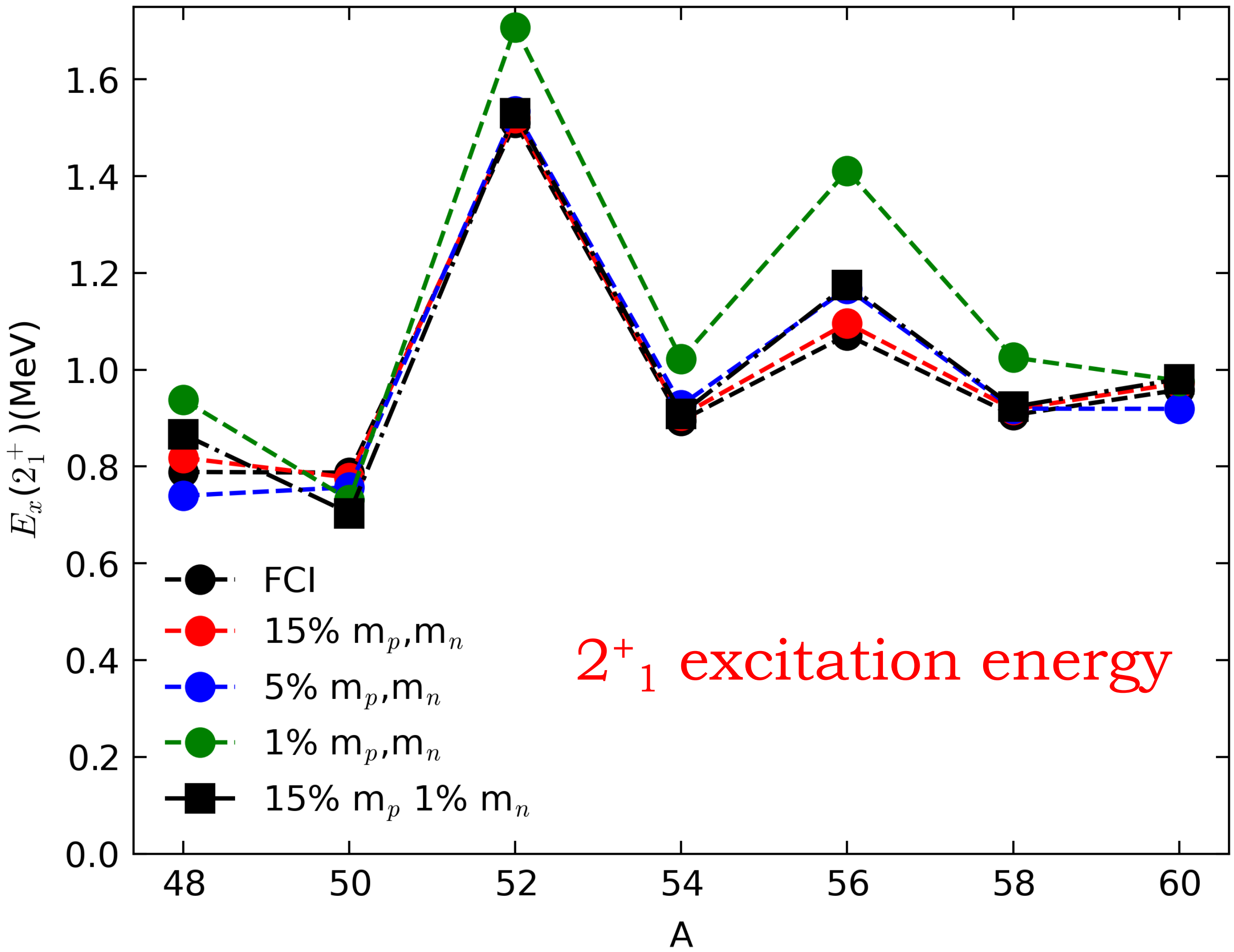
e weak-entanglement approximation capture shape transitions?

We consider the chromium isotopes: at N = 28 (A=52) should be spherical, otherwise deformed

This is valence space, in *pf* shell (with GX1A)

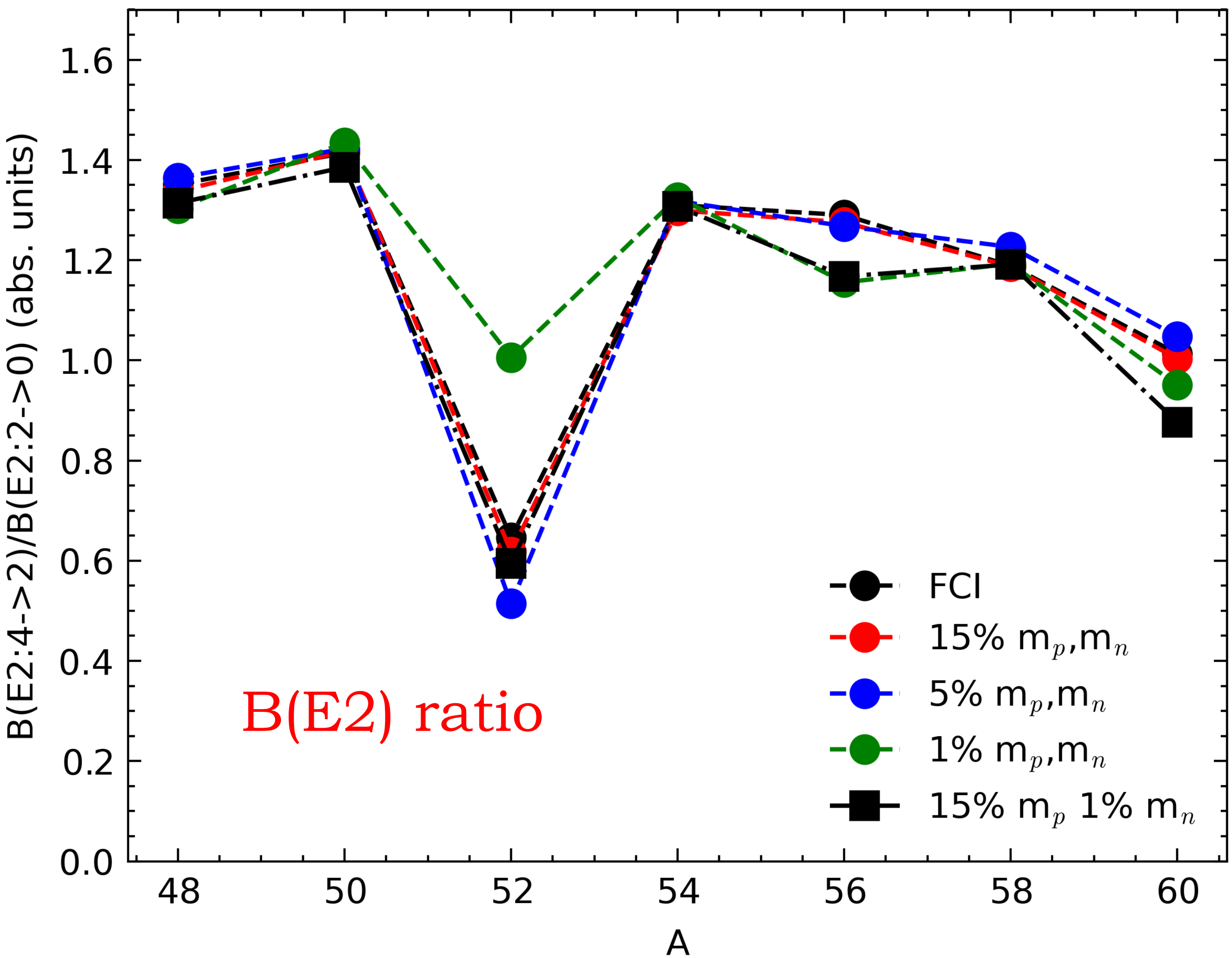


Shape transitions in chromium isotopes



This is valence space, in *pf* shell (with GX1A)

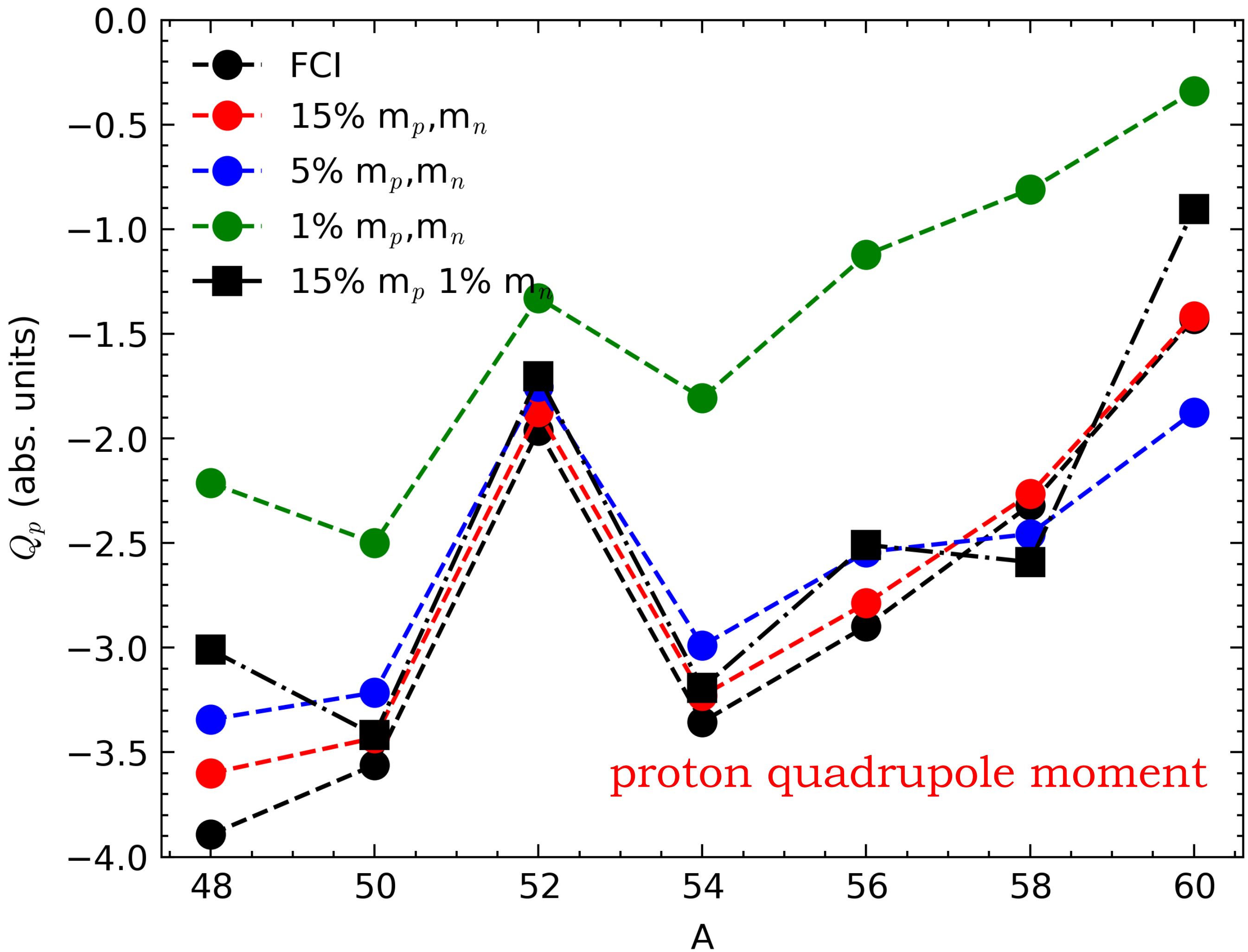
Shape transitions in chromium isotopes



This is valence space, in *pf* shell (with GX1A)

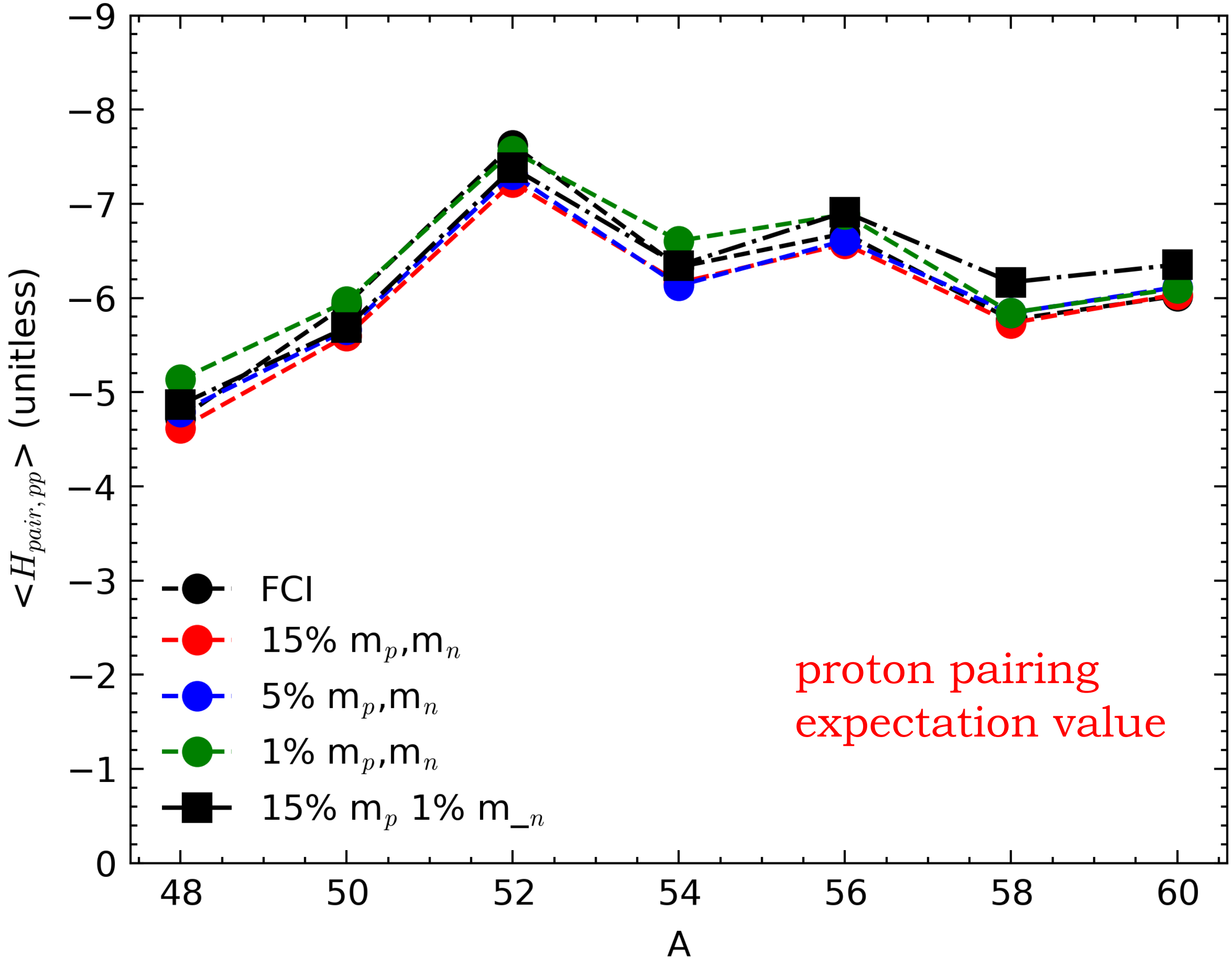
Shape transitions in chromium isotopes

SAN DIEGO STATE UNIVERSITY



This is valence space, in *pf* shell (with GX1A)

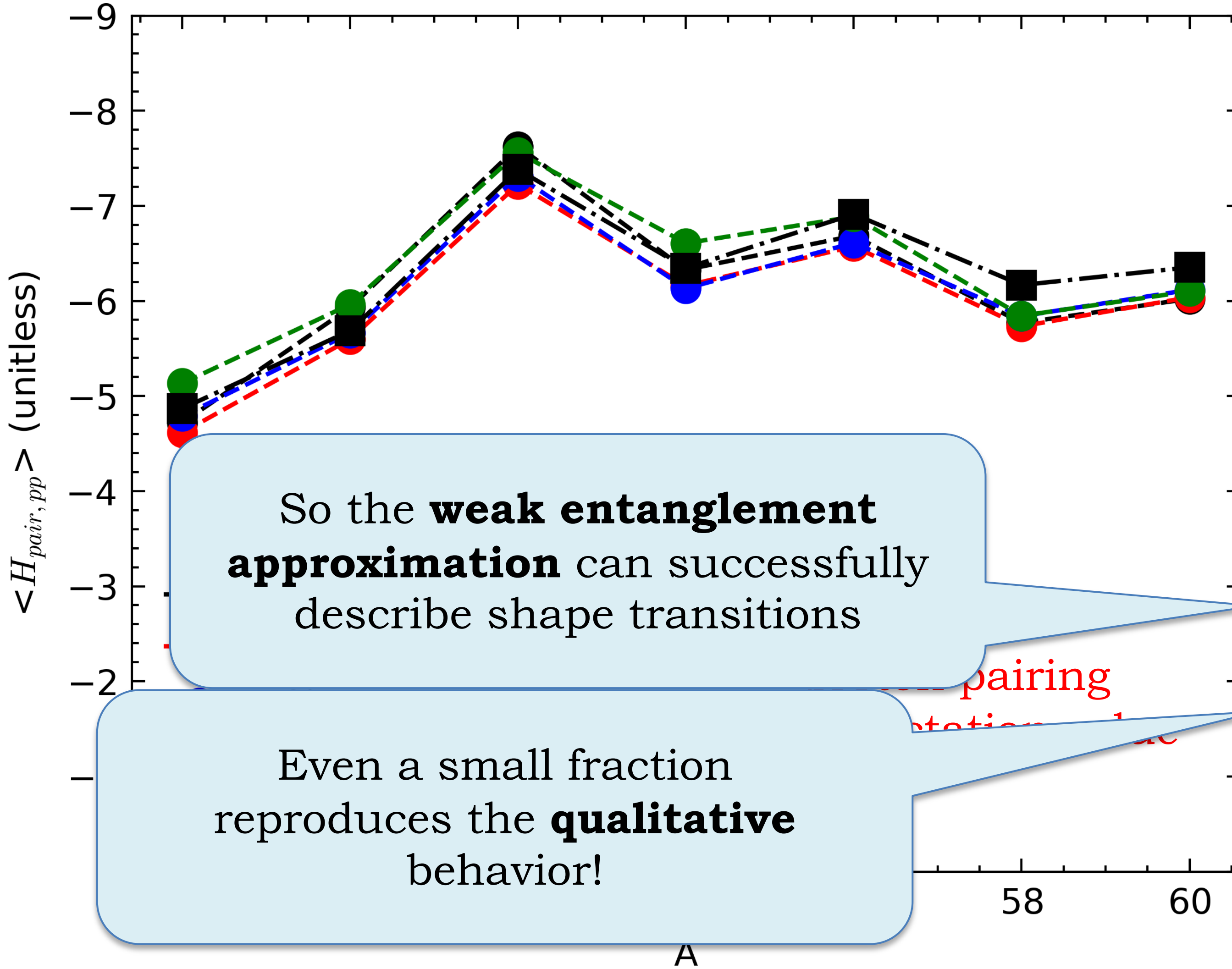
Shape transitions in chromium isotopes



This is valence space, in *pf* shell (with GX1A)

Shape transitions in chromium isotopes

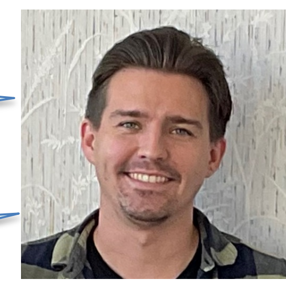
San Diego State University



This is valence space, in *pf* shell (with GX1A)

So the **weak entanglement approximation** can successfully describe shape transitions

Even a small fraction reproduces the **qualitative** behavior!



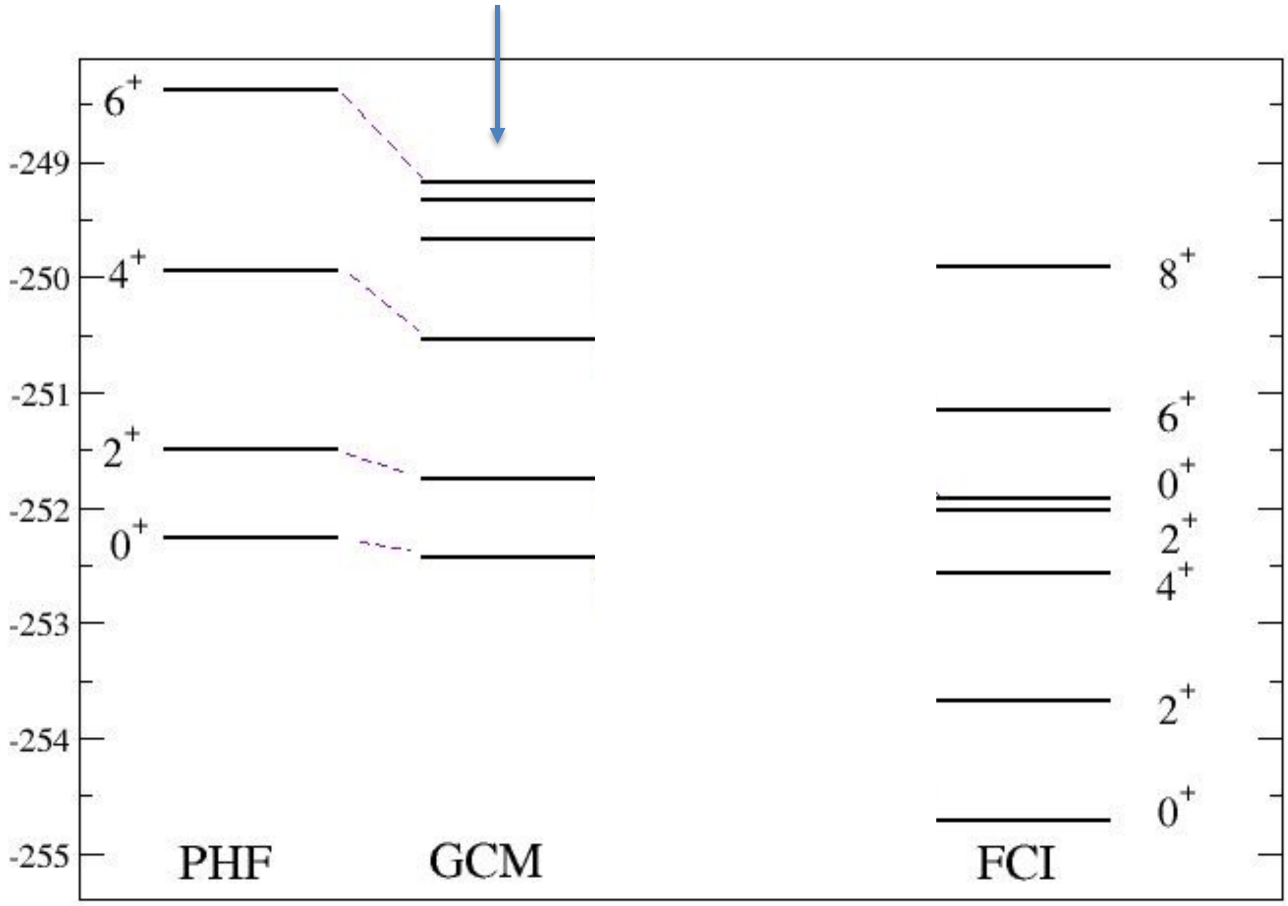
SAN DIEGO STATE UNIVERSITY

(if time….)

We can also apply these ideas to beyond-mean-field,

e.g., PHF, GCM, DNO-SM

7 reference
Slater determinants



^{60}Zn

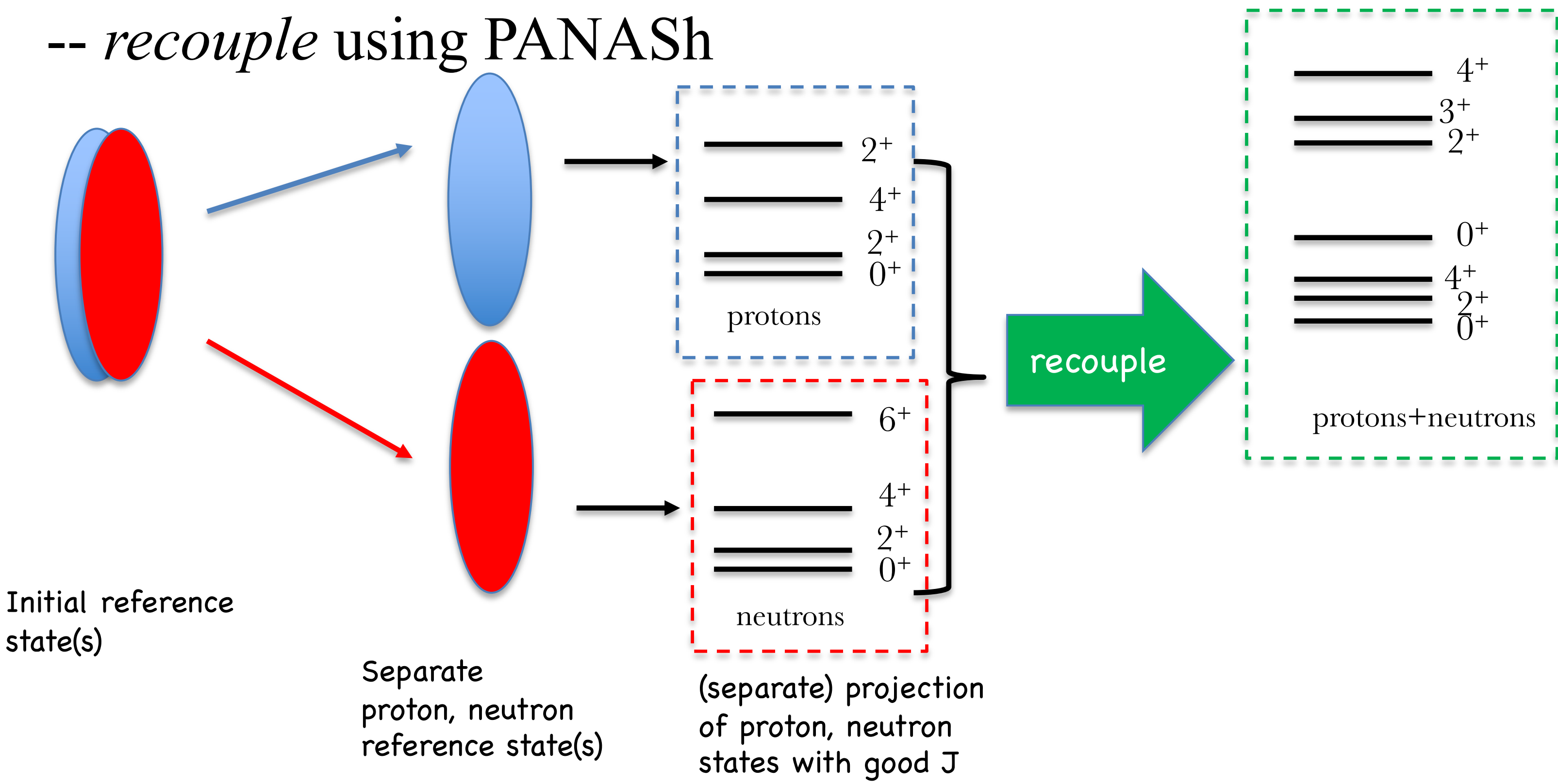
This is valence space again,
in *pf* shell (with GX1A)

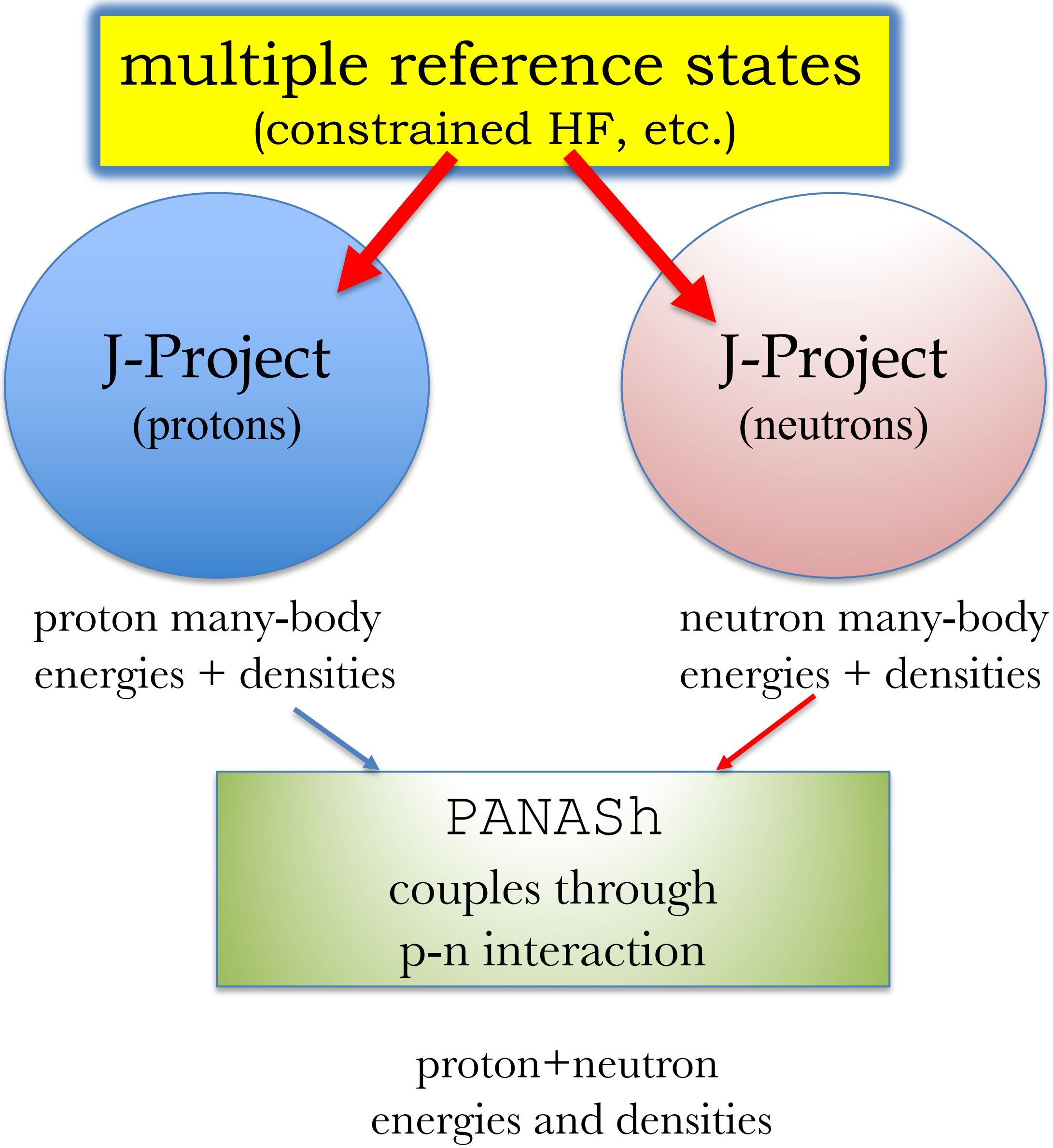
SPR:

-- *separate* proton and neutron reference states

-- *project*

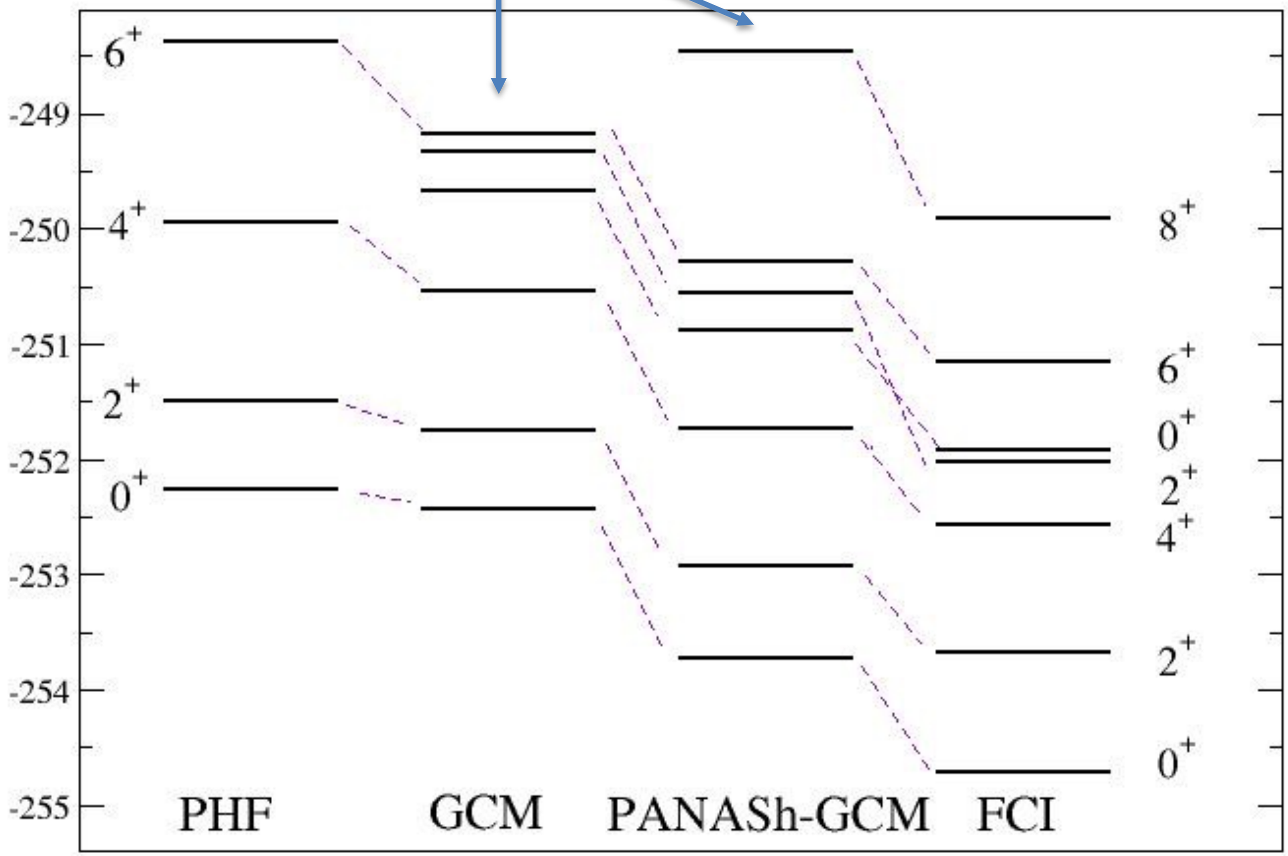
-- *recouple* using PANASh





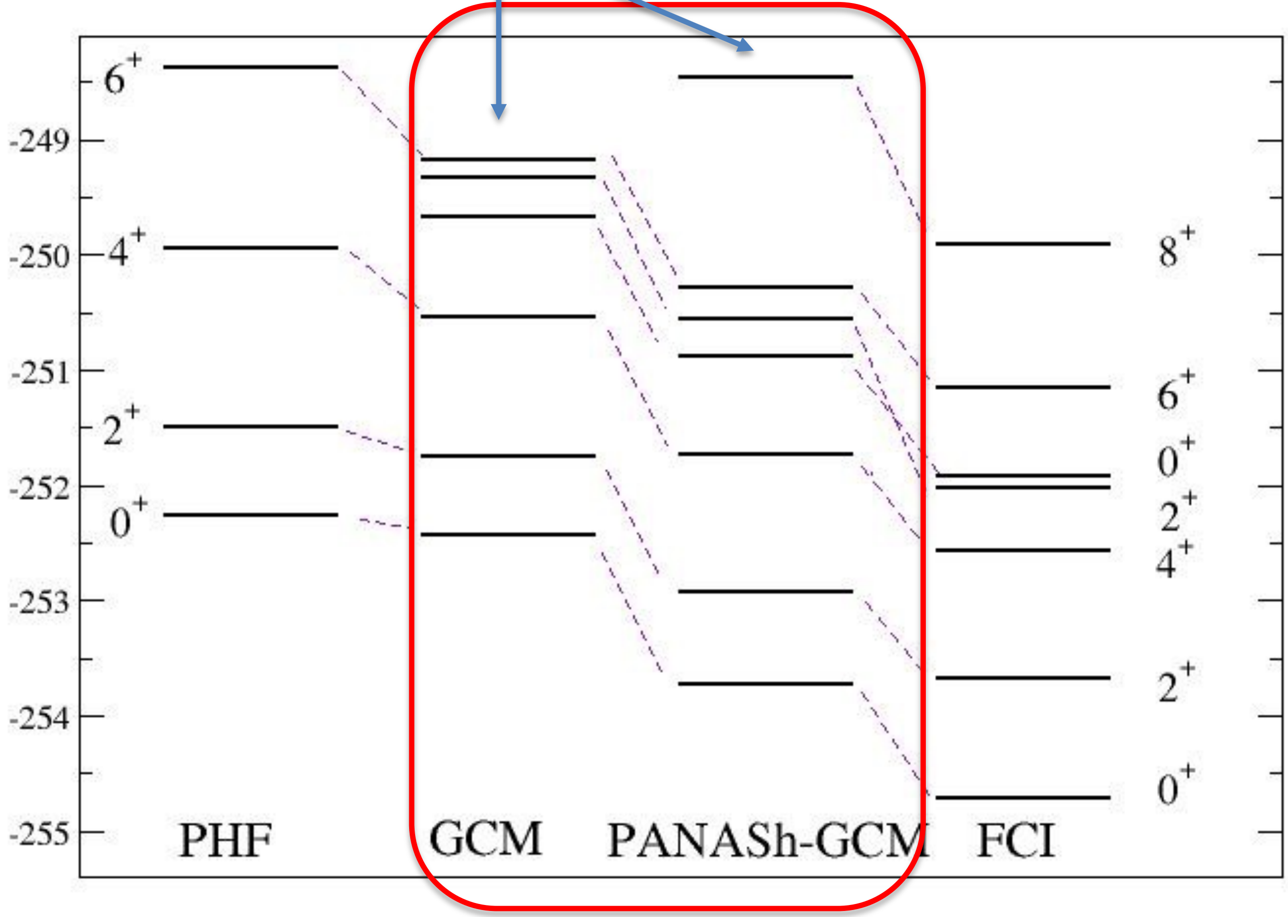
San Diego State University

7 reference
Slater determinants



^{60}Zn

7 reference
Slater determinants



^{60}Zn

Both use same set of reference states

Conclusions

SAN DIEGO STATE UNIVERSITY

- Shell-model wave functions have **weak entanglement** between proton and neutron partitions
- The ground state is dominated by low-energy components in each partition

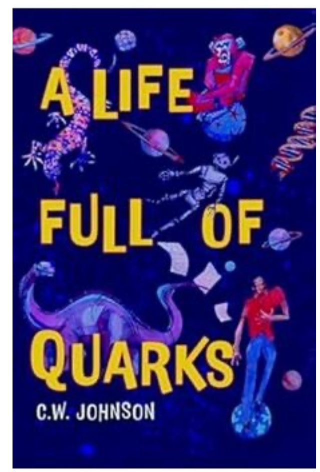
This suggests a practical "importance truncation" of the shell model

- We get a good description of low-lying spectra with a tiny fraction of the Hilbert space
- In particular, 'shape transitions' can be reproduced
- This approach can 'accelerate' GCM-like calculations

We are working on:

- Improving proton/neutron components
- Improving transitions (so far mediocre, but we understand)
- Going to larger valence spaces
- Applying to no-core calculations

Also sponsored by:



lifefullofquarks.com