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Extending the reach of the shell model

Calvin W. Johnson
Oliver C. Gorton

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by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, with support from the ACT-UP award"

TRIUMF ab initio workshop Feb 28, 2023

"It's not enough to just show up. You have to have a business plan."

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THE THEME OF THIS TALK…

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

I am interested in more than '**proof of principle**': I want '**proof of practicality**'

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Today focus on
"empirical" shell model
with an eye towards NCSM
(*ab initio)*

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

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APPLICATIONS

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- **Dark matter targets**: some targets for dark matter (e.g. ^{40}Ar) are in very large model spaces. (Similarly for neutrino targets)

* **Beta decays**: beta-delayed neutron emission in fission fragments (with Escher at LLNL); independently, look at beta decays of neutron-rich nuclides relevant to FRIB.

* **Hadronic parity violation**: Experimental measurement of the anapole moment in heavy nuclides is underway (D. DeMille et al; Also TRIUMF's RadMol experiment)

* **Inputs for reactions in medium to heavy nuclei**, including spectroscopic factors.

THE "SHELL MODEL"

A.K.A., CONFIGURATION-INTERACTION

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We want to solve *Schrödinger's equation*:

$$\left(\sum_i -\frac{\hbar^2}{2m}\nabla^2 + U(r_i) + \sum_{i<j} V(\vec{r}_i - \vec{r}_j)\right)\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3\ldots) = E\Psi$$

but as a matrix equation

$$\hat{\mathbf{H}}\left|\Psi\right\rangle = E\left|\Psi\right\rangle$$

The matrix formalism:
expand in some (many-body) basis

$$\hat{\mathbf{H}}\left|\Psi\right\rangle = E\left|\Psi\right\rangle$$

$$\left|\Psi\right\rangle = \sum_{\alpha} c_{\alpha}\left|\alpha\right\rangle \qquad H_{\alpha\beta} = \left\langle\alpha\left|\hat{\mathbf{H}}\right|\beta\right\rangle$$

$$\sum_{\beta} H_{\alpha\beta} c_{\beta} = E c_{\alpha}$$

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$$\sum_{\beta} H_{\alpha\beta} c_{\beta} = E c_{\alpha}$$

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Choice of wave function basis

That's because the subgroup for J_z is abelian

M-scheme: basis states with fixed total J_z

Simple and easy to construct/work with

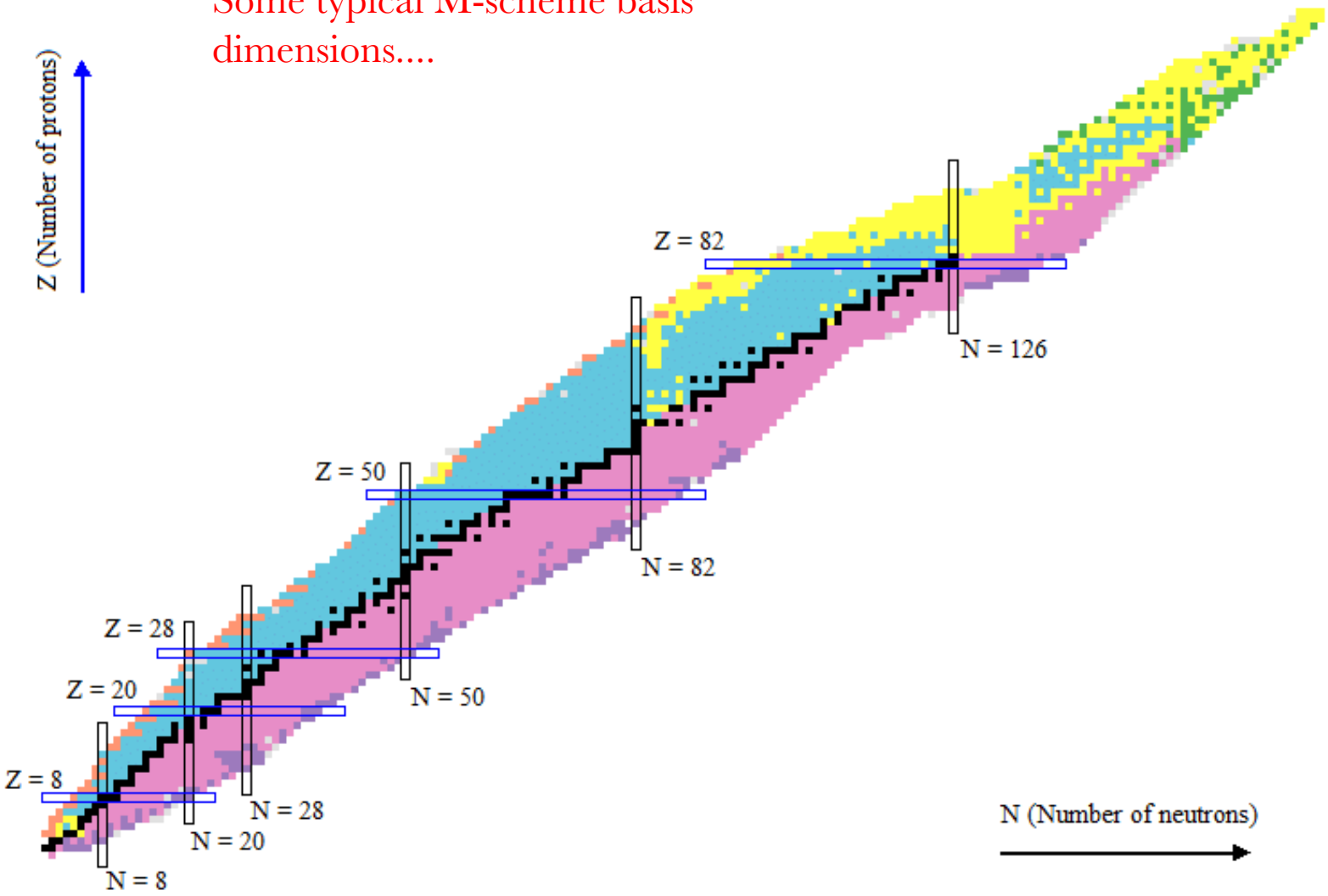
One can make each "Slater determinant" have good M

Requires large dimension basis

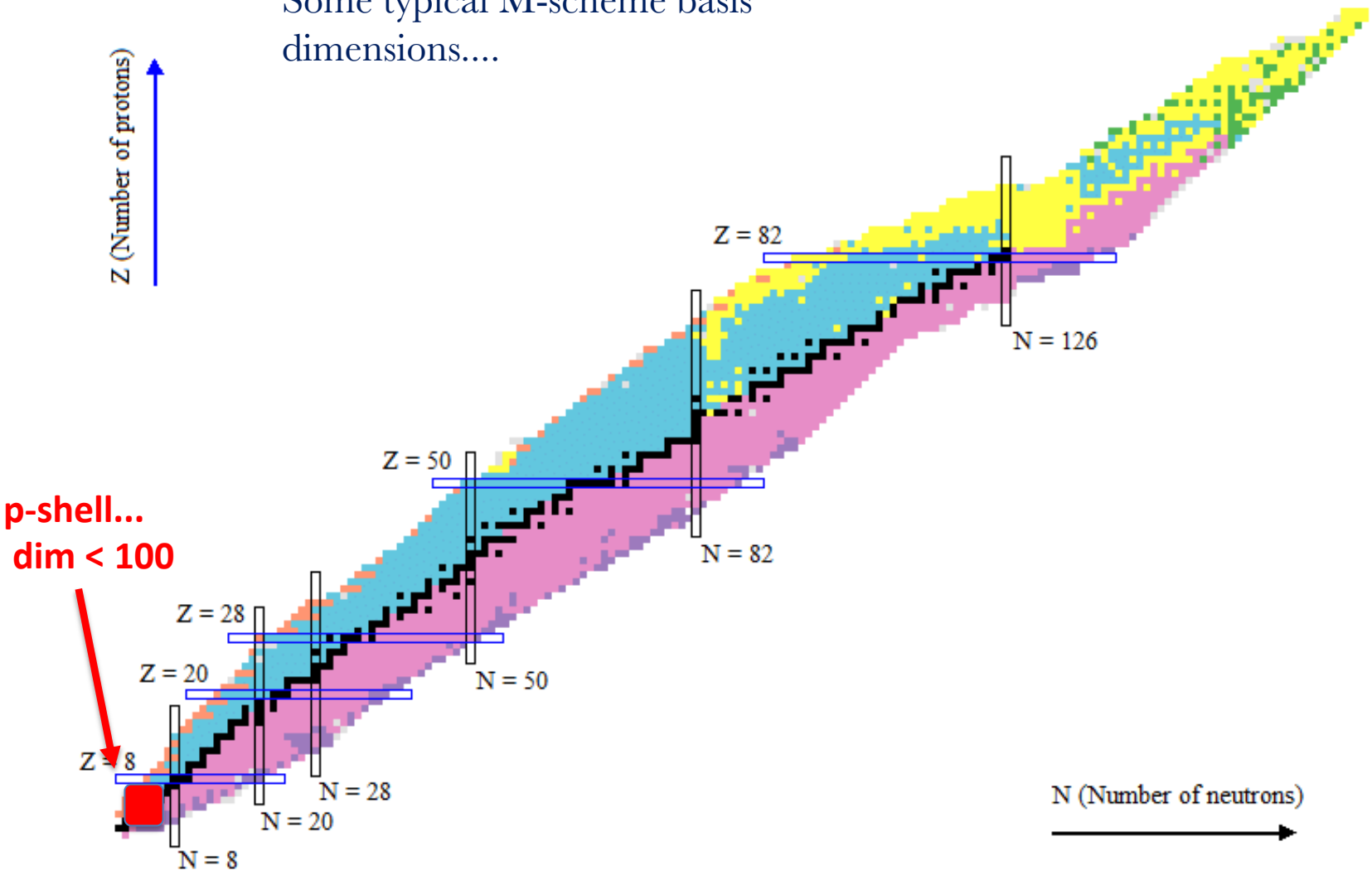
n_i	1	2	3	4	5	6	7
α=1	1	0	0	1	1	0	1
α=2	1	0	1	0	0	1	1
α=3	0	1	1	1	0	1	0

Eugene Wigner

Each of these single-particle states have a fixed value of 'm' and one obtains total 'M' by just summing

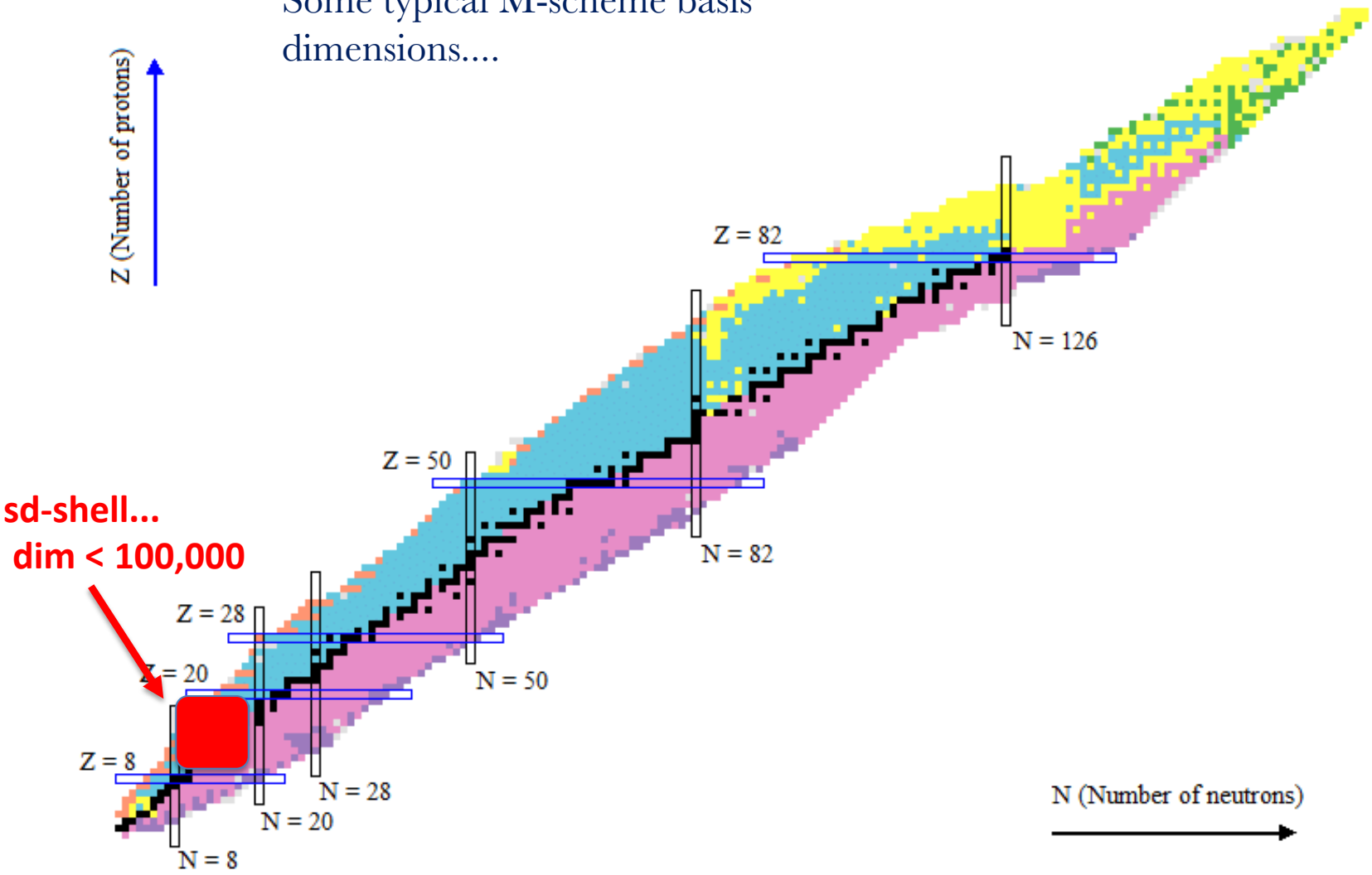

Some typical M-scheme basis dimensions....
Z (Number of protons)
Z = 82
N = 126
Z = 50
N = 82
Z = 28
Z = 20
N = 50
Z = 8
N = 28
N = 20
N = 8
N (Number of neutrons)

Some typical M-scheme basis dimensions....



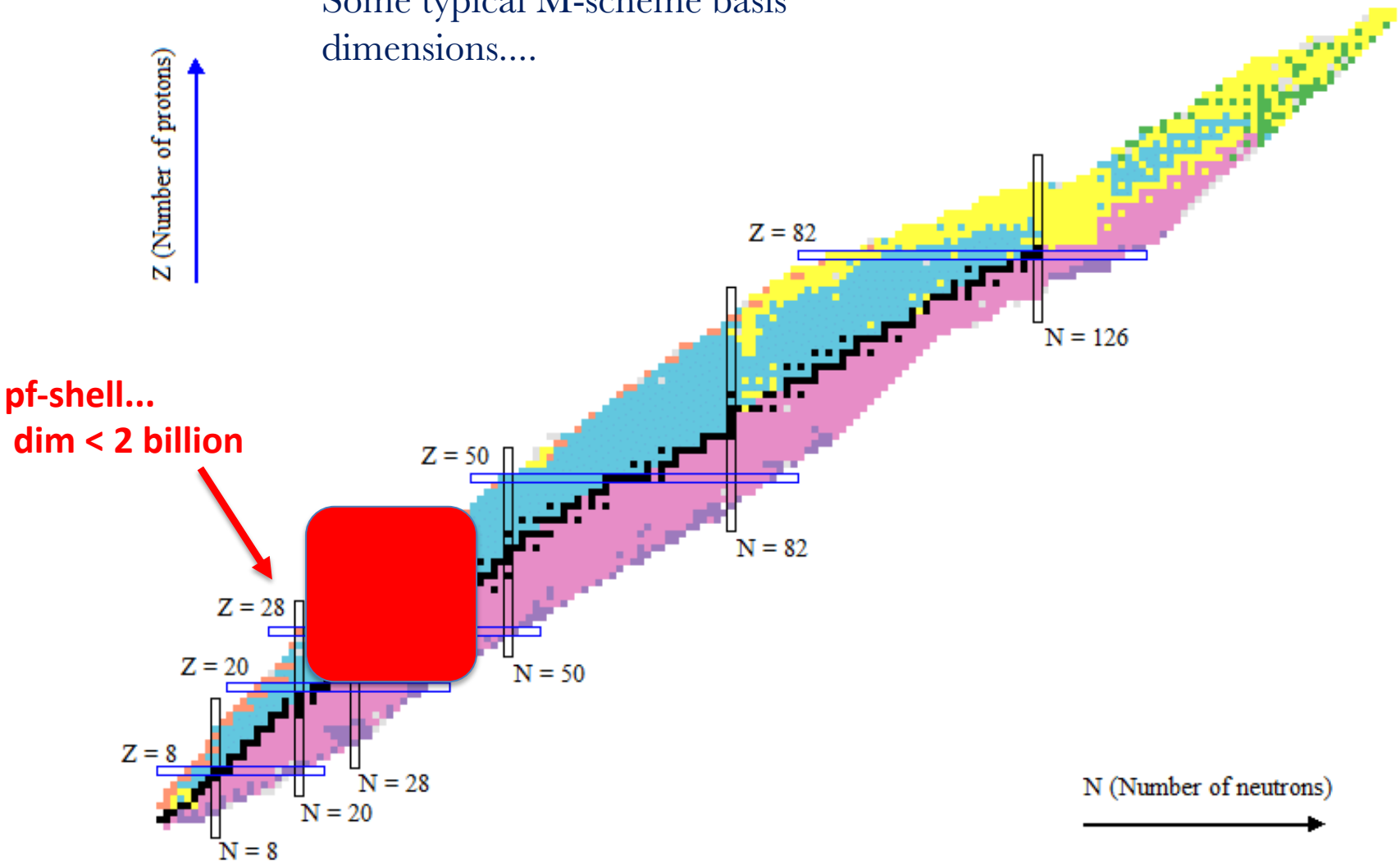
p-shell...
dim < 100

Some typical M-scheme basis dimensions....



sd-shell...
dim < 100,000

Some typical M-scheme basis dimensions....



pf-shell...
dim < 2 billion

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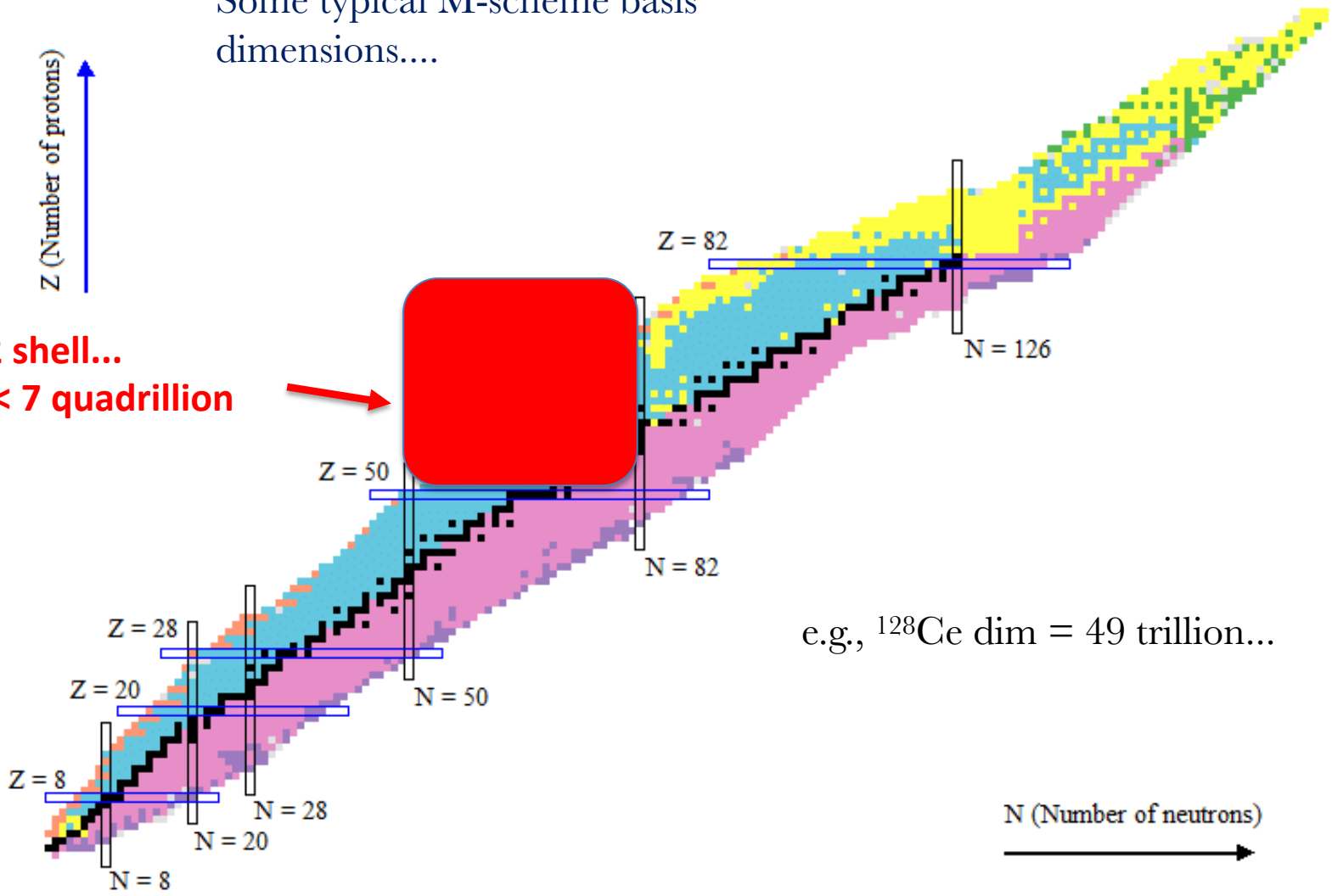
Some typical M-scheme basis dimensions....



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

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A sampling menu of dimensionalities

^{12}C N_{max} = 4 dim 1 million

^{12}C N_{max} = 6 dim 30 million

^{12}C N_{max} = 8 dim 500 million

^{12}C N_{max} = 10 dim 7.8 billion

^{12}C N_{max} = 12 dim 81 billion

Largest (?) known calculation, ^{6}Li, N_{max}=22, **25 billion**

(Forssen *et al*, PRC **97**, 034328 (2018). with `pANTOINE`)

A Problem….

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Despite sparsity, nonzero matrix elements can require TB of storage

Nuclide	Space	Basis dim	matrix store
^{56}Fe	*pf*	501 M	3.5 Tb
^{7}Li	N_{max}=12	252 M	3.6 Tb
^{7}Li	N_{max}=14	1200 M	23 Tb
^{12}C	N_{max}=6	32M	0.2 Tb
^{12}C	N_{max}=8	590M	5 Tb
^{12}C	N_{max}=10	7800M	111 Tb
^{16}O	N_{max}=6	26 M	0.14 Tb
^{16}O	N_{max}=8	990 M	9.7 Tb

Possible solution:

Spread nonzero matrix elements over many MPI compute nodes

(i.e., code MFDn by J. Vary et al.)

A Problem….

San Diego State University

Despite sparsity, nonzero matrix elements can require TB of storage

So, are we stuck running on a supercomputer?
Just to store the matrix?

			matrix store
			3.5 Tb
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Li	N_{max}=14	1200 M	23 Tb
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Not necessarily!

…ic
…spread nonzero matrix elements over many MPI compute nodes

(i.e., code MFDn by J. Vary et al.)

A Problem….

San Diego State University

Despite sparsity, nonzero matrix elements can require TB of storage

So, are we stuck running on a supercomputer? Just to store the matrix?

Not necessarily!

"Divide-and-conquer"

that is, break problem into smaller, easier pieces and solve each separately

			matrix store
			3.5 Tb
			3.6 Tb
Li	N_{max}=14	1200 M	23 Tb
^{12}C	N_{max}=6		
^{12}C	N_{max}=8		
^{12}C	N_{max}=10		
^{16}O	N_{max}=6		
^{16}O	N_{max}=8	990 M	9.7 Tb

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

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

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

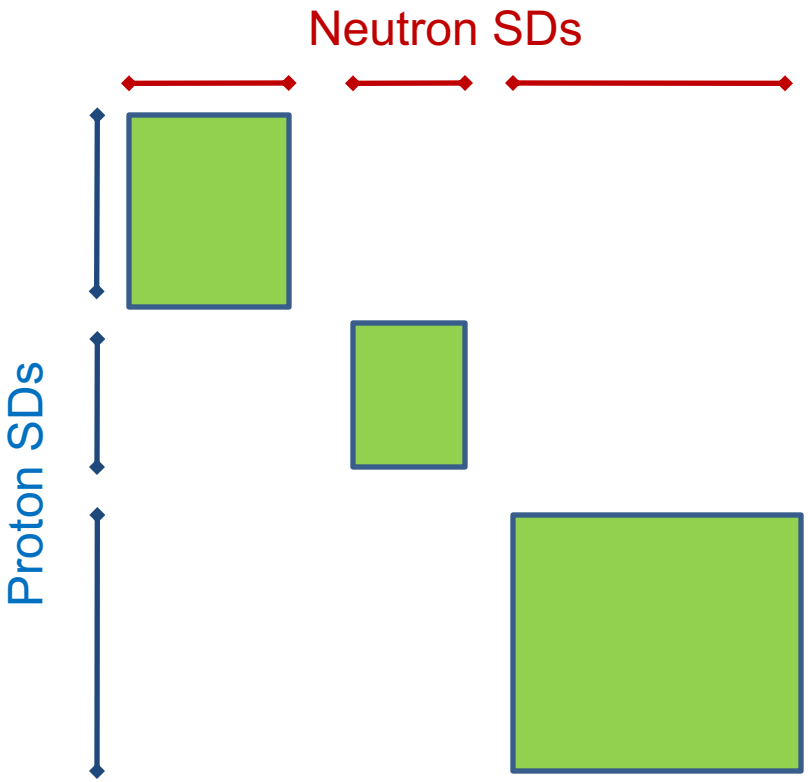
$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

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

FACTORIZATION

Reuse can be **exploited using exact factorization**
enforced through *additive/multiplicative quantum numbers*

$$|\alpha\rangle = |\alpha_p\rangle \times |\alpha_n\rangle$$



Example N = Z nuclei

Nuclide	Basis dim	# pSDs (=#nSDs)
^{20}Ne	640	66
^{24}Mg	28,503	495
^{28}Si	93,710	924
^{48}Cr	1,963,461	4895
^{52}Fe	109,954,620	38,760
^{56}Ni	1,087,455,228	125,970

SOME SHELL-MODEL CODES

Matrix storage:

Oak Ridge-Rochester (small matrices)

Glasgow-Los Alamos (M-scheme, stored on disk; introduced Lanczos)

OXBASH /Oxford-MSU (J-scheme, stored on disk)

MFDn/ Iowa State (M-scheme, stored in RAM)

MCSM/ Tokyo (J-scheme from selected states)

Importance Truncation SM/Darmstadt (M-scheme from selected states)

Sym Adapted SM / LSU

Factorization/on-the-fly:

ANTOINE Strasbourg (M-scheme; originator of on-the-fly)

NATHAN Strasbourg (J-scheme)

NuShell/NuShellX (J-scheme)

MSHELL64 / KSHELL Tokyo (M-scheme)

BIGSTICK/ LSU-SDSU-Livermore

The BIGSTICK public shell-model code!

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Download from: github.com/cwjsdsu/BigstickPublick

Manual at arXiv:1801.08432

Authors: CWJ, Erich Ormand, K. McElvain, H.Z. Shan, R. Zbikowski

Uses "factorization" algorithm: Johnson, Ormand, and Krastev, Comp. Phys. Comm. 184, 2761(2013)

Runs on both desktop and parallel machines

--can run at least dimension 300M+ on desktop

--has done *dimension 20 billion*+ on supercomputers

FACTORIZATION

STATE
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Reuse can be **exploited using exact factorization**
enforced through *additive/multiplicative quantum numbers*

Comparison of nonzero matrix storage with factorization

Nuclide	Space	Basis dim	matrix store	factorization
^{56}Fe	*pf*	501 M	3500 Gb	0.72 Gb
^{7}Li	N_{max}=12	252 M	3800 Gb	61 Gb
^{7}Li	N_{max}=14	1200 M	23 Tb	624 Gb
^{12}C	N_{max}=6	32M	196 Gb	3.3 Gb
^{12}C	N_{max}=8	590M	5000 Gb	65 Gb
^{12}C	N_{max}=10	7800M	111 Tb	1.4 Tb
^{16}O	N_{max}=6	26 M	142 Gb	3.0 Gb
^{16}O	N_{max}=8	990 M	9700 Gb	130 Gb

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

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

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

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

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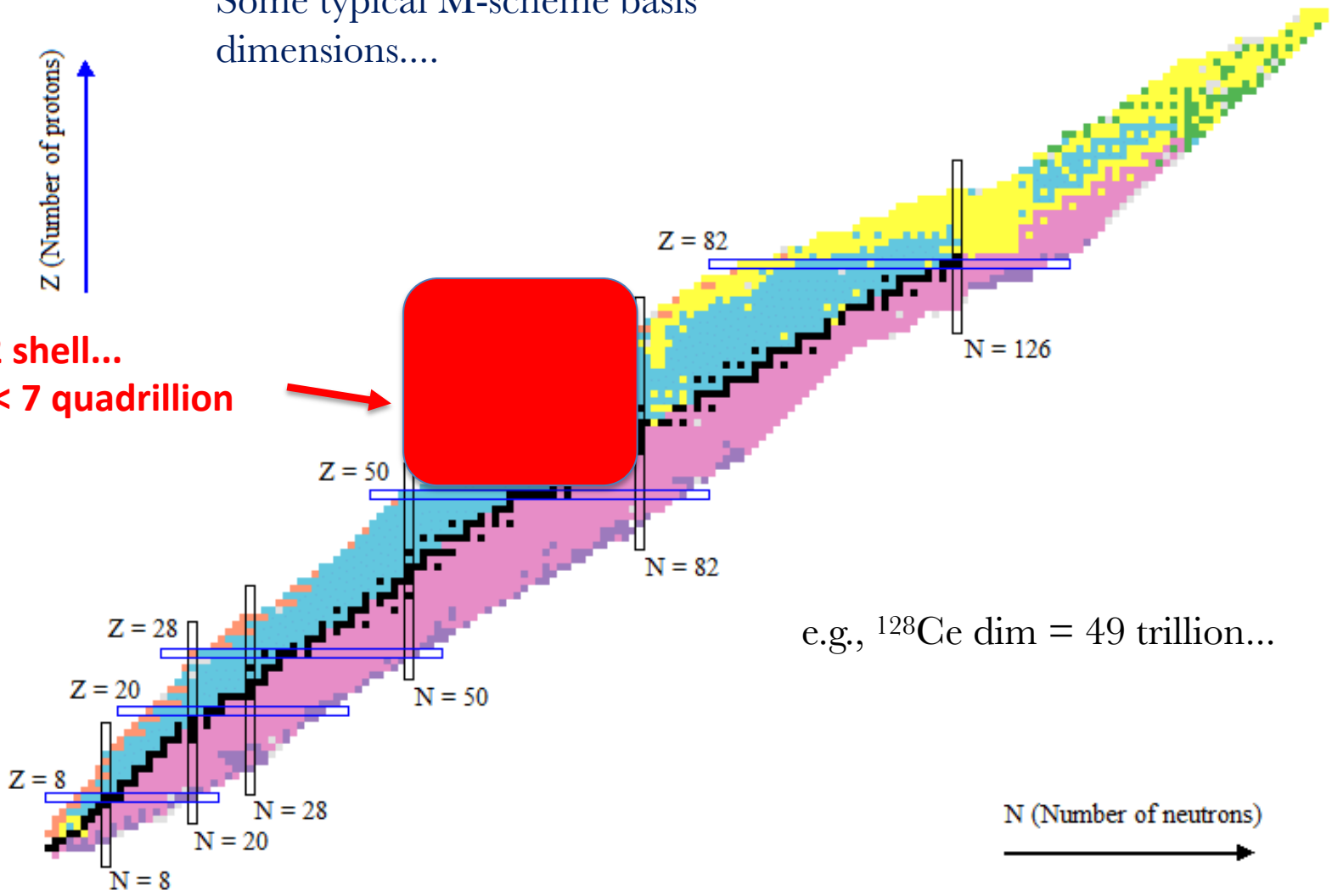
Some typical M-scheme basis dimensions....



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

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It is easy to get to model spaces beyond our reach:

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

^{128}Te: dim 13 million (laptop)

^{127}I: dim 1.3 billion (small supercomputer)

^{128}Xe: dim 9.3 billion (supercomputer)

^{129}Cs: dim 50 billion (haven't tried!)

^{130}Ba: dim 200 billion!!

^{128}Ce: dim 49 trillion!!!

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?

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

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

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

No longer single “Slater determinants” but linear combinations…

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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)

Why we think this could work:
Decompose full wfn into proton, neutron components

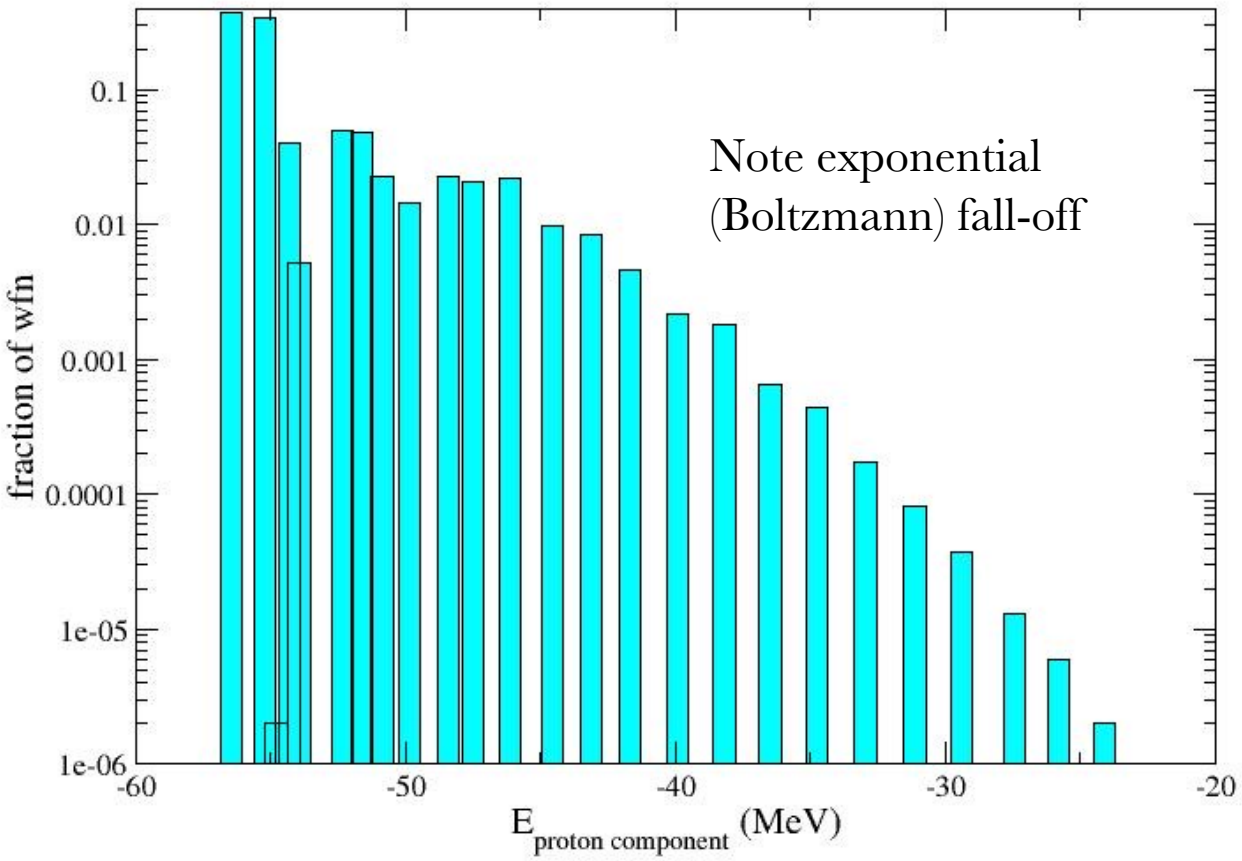
$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

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

(one can compute this very efficiently with the Lanczos algorithm, using just the **proton part of the full Hamiltonian**)

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

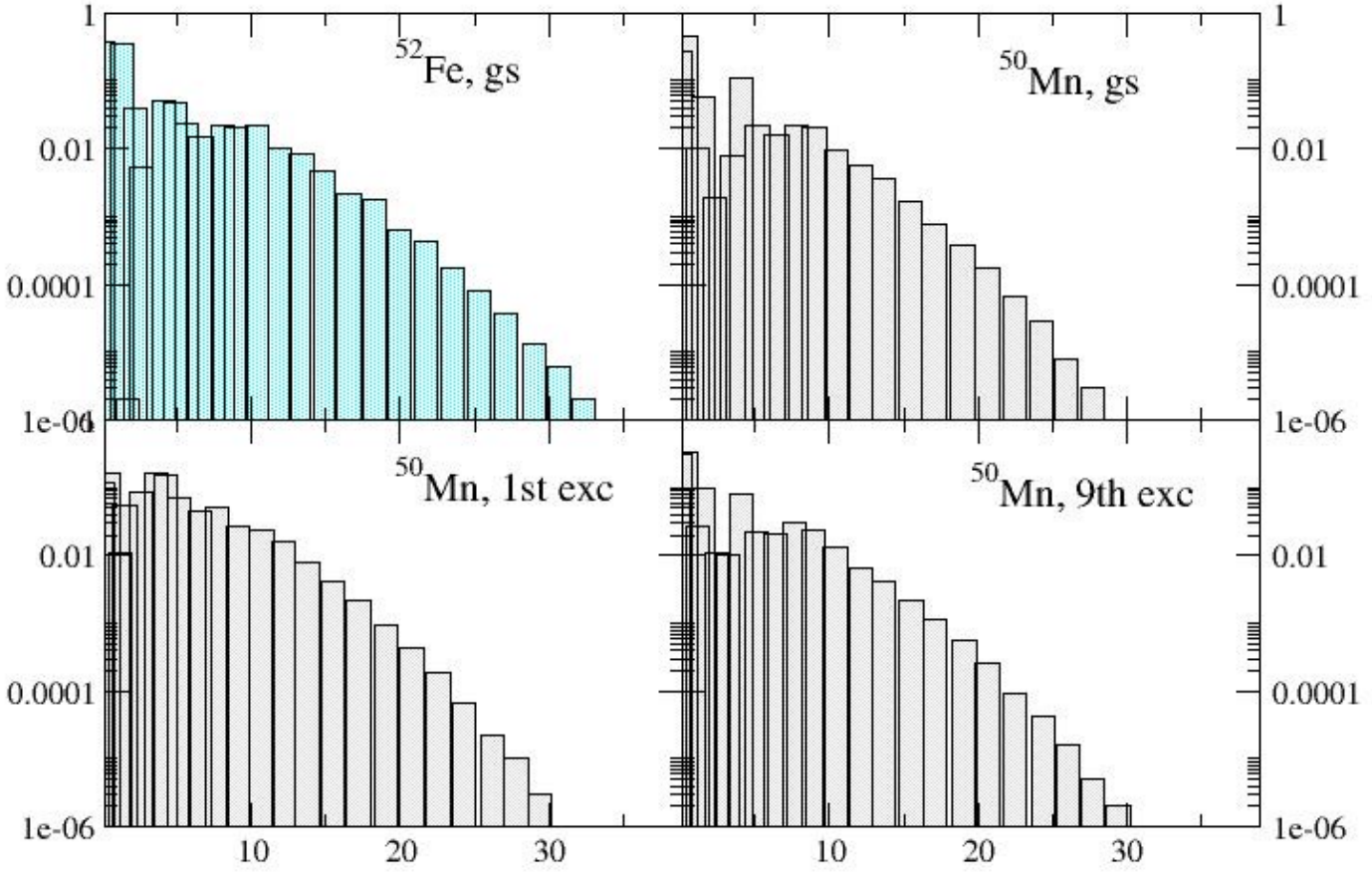
decomposition of g.s.



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

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Example application:

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

^{129}Cs: M-scheme dim 50 billion (haven't tried!)

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

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

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

Oliver Gorton

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Oliver Gorton

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BIGSTICK (protons)

BIGSTICK (neutrons)

proton many-body energies + densities

neutron many-body energies + densities

PANASh couples through p-n interaction

proton+neutron energies and densities

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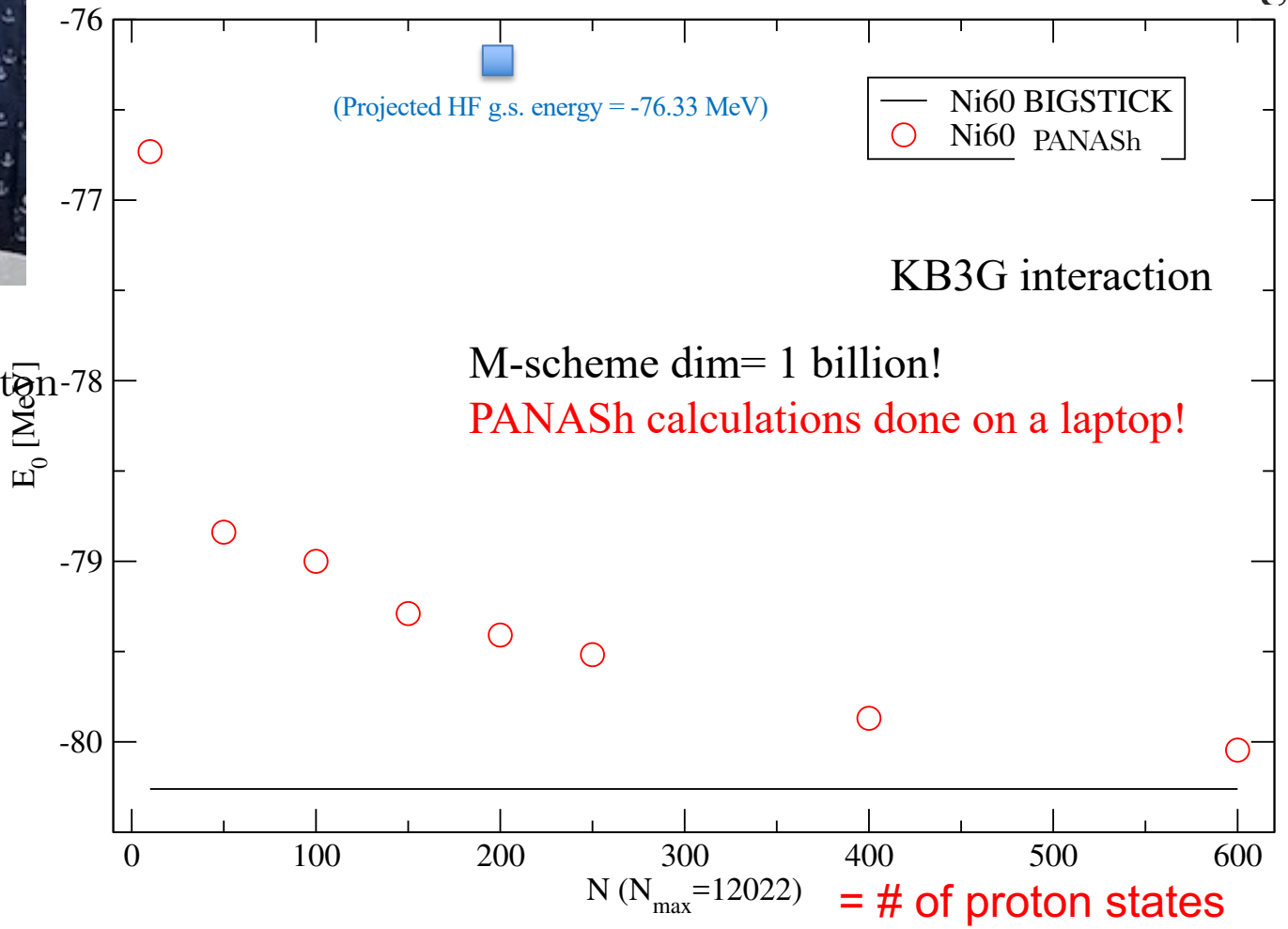
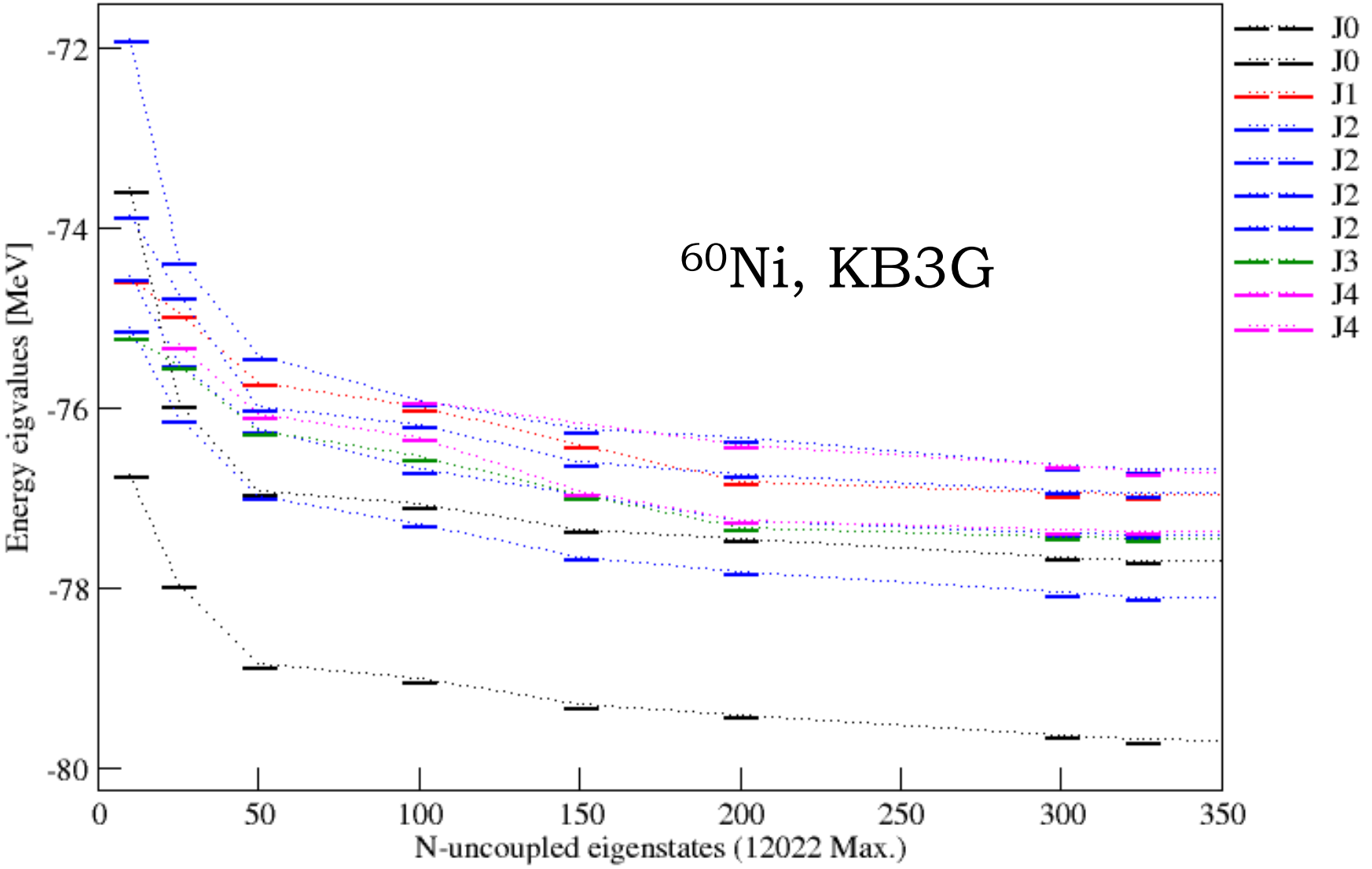
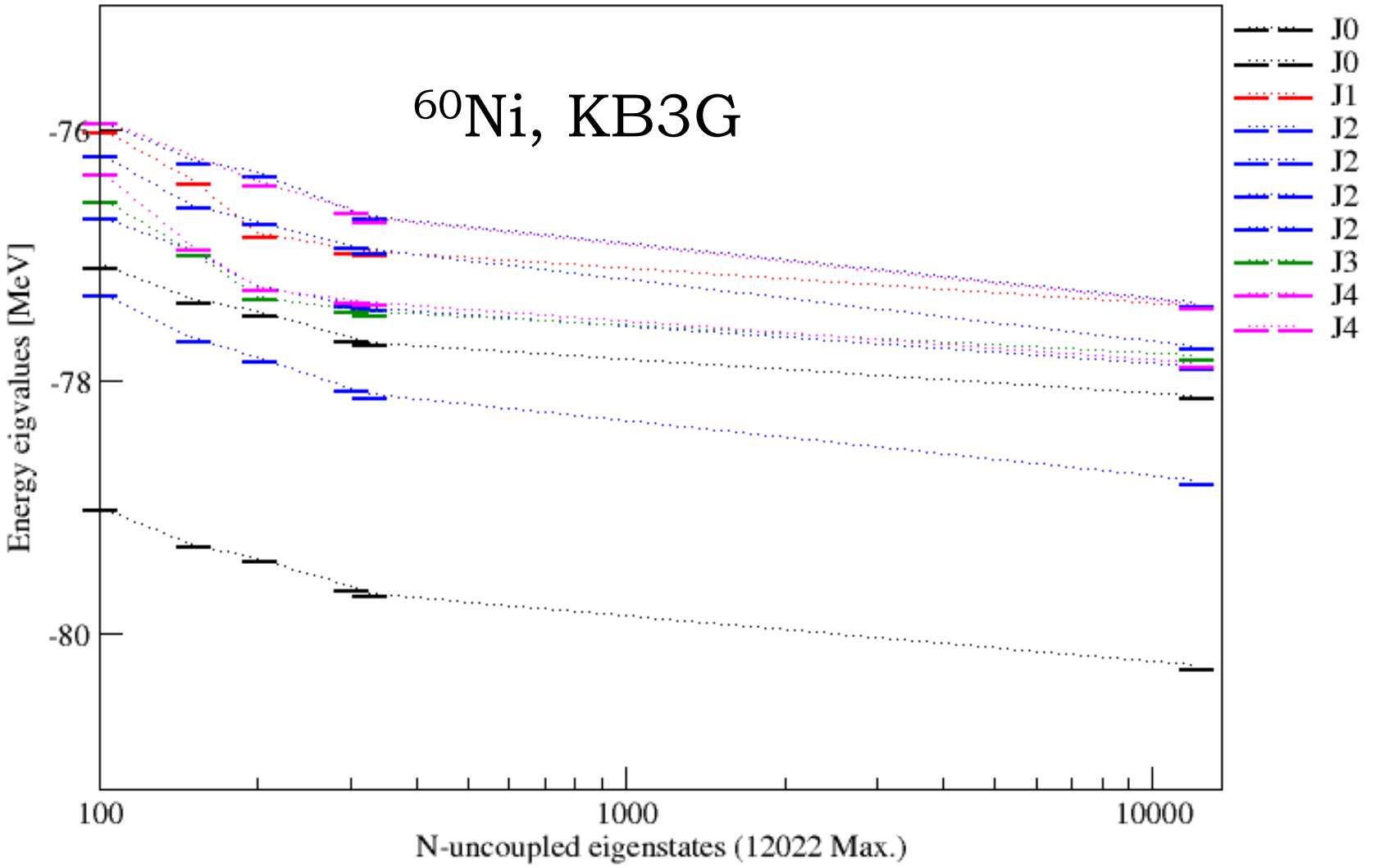
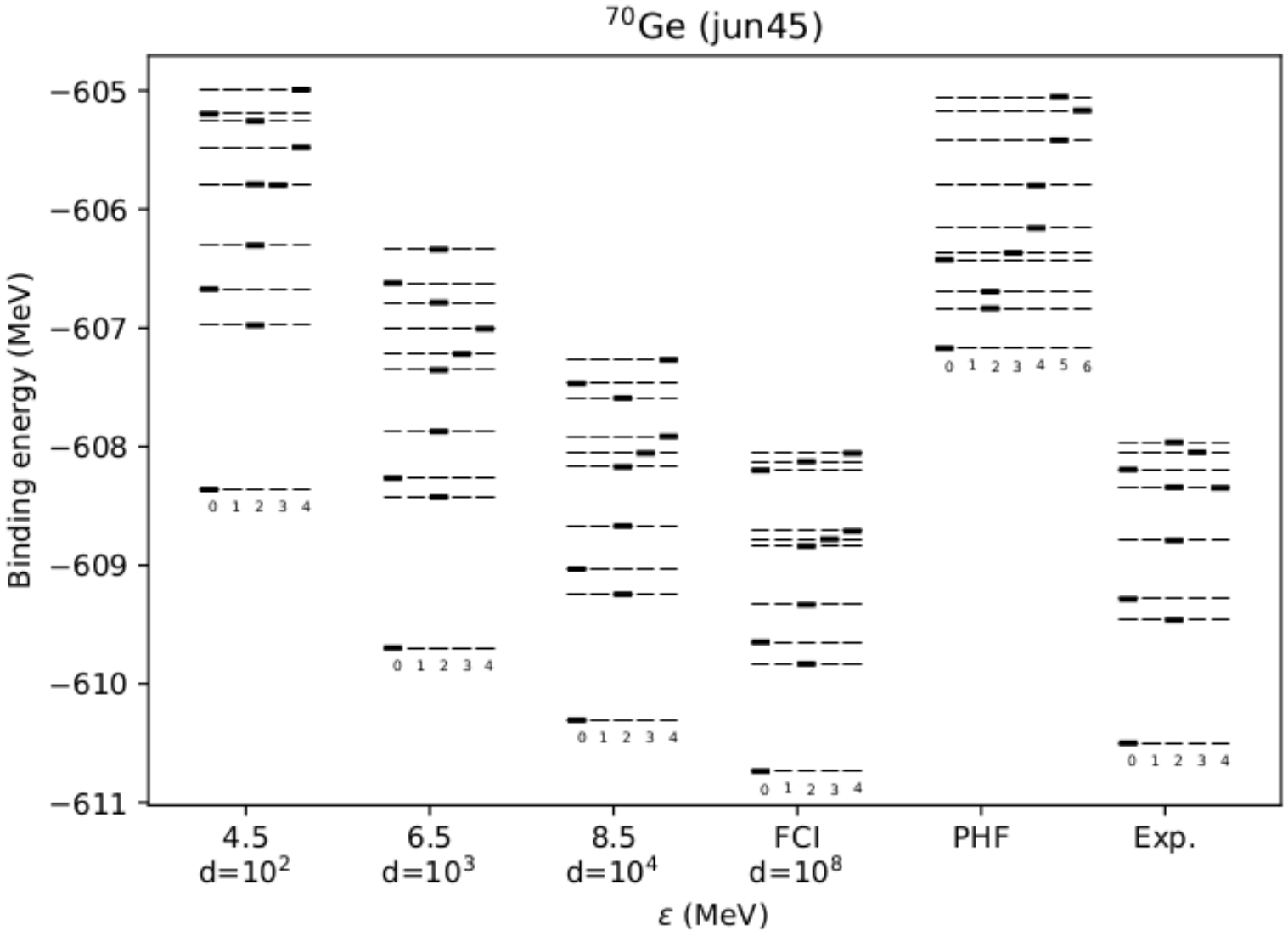
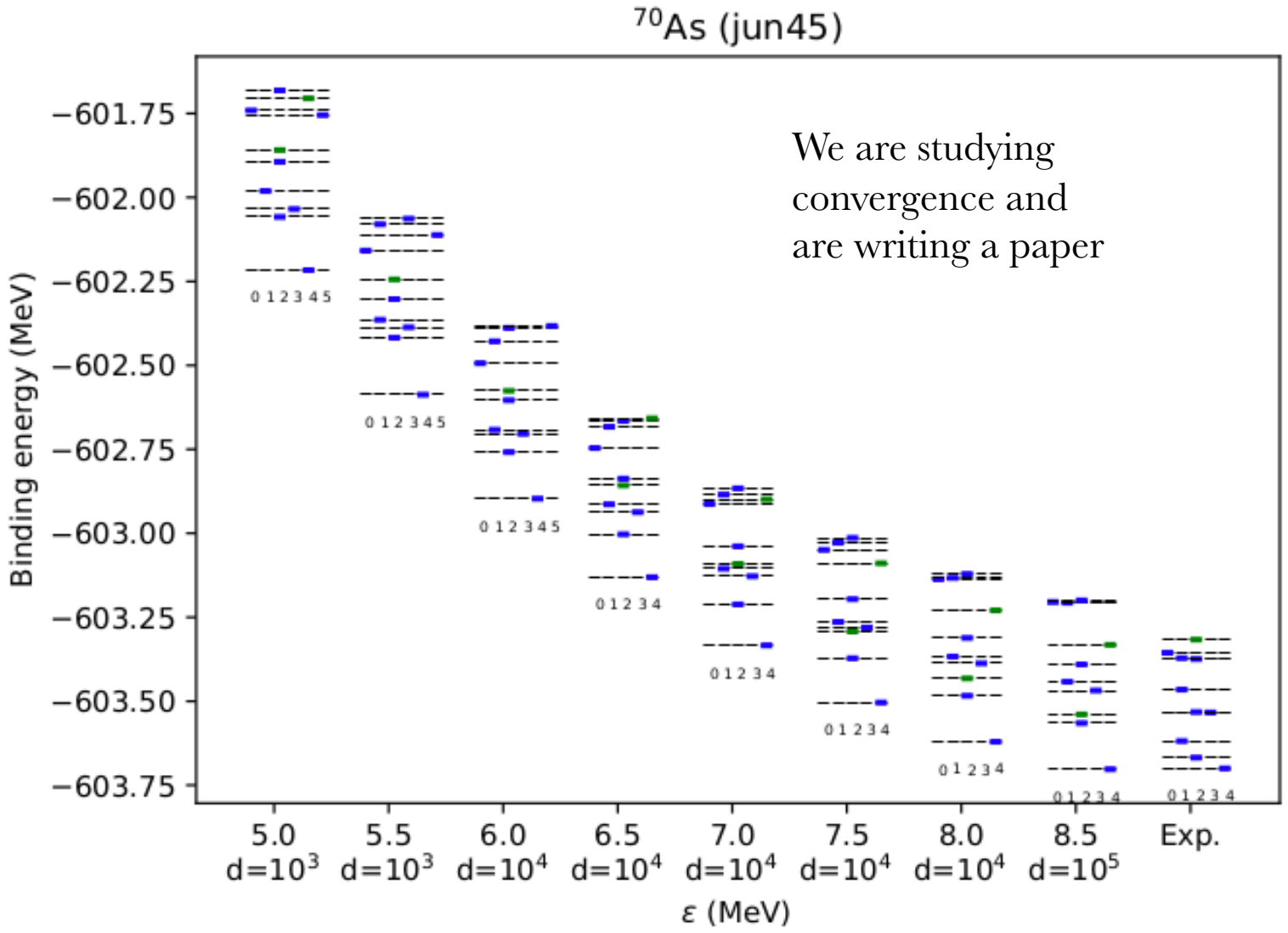
Oliver Gorton




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

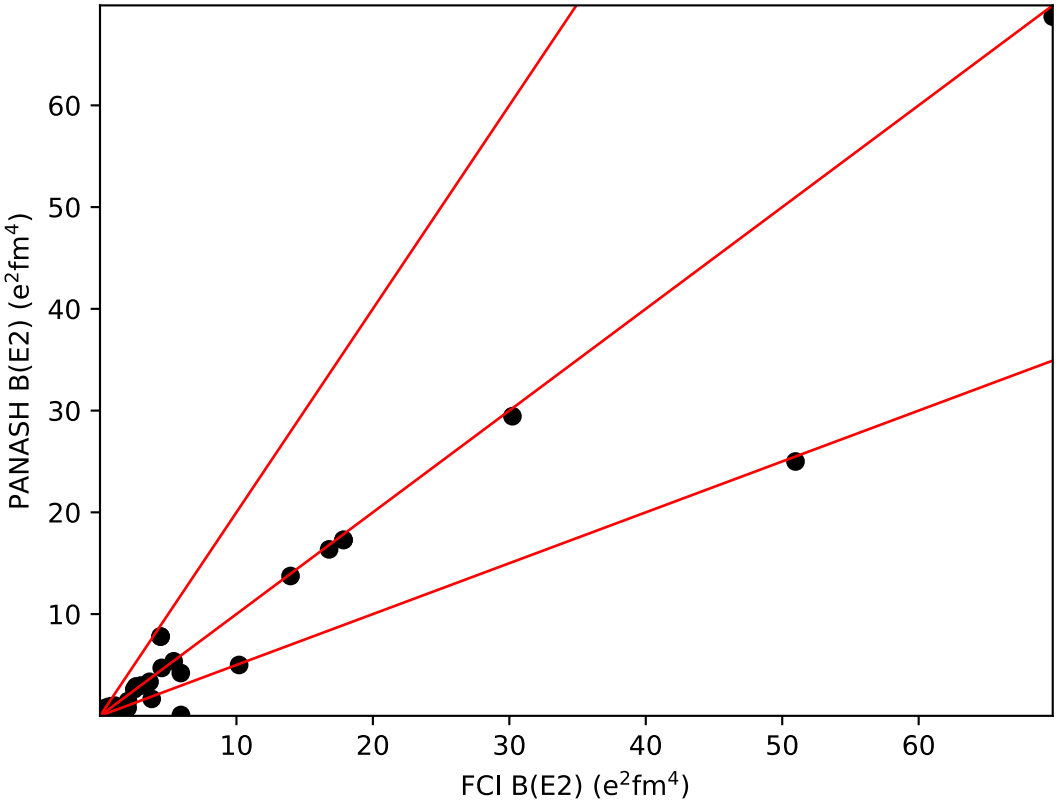

^{60}Ni, KB3G
Energy eigvalues [MeV]
-76
-78
-80
100
1000
10000
N-uncoupled eigenstates (12022 Max.)
J0
J0
J1
J2
J2
J2
J2
J3
J4
J4


^{70}Ge (jun45)
Binding energy (MeV)
−605
−606
−607
−608
−609
−610
−611
0 1 2 3 4
0 1 2 3 4
0 1 2 3 4
0 1 2 3 4
0 1 2 3 4 5 6
0 1 2 3 4
4.5
d=10^2
6.5
d=10^3
8.5
d=10^4
FCI
d=10^8
PHF
Exp.
ε (MeV)



We are studying convergence and are writing a paper

We can also compute EM and weak transitions



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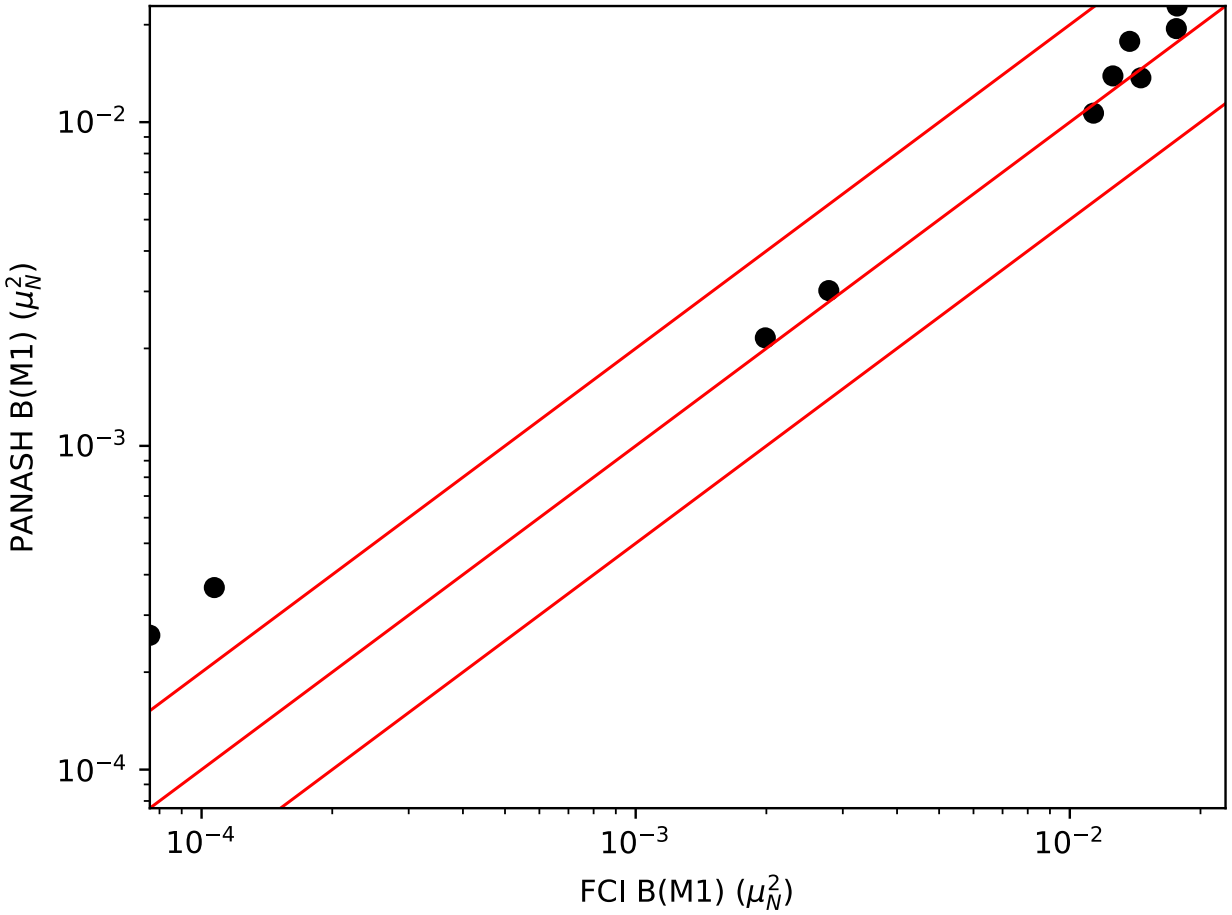
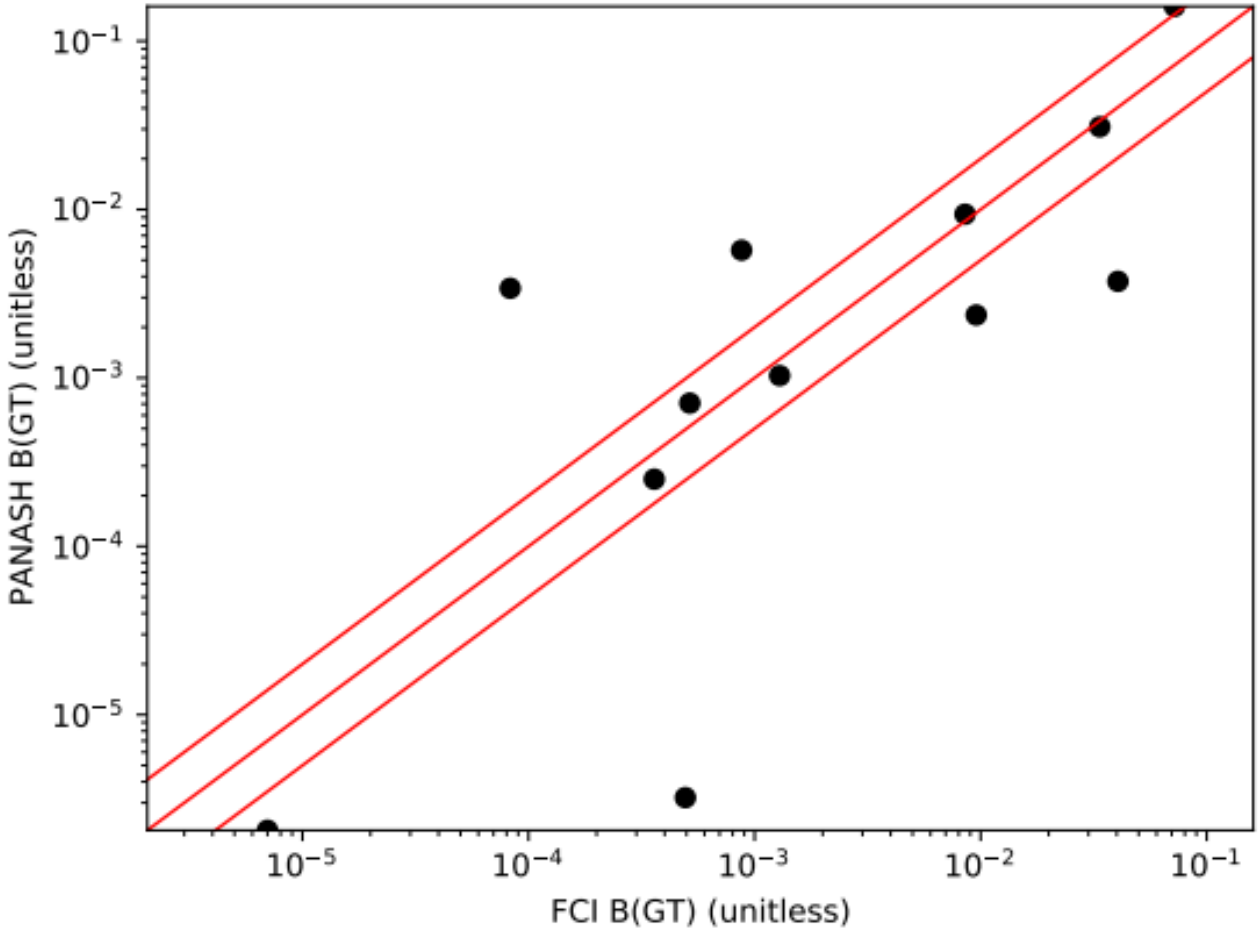
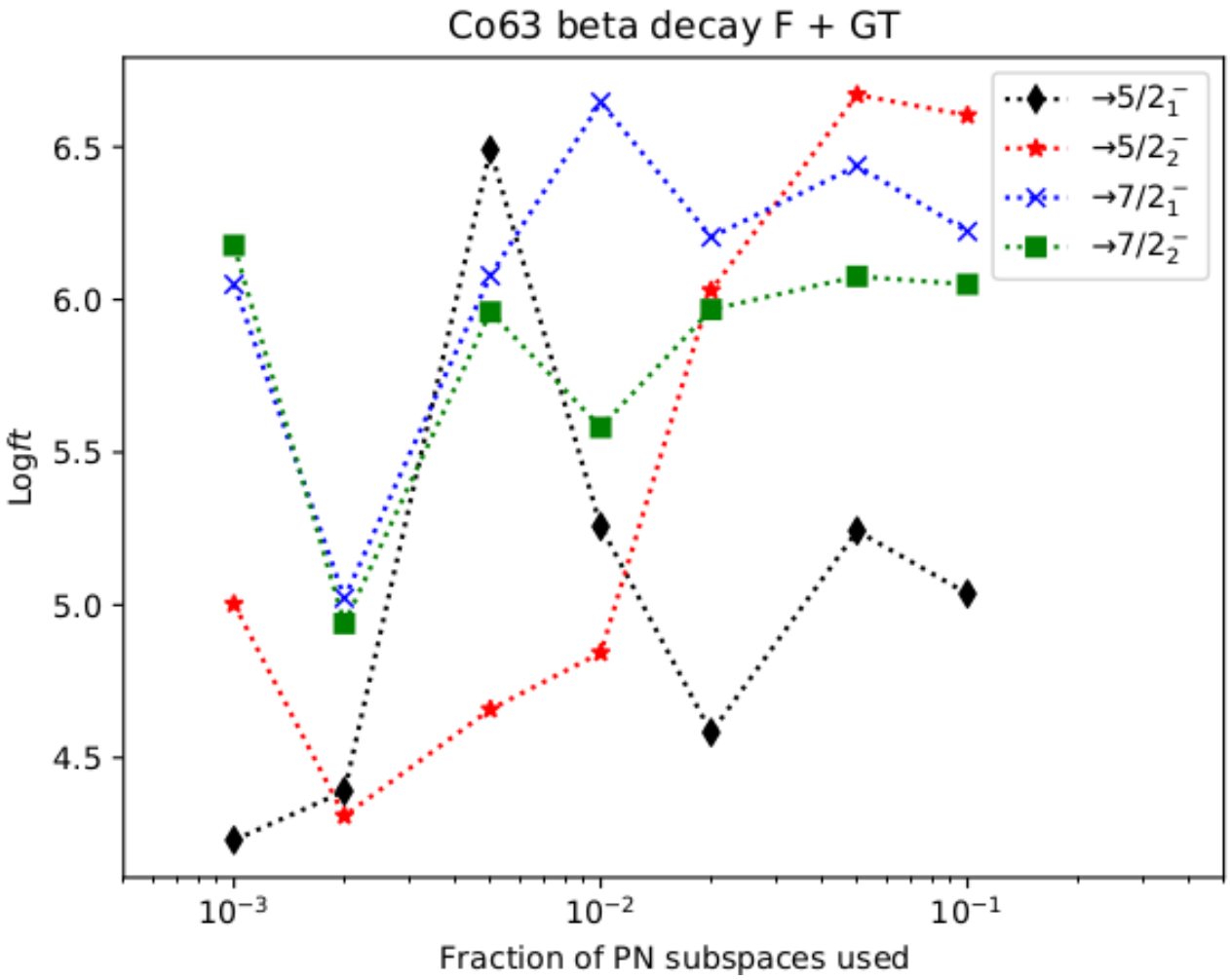


We can also compute EM and weak transitions



We can also compute EM and weak transitions



We can also compute EM and weak transitions

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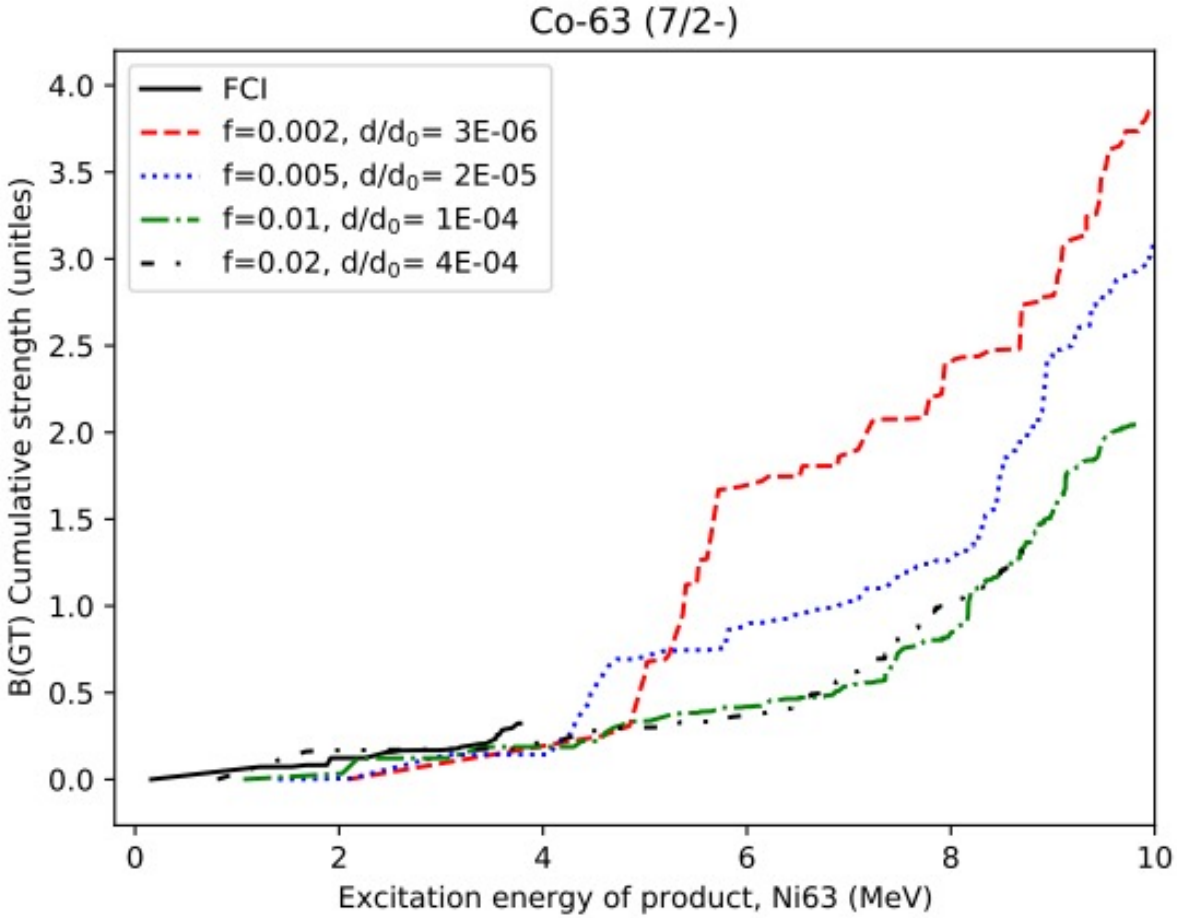
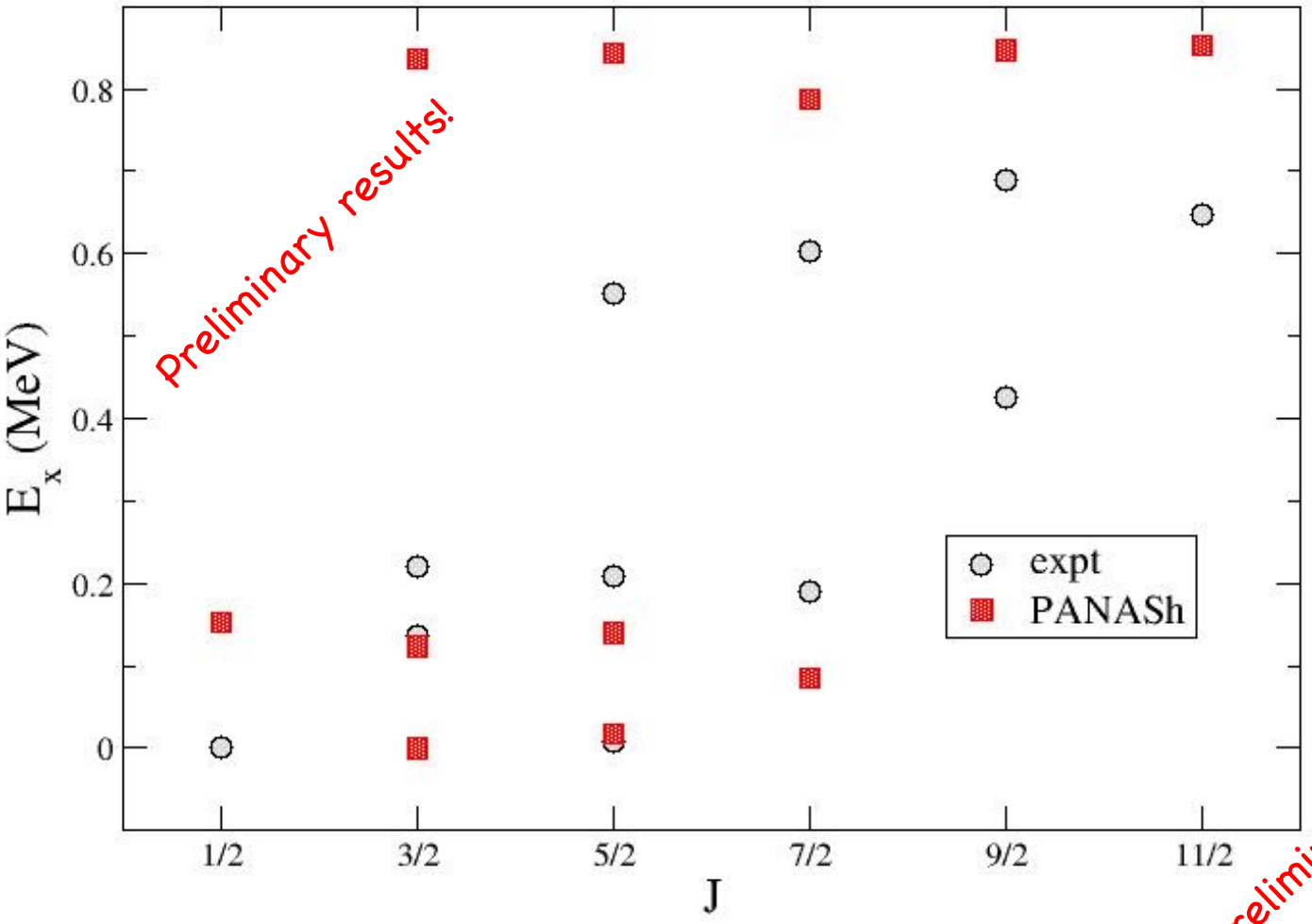
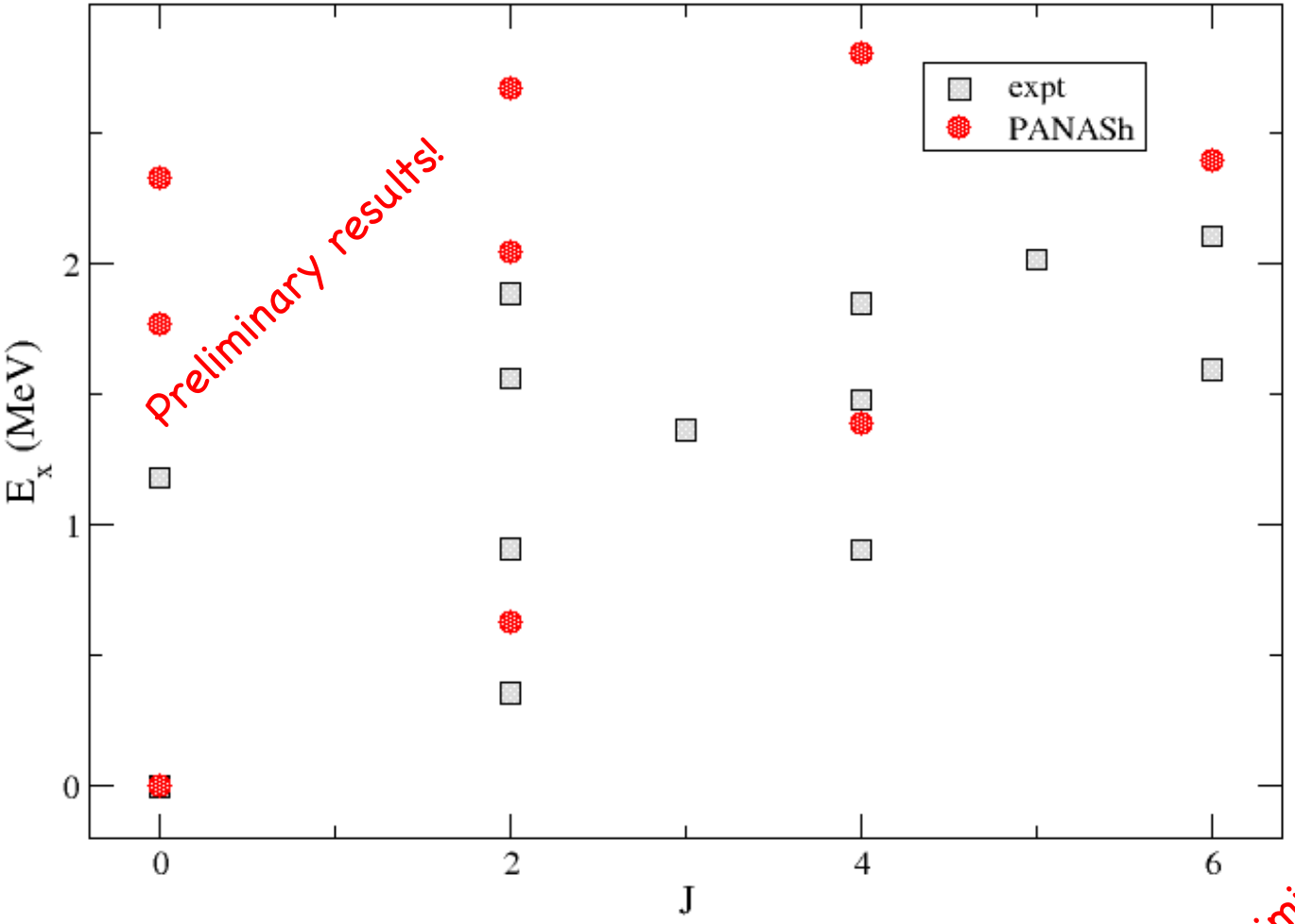


'Aspirational' calculation: ^{129}Cs in 50-82 space (force from Nowacki)
full space dimension: 50 billion!



Preliminary results!

‘Aspirational’ calculation: ^{130}Ba in 50-82 space (force from Nowacki)
full space dimension: 200 billion!



Preliminary results!

Moving forward

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We (mostly Oliver Gorton) are working to further improve parallelization, to speed-up applications.

Moving forward

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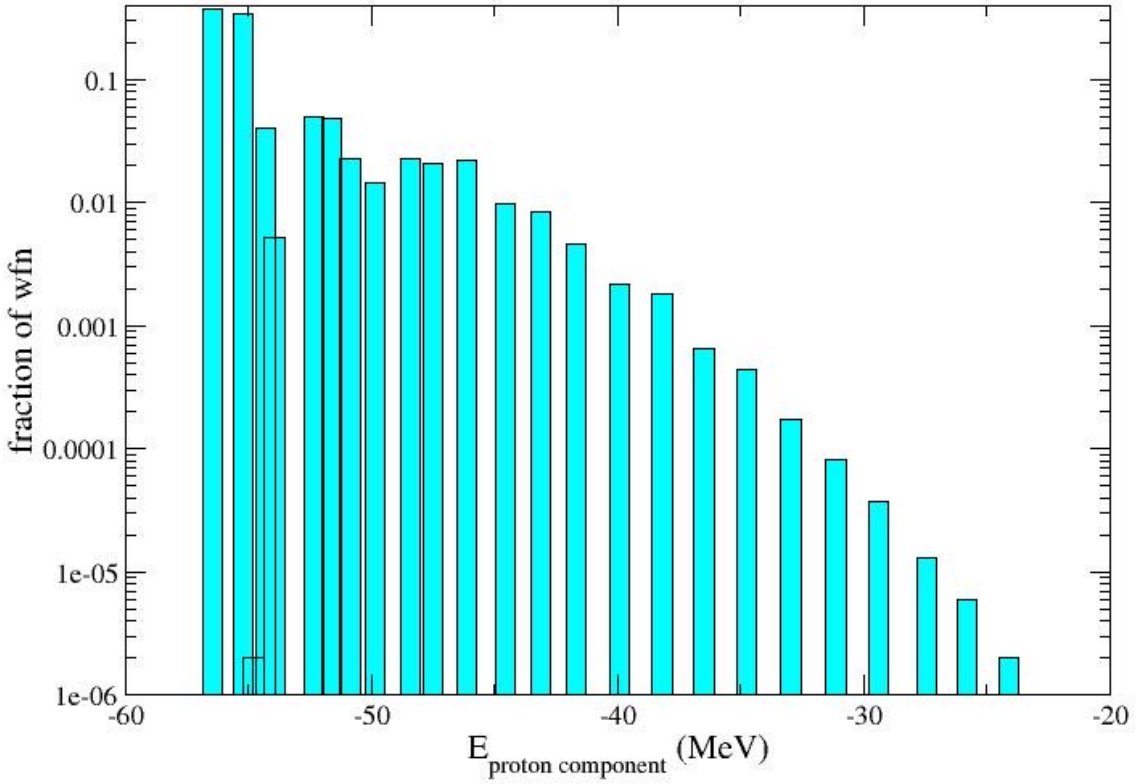
Can we use the statistical behavior to improve extrapolations/convergence?



Moving forward

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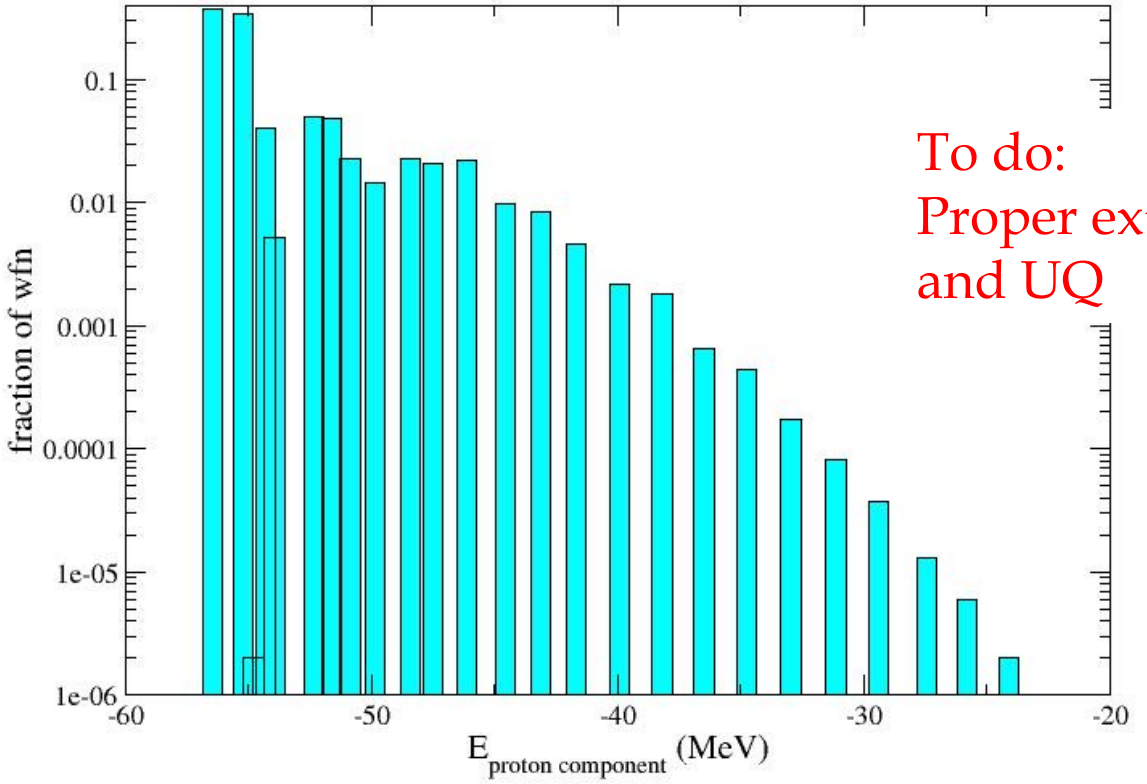
Can we use the statistical behavior to improve extrapolations/convergence?



To do:
Proper extrapolation and UQ

Moving forward

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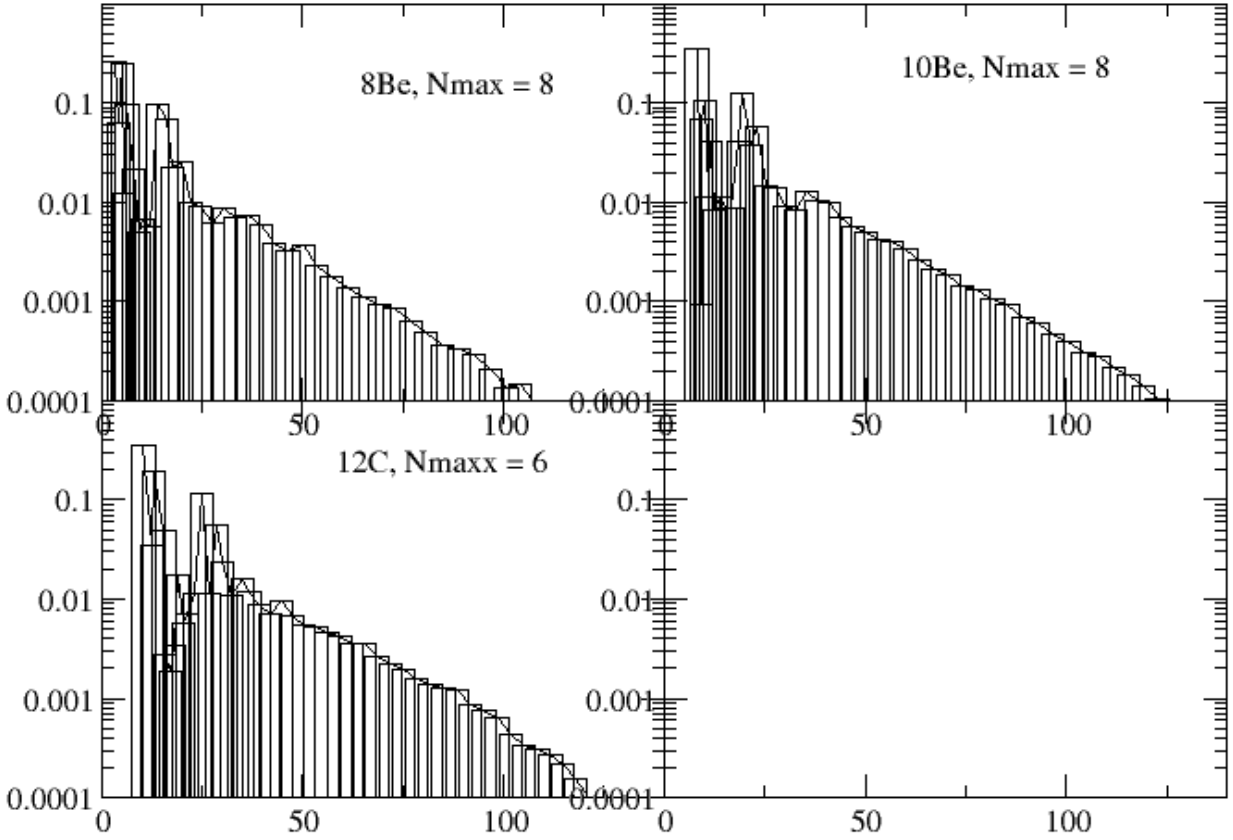
Can we apply to the no-core shell model?



Back to the chart of the nuclides…

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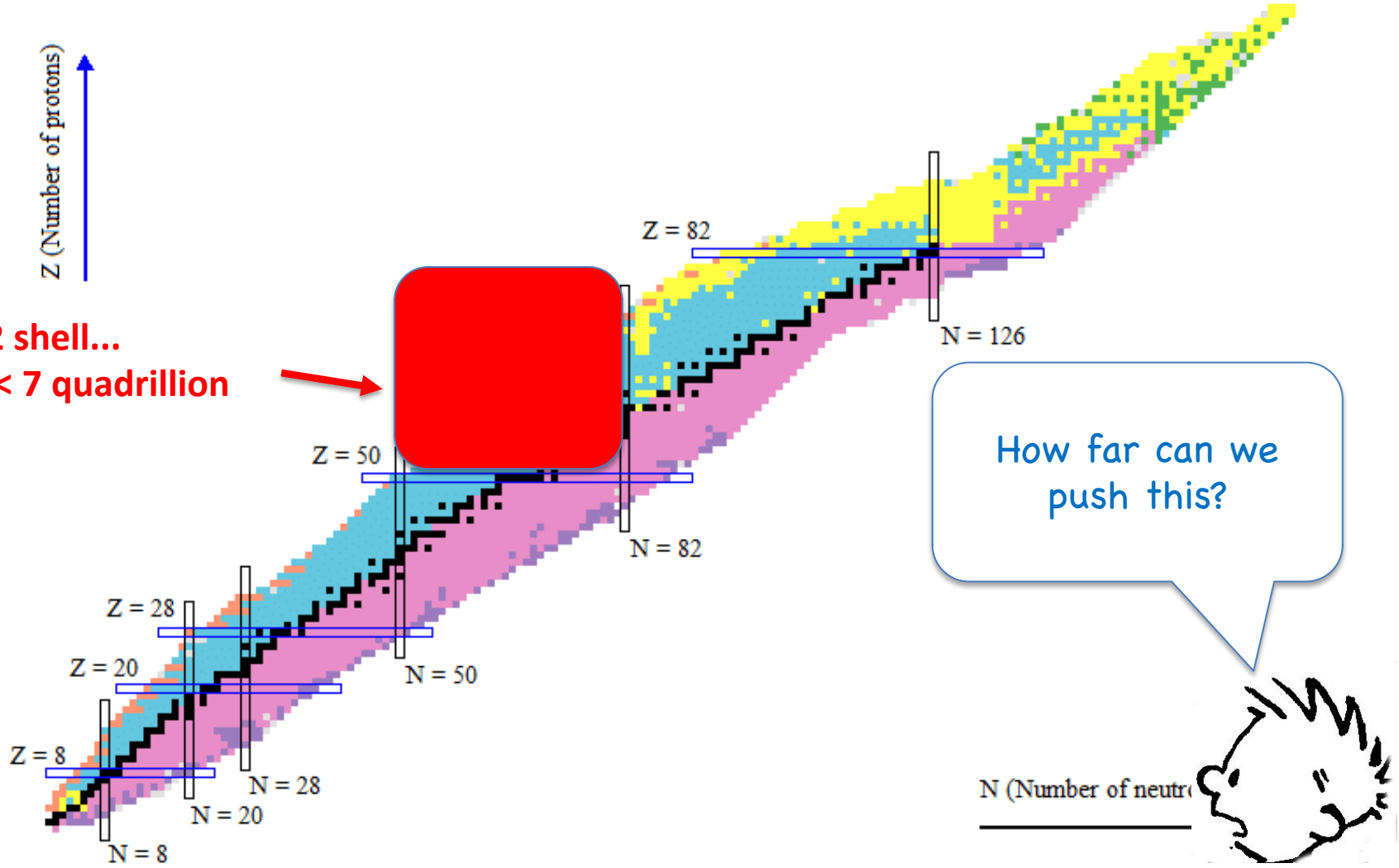
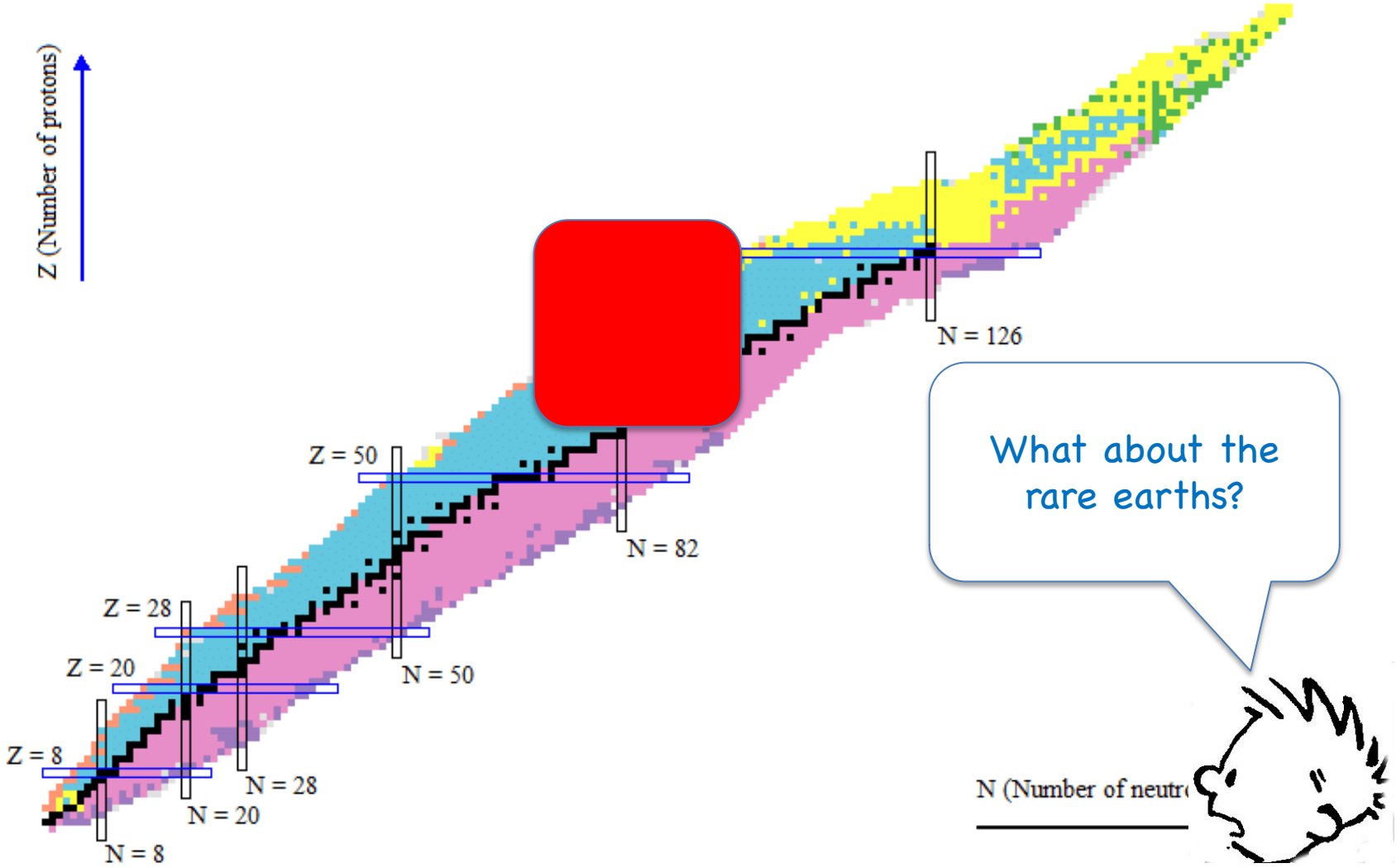
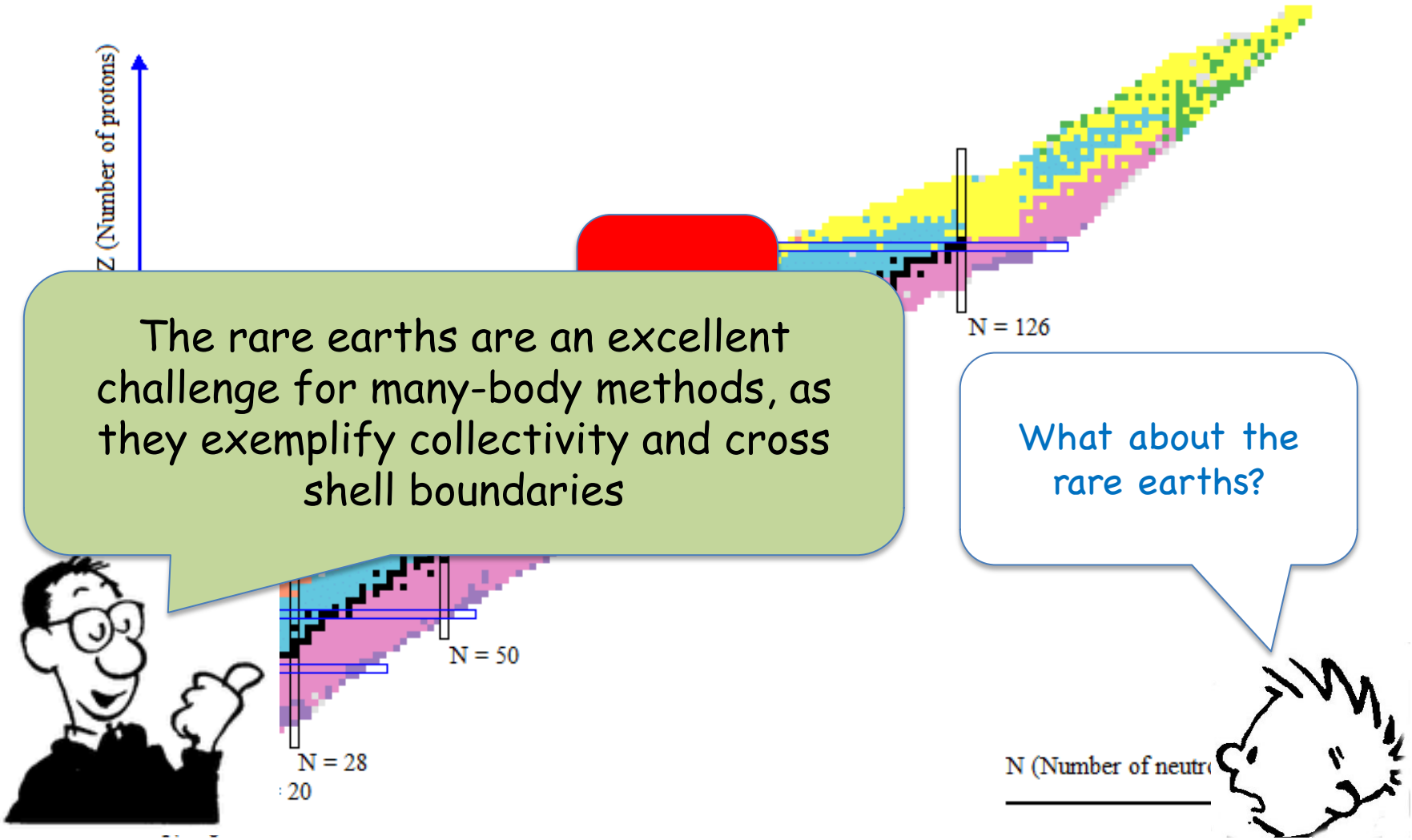



Z (Number of protons)
N = 126
Z = 50
N = 82
Z = 28
Z = 20
N = 50
Z = 8
N = 28
N = 20
N = 8
What about the rare earths?
N (Number of neutr


Z (Number of protons)
N = 126
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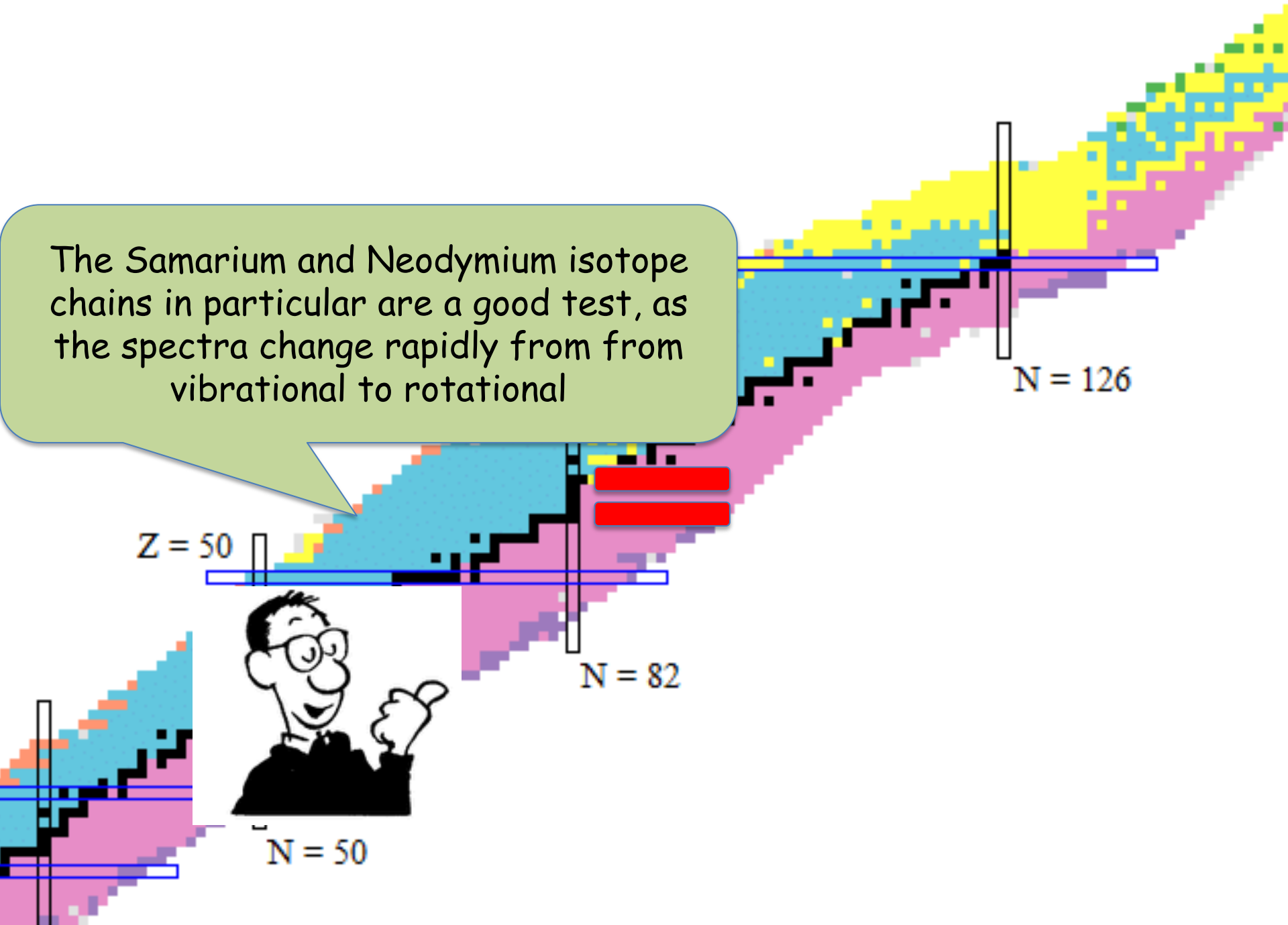
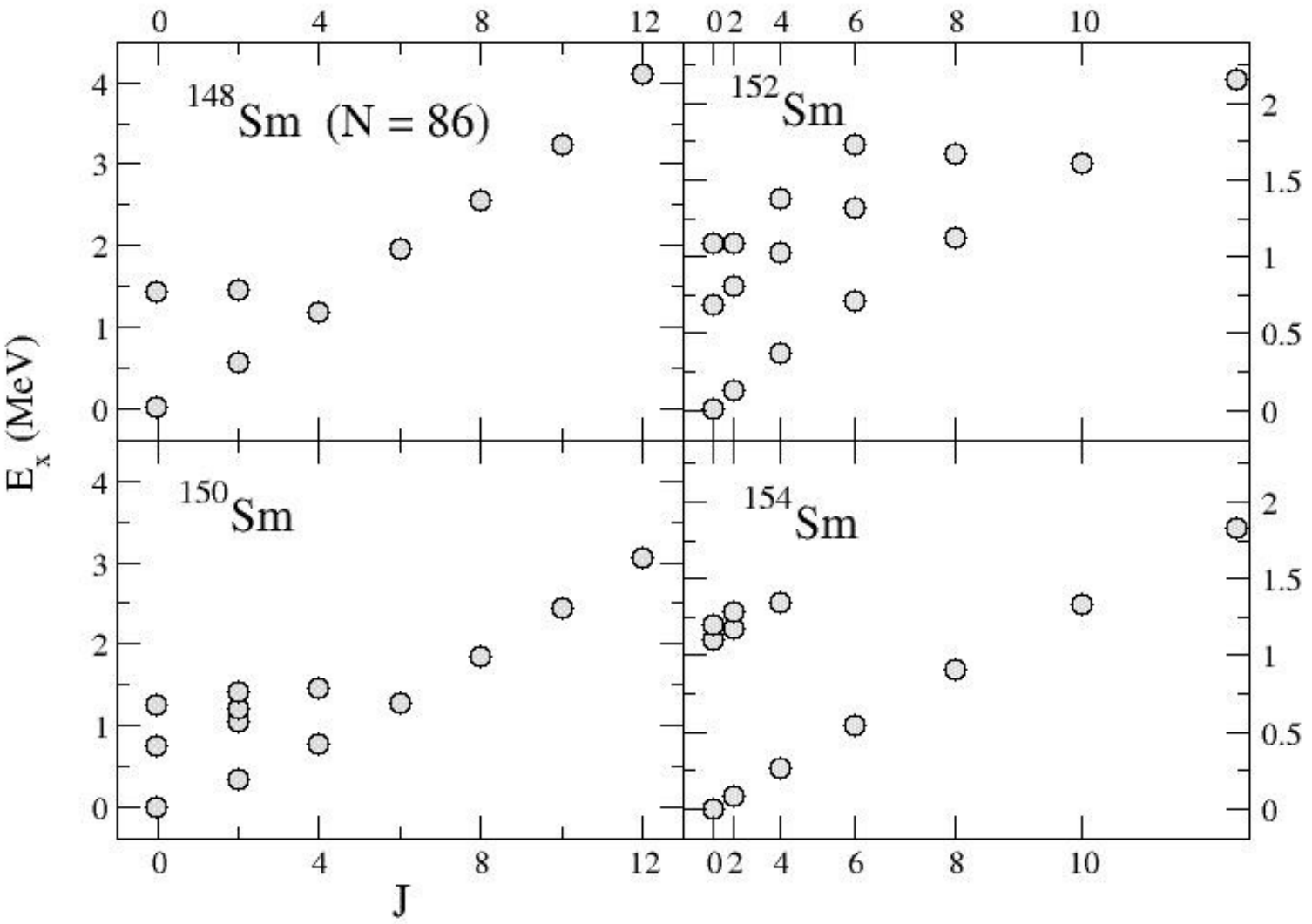
20
N (Number of neutr
The rare earths are an excellent challenge for many-body methods, as they exemplify collectivity and cross shell boundaries
What about the rare earths?

The Samarium and Neodymium isotope chains in particular are a good test, as the spectra change rapidly from from vibrational to rotational



Vibrational spectra -> Rotational spectra



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I use an interaction from Gilbreath et al, PRC **97**, 014315 (2018), which uses the 'Shell-model Monte Carlo' to investigate changes in deformation. The SMMC can handle huge spaces, but

-- is better for thermal properties rather than individual energies

-- requires a 'sign-problem-free' multipole-multipole + pairing force

I can use a more general force, but this force is *approximately* correct for this mass region (but not guaranteed to fully reproduce the spectra…)

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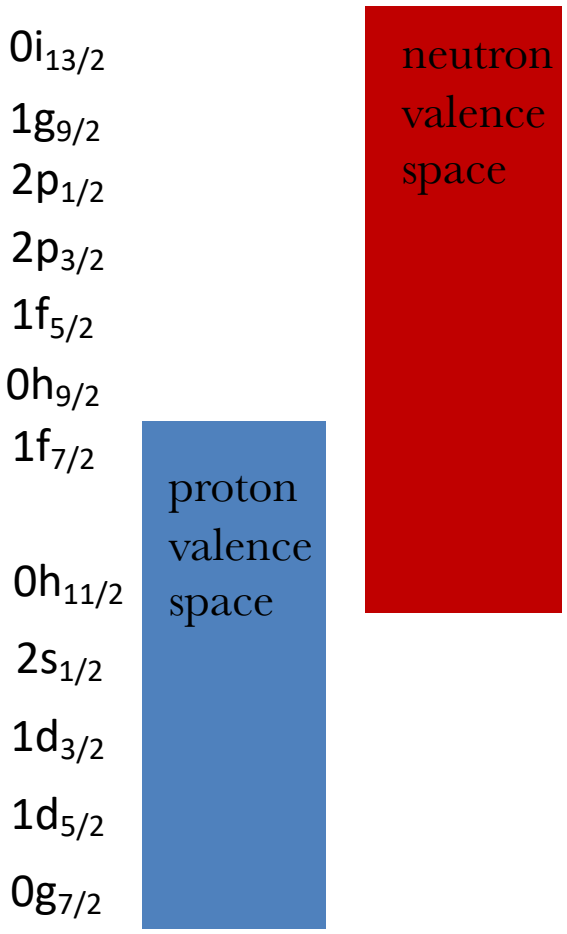
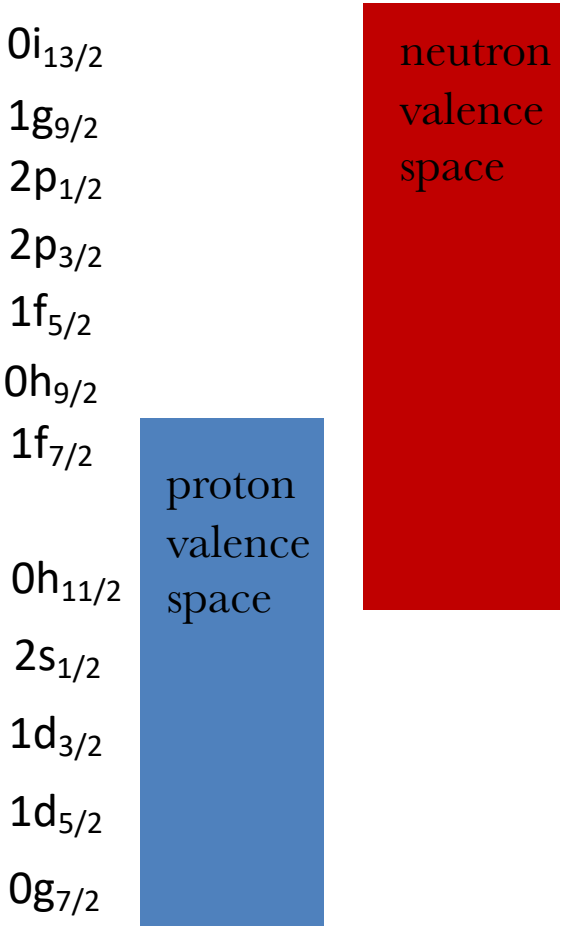
I can use a m
this force is
for this mass
to fully reproduce the spectra

Ideally use IMSRG interaction...

Single-particle orbits



Single-particle orbits



But for naïve application of PANASh, this space is a little too large!

^{148}Sm:

12 valence protons, dim = 150M
16 valence neutrons, dim = 800M (est)

Note: BIGSTICK code less efficient for single-species calculations

What about other approaches?

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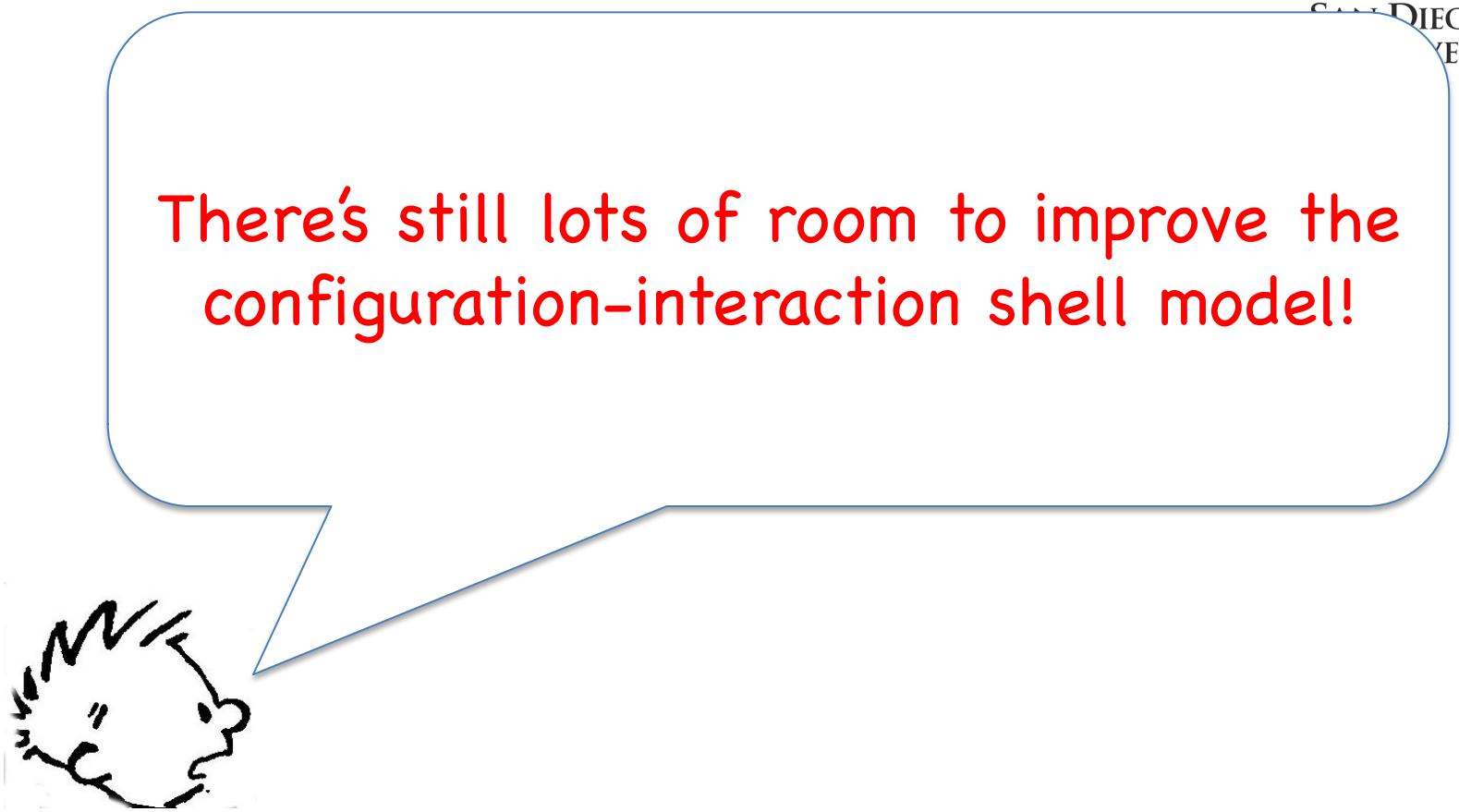
-- projected generator coordinate – cf B. Bally's talk Wed afternoon

(projected Hartree-Fock isn't a bad starting point:

Lauber, Frye, and Johnson, J. Phys. G. **48**, 095107 (2021).)

Could also do an energy truncation on the basis:

Horoi, Brown, and Zelevinsky, PRC 50, R2274(R) (1994)


There's still lots of room to improve the configuration-interaction shell model!