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Shell model calculations for neutrino and BSM physics

Calvin W. Johnson

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INT-23-85W, April 17, 2023

An all-too-common view:

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An all-too-common view:

Dark matter, string theory, neutrino physics….

An all-too-common view:

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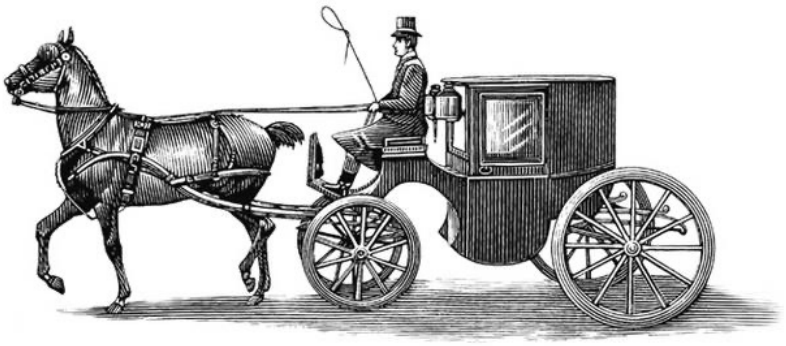

Dark matter, string theory, neutrino physics….

Nuclear structure physics

An all-too-common view:

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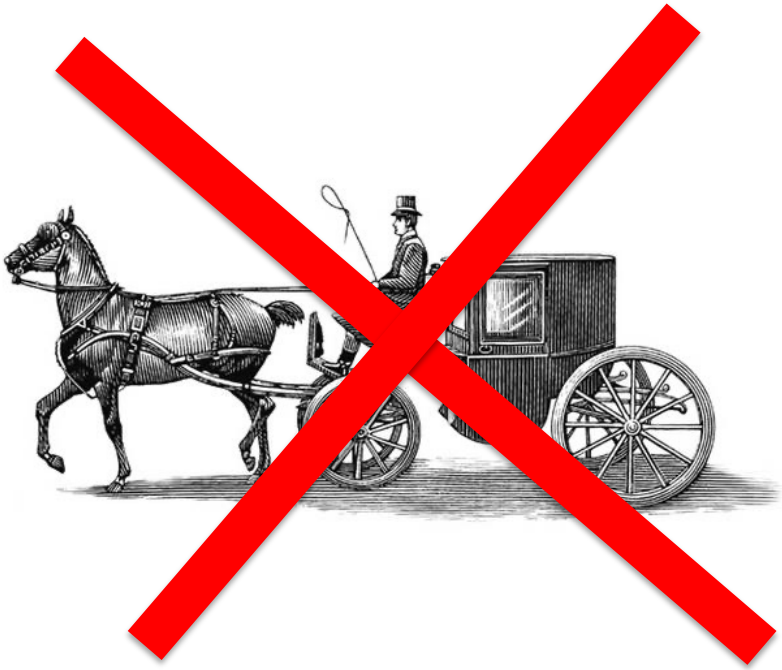

Dark matter, string theory, neutrino physics….

Nuclear structure physics

A better view:

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Dark matter, string theory, neutrino physics….

Nuclear structure physics

A better view:

Modern nuclear structure physics is rigorous, vigorous, and *the launchpoint for many other investigations.*

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To detect dark matter,
one needs **nuclear cross-sections**.
For neutrino physics, **nuclear cross-sections**.
For neutrinoless ββ decay, **need nuclear matrix element**
For parity/time-reversal violation (e.g. EDM),
need nuclear matrix element….

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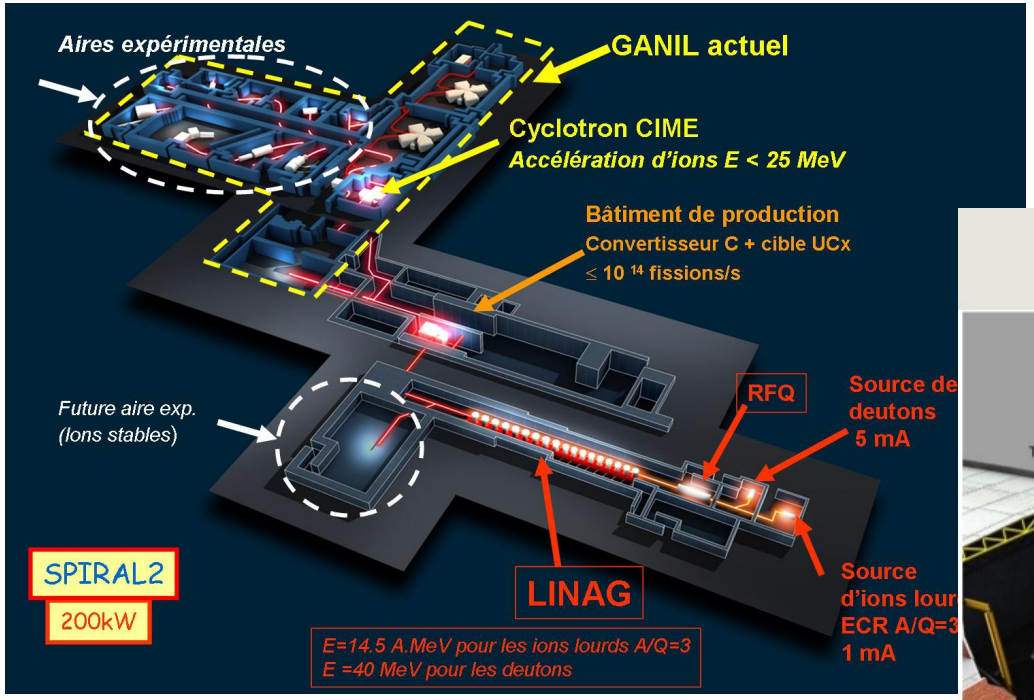
To detect dark matter,
one needs **nuclear cross-sections**.

(e.g., "`dmscatter`: a fast program for WIMP-nucleus scattering,"
O. C. Gorton, **CWJ, et al**, Comp. Phys. Comm. **284**, 108597 (2023))



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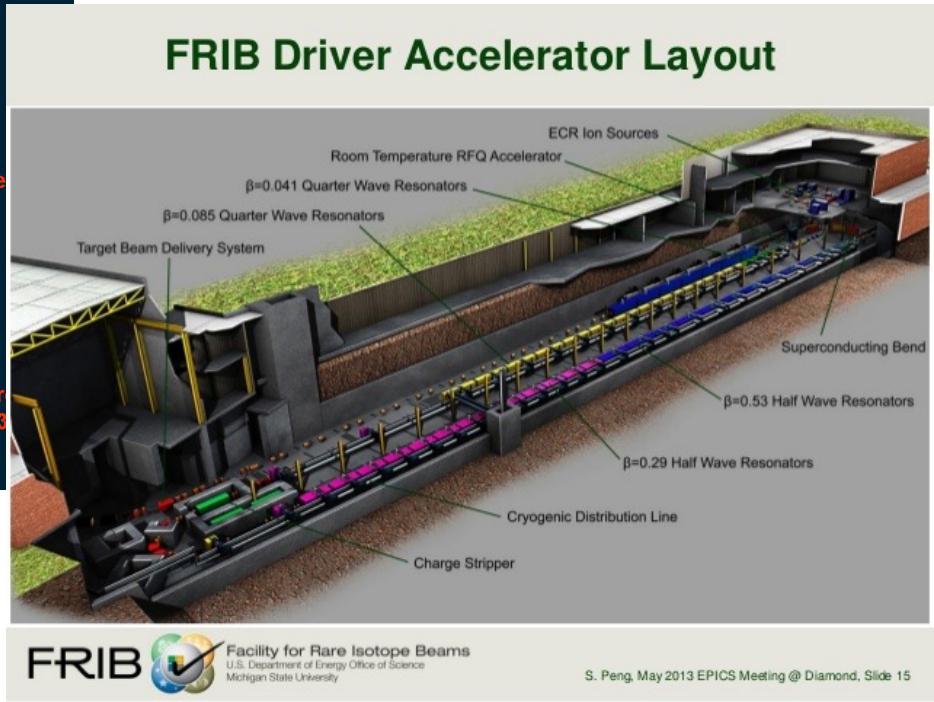
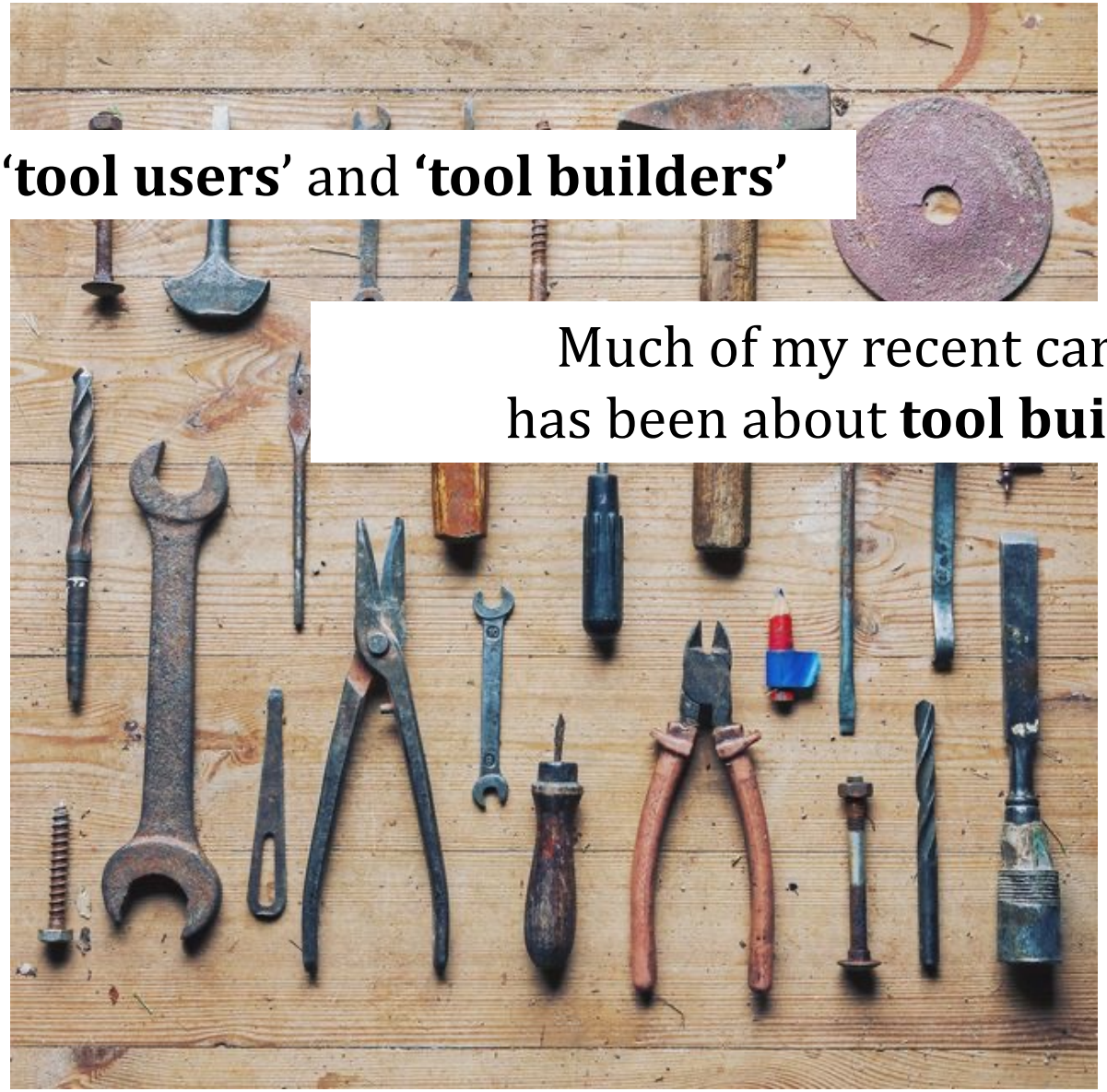


…and of course, hadronic reactions as found, e.g., at rare isotope facility: **origin of the elements, extreme & exotic behavior, etc.**

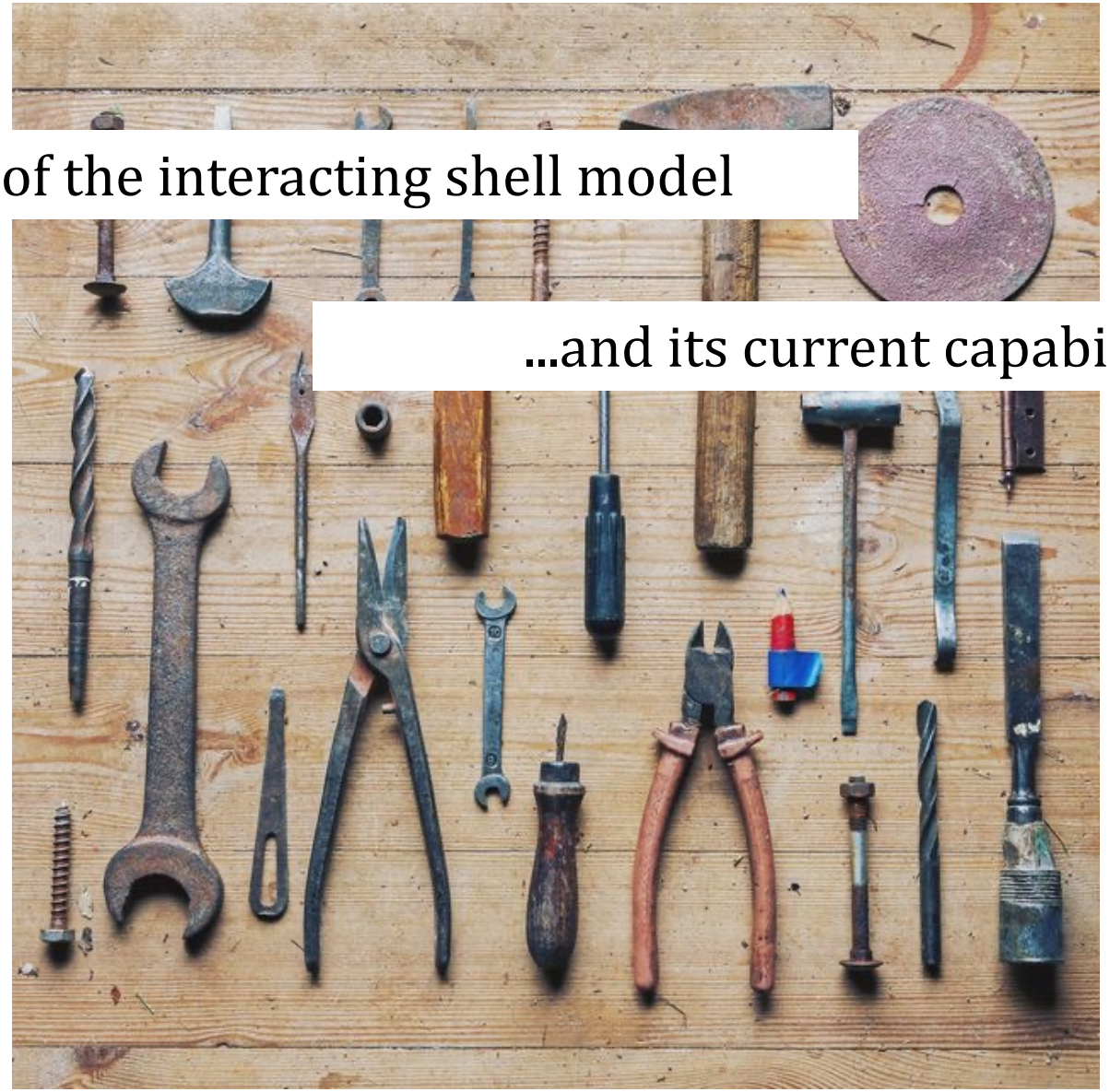
THE THEME OF THIS TALK…



There are '**tool users**' and '**tool builders**'

Much of my recent career has been about **tool building**

PART I



Overview of the interacting shell model

...and its current capabilities

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To compute electromagnetic and weak transition rates, we use Fermi's (actually Dirac's) Golden Rule from time-dependent perturbation theory:

$$R_{i\to f} = \frac{2\pi}{\hbar}\left|\langle f|\hat{O}|i\rangle\right|^2 \frac{dN_f}{dE}$$

Transition probability (strength)

$$\langle f|\hat{O}|i\rangle = \sum_{a,b}\langle a|\hat{O}|b\rangle\langle f|\hat{c}_a^+\hat{c}_b|i\rangle$$

Many-body matrix element

One-body matrix element

One-body density matrix elements between many-body states

(can also generalize to two-body transition operators)

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One-body matrix element

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To get the many-body states, we use the matrix formalism (a.k.a *configuration-interaction)*

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

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

$$\sum_{\beta} H_{\alpha\beta}c_{\beta} = Ec_{\alpha} \quad \text{if} \quad \langle\alpha|\beta\rangle = \delta_{\alpha\beta}$$

The single particle states are in 'orbitals' or 'shells', hence 'shell model'

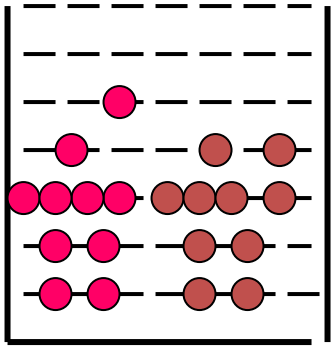
- How the basis states are represented

Product wavefunction ("Slater Determinant")

$$\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3\ldots) = \phi_{n_1}(\vec{r}_1)\phi_{n_2}(\vec{r}_2)\phi_{n_3}(\vec{r}_3)\ldots\phi_{n_N}(\vec{r}_N)$$

Each many-body state can be *uniquely* determined by a list of "occupied" single-particle states = "occupation representation"

$$|\alpha\rangle = \hat{a}^+_{n_1}\hat{a}^+_{n_2}\hat{a}^+_{n_3}\ldots\hat{a}^+_{n_N}|0\rangle$$



A brief and incomplete history

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1949: Goeppert-Mayer and Axel, Jensen & Suess show spin-orbit splitting explain magic numbers. Single-particle picture describes many measured magnetic moments. (*Non-interacting shell model*)

1956: Edith Halbert and J. B. French perform early configuration-interaction *(interacting shell model*) calculations.

1965: Cohen-Kurath empirical interaction for **valence** *p*-shell
1977: Whitehead introduces Lanczos method
1984: Wildenthal interaction for **valence** *sd*-shell
1991: FPD6 interaction for **valence** *pf* shell

Issues:

$$\sum_{\beta} H_{\alpha\beta} c_{\beta} = E c_{\alpha} \qquad |\Psi\rangle = \sum_{\alpha} c_{\alpha} |\alpha\rangle$$

- Origin of Hamiltonian matrix elements

Semi-phenomenological vs. *ab initio*
(fit to *A*-body vs. fit to few-body)

- Representation and selection of basis

(basis "scheme" and model space)

- Computation with Hamiltonian matrix element

Storage vs. construction "on-the-fly"

Modern many-body calculations

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Ab initio approaches include coupled-cluster, Green's-function Monte Carlo, and the **no-core shell model** (NCSM)

See talk by J. Sobczyk

No-core shell model: in harmonic oscillator basis, "all" particles active (up to N_{max} h.o. excitation quanta), with high-precision interaction (e.g. chiral EFT, HOBET, etc.) fit to *few-body* data

e.g. *p*-shell nuclides up to N_{max} = 10 … 22

cf. Barrett et al, *Progress in Particle and Nuclear Physics* **69**, 131 (2013)

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Ab initio/ "No-core shell model": take to infinite limit

Two parameters: h.o. basis frequency Ω
and model space cutoff N_{max}

Naïve expectation: take N_{max} -> infinity
Converged results independent of Ω

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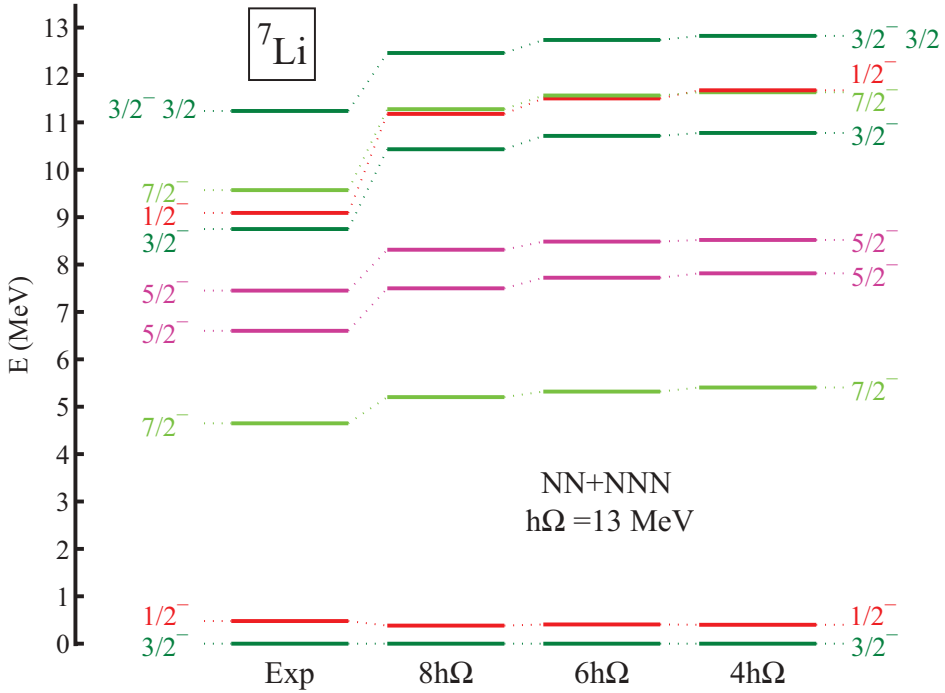
Some highlight achievements:

- Can get spectra of light nuclei ”from first principles”

PHYSICAL REVIEW C **87**, 014327 (2013)



Maris , Vary, Navratil
PRC **87**, 014327 (2013)

chiral 2+3 body forces

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Some highlight achievements:

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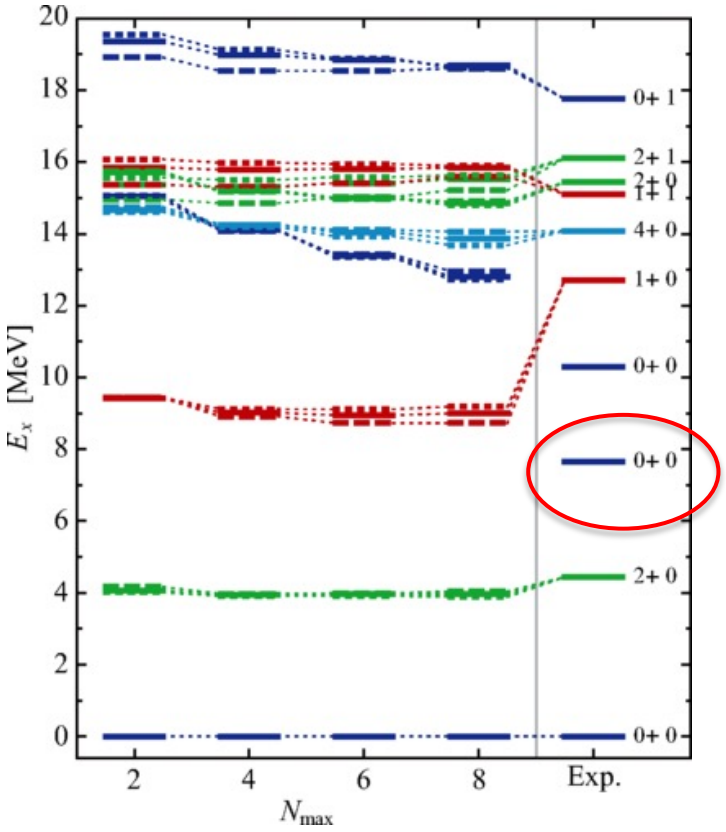

Hoyle state

Maris *et al* PRC **90**, 014314 (2014)

^{12}C with chiral 2+3 body forces

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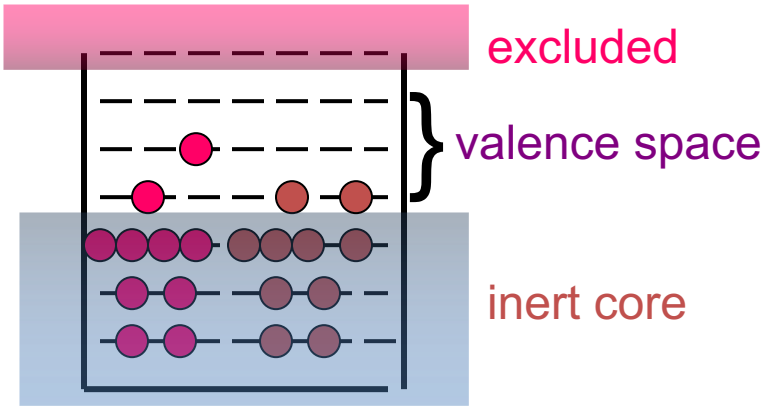
"Phenomenological" calculations work in a fixed space, usually with a core



cf. Caurier et al, Rev. Mod. Phys. **77**, 427 (2005)

Phenomenological/empirical shell model:
Fixed valence space calculations with frozen core

Interaction matrix elements start from 'realistic' force
(usually modified by a G-matrix calculation)
matrix elements adjusted to reproduce many-body spectra

-- can tackle heavier nuclides
-- but lose physical interpretation of, e.g., s.p. wfn
-- no theory to expand model space

cf. Caurier et al, Rev. Mod. Phys. **77**, 427 (2005)

Modern many-body calculations

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New: “Non-empirical” or “ab initio valence space” Valence space calculations; start from ab initio and transformed via in-medium similarity-renormalization-group (next talk by Baishan Hu).

(In principle, more predictive than standard ‘empirical’ shell model; can choose valence space.)

S. R. Stroberg, et al., *Annual Review of Nuclear and Particle Science* **69**, 307 (2019)

Choice of wave function basis

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One chooses between *a few, complicated states*
or *many simple states*

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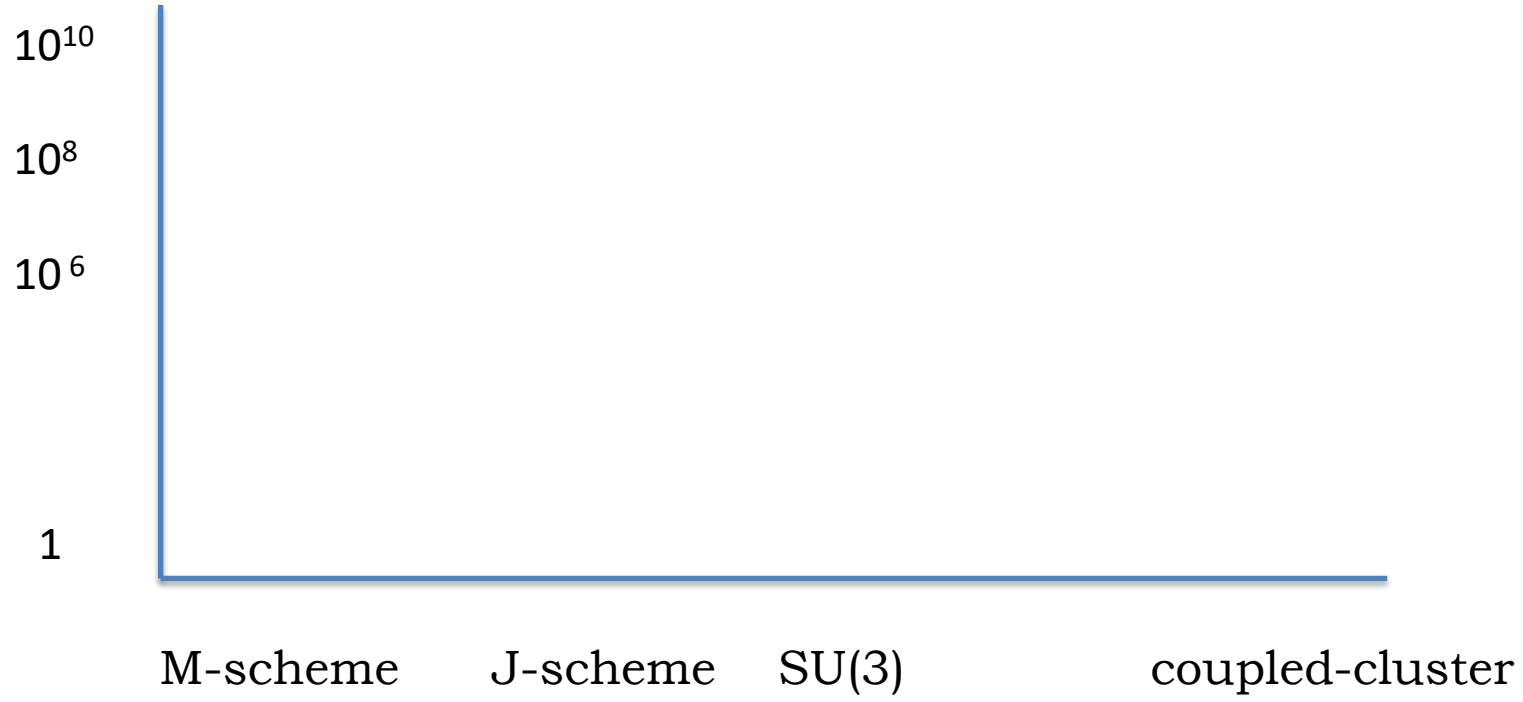

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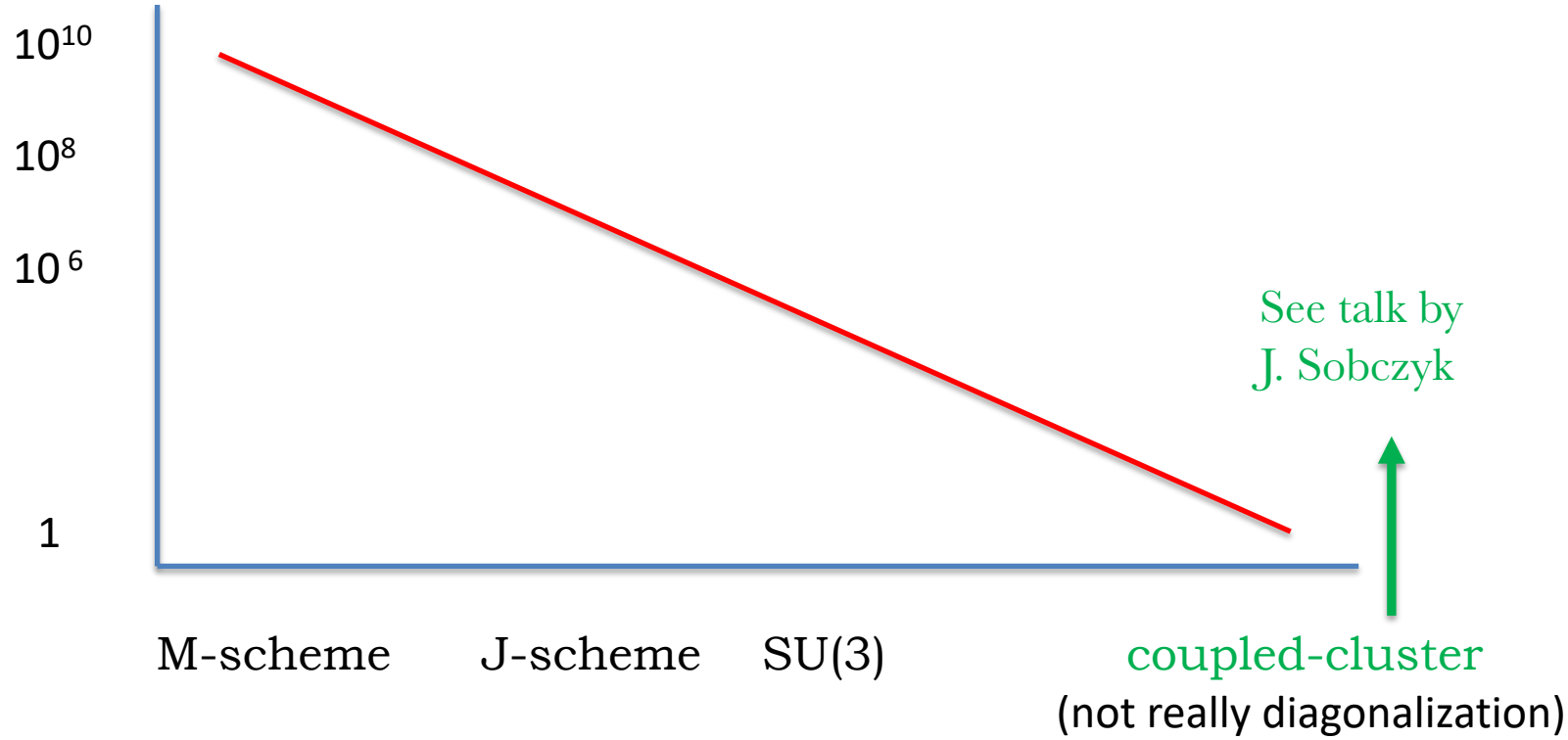

Choice of wave function basis

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One chooses between *a few, complicated states*
or *many simple states*

M-scheme: basis states with fixed total J_z
Simple and easy to construct/work with
Requires large dimension basis

J-scheme: basis states with fixed total J
Enforced rotational symmetry, smaller dimensions
Generally built from *M*-scheme states

Choice of wave function basis

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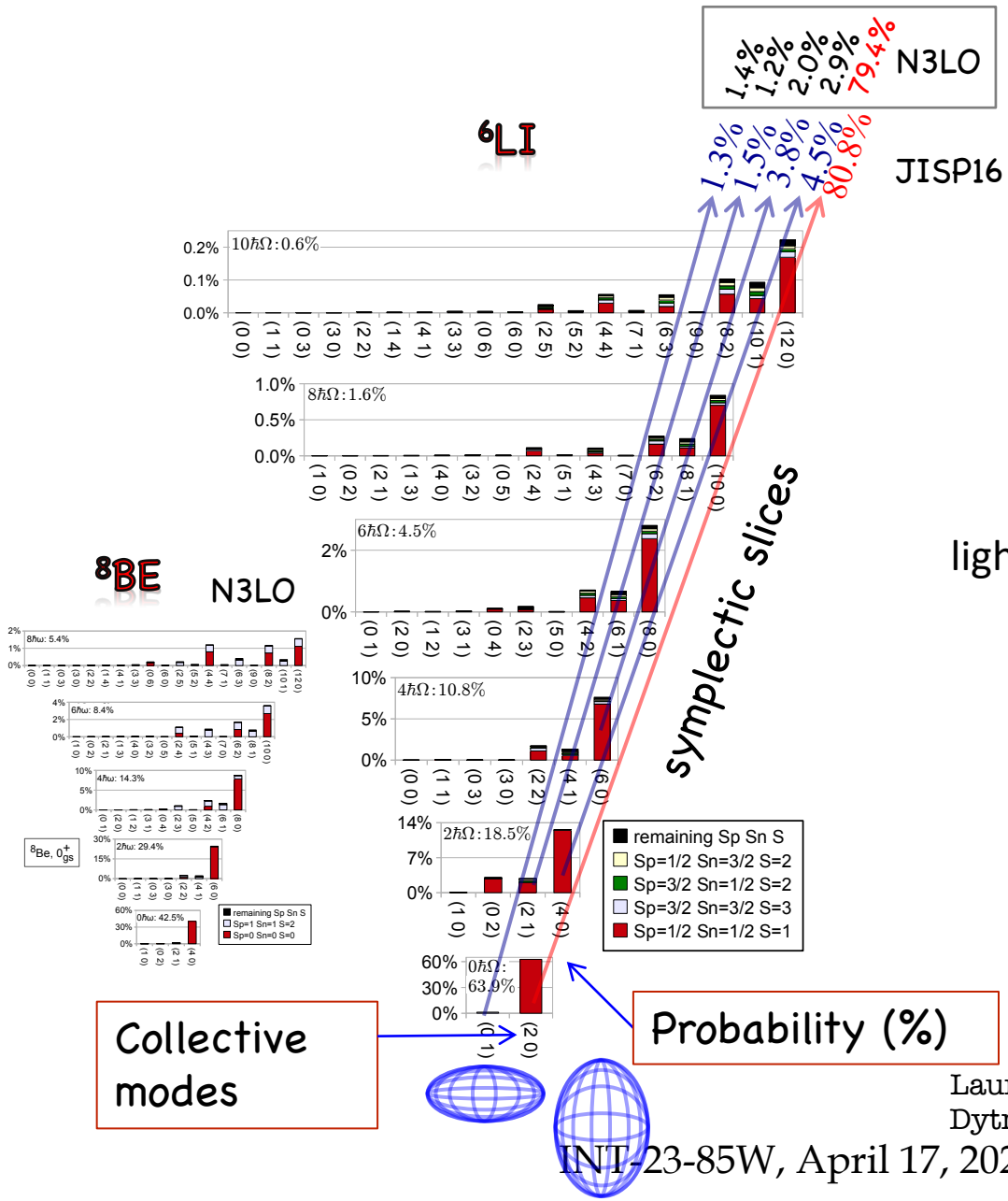
One chooses between *a few, complicated states*
or *many simple states*

Symmetry-adapted (SU(3), Sp(3,R), etc):
States from selected group irreps

Enforced symmetries, rotational + translational, smaller dimensions

Often built from *M*-scheme states or by recursion

Symplectic Sp(3,R) Symmetry



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(From K. Launey, LSU)

From first principles: light/intermediate-mass nuclei, low-lying states

Launey et al., Prog. Part. Nucl. Phys. 89 (2016) 101
Dytrych et al., Phys. Rev. Lett. 111 (2013) 252501

Collectivity features

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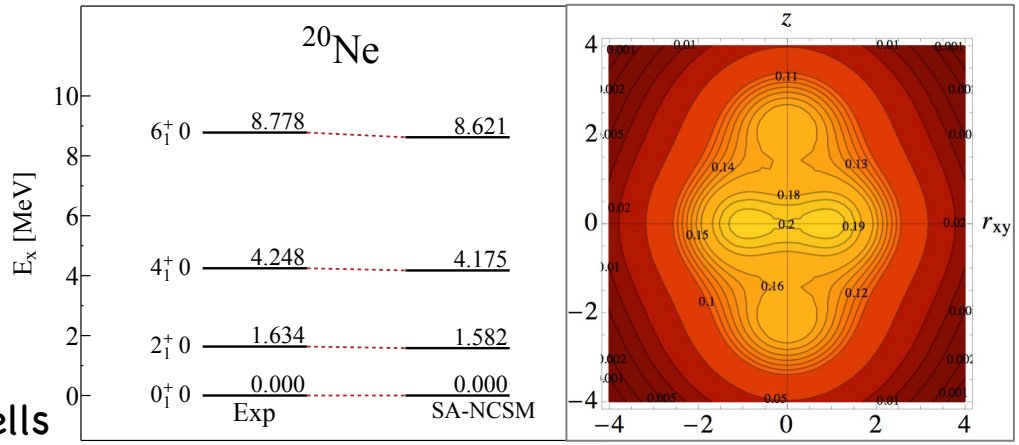


13 shells

SA-NCSM (selected model space): 50 million SU(3) states

Complete model space: 1000 billion states

^{18}Ne, B(E2: $2^+ \to 0^+$)

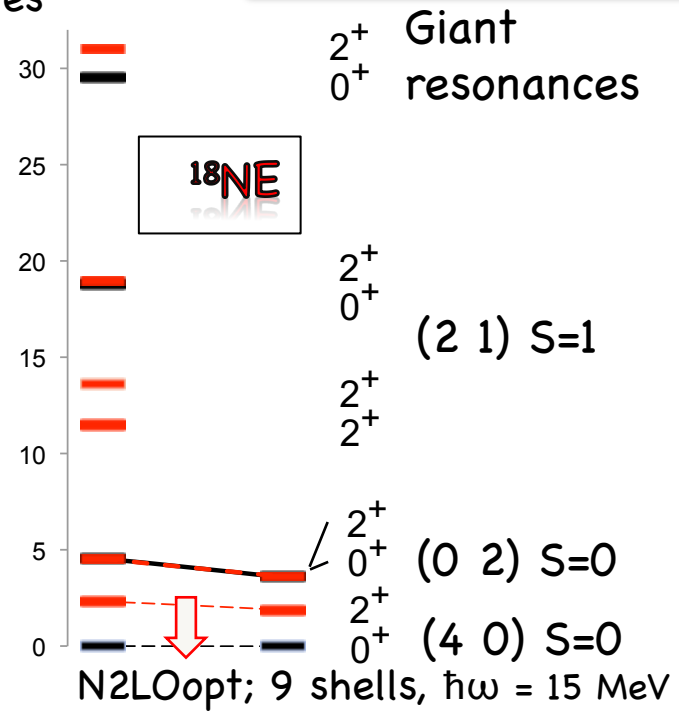
Experiment…… 17.7(18) W.u.

9 shells …… 1.13 W.u.

33 shells ……. 13.0(7) W.u.

(no effective charges)

Ne & Mg isotopes



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It's also important to know:

Computational burden is *not* primarily the dimension but is the # of nonzero Hamiltonian matrix elements.

Loop over α:

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

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J-scheme matrices are smaller but much denser than M-scheme, and "symmetry-adapted" (i.e. SU(3)) matrices are smaller (and denser) still.

example: ^{12}C $N_{max} = 8$

scheme	basis dim
M	0.6×10^9
J (J=4)	9×10^7
SU(3)	9×10^6

(truncated)

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example: ^{12}C $N_{max} = 8$

scheme	basis dim	# of nonzero matrix elements
M	0.6×10^9	5×10^{11}
J (J=4)	9×10^7	3×10^{13}
SU(3)	9×10^6	2×10^{12}

(truncated)

Dytrych, et al. *Computer Physics Comm* **207**, 202 (2016)

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example: ^{12}C $N_{max} = 8$

scheme	basis dim	# of nonzero matrix elements	
M	0.6×10^9	5×10^{11}	4 Tb of memory!
J (J=4)	9×10^7	3×10^{13}	240 Tb of memory!
SU(3)	9×10^6	2×10^{12}	16 Tb of memory!

(truncated)

Dytrych, et al. *Computer Physics Comm* **207**, 202 (2016)

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Older codes (e.g., OXBASH) stored nonzero matrix elements on hard drive -> I/O as bottleneck

More recent codes (e.g., MFDn) store nonzero matrix elements in RAM -> requires supercomputer

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Alternate approach: “on-the-fly/factorization”
pioneered by ANTOINE code
used by NuShellX, **BIGSTICK**, KSHELL codes

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Alternate approach: “on-the-fly/factorization”
pioneered by ANTOINE code
used by NuShellX, **BIGSTICK**, KSHELL codes

“On-the-fly” uses the fact that only two (or three) particles at a time interact; the rest are spectators

-> ”loop over spectators”

A description of the “factorization” algorithm:

CWJ, W. Ormand, P. Krastev, Comp. Phys. Comm. **184**, 2761(2013)

J-scheme matrices are smaller but much denser than M-scheme, and "symmetry-adapted" (i.e. SU(3)) matrices are smaller still.

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SU(3)	9×10^6	2×10^{12}	16 Tb of memory!
(truncated)		On-the-fly requires only 43 Gb!	

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Links to free, open-source many-body codes:

fribtheoryalliance.org

In particular `BIGSTICK`, available from:
github.com/cwjsdsu/BigstickPublick

Manual at arXiv:1801.08432

Also: NuShellX (MSU)
KSHELL (Tokyo)
ANTOINE

The BIGSTICK public shell-model code!

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Download from: github.com/cwjsdsu/BigstickPublick

100-page 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

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Despite advances, it is easy to get to model spaces beyond our reach:

N_{max} calculations:

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

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

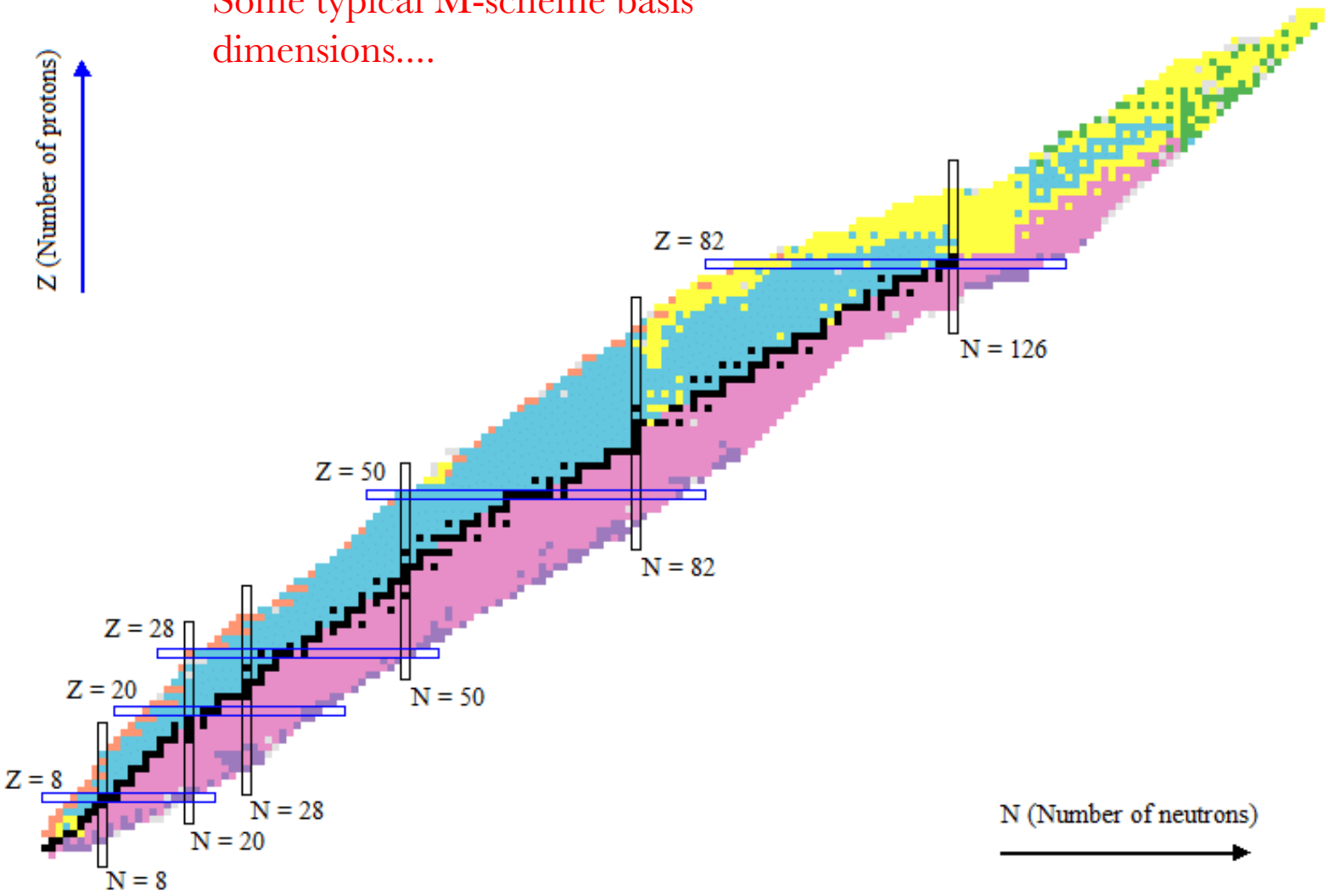
^{12}C $N_{max} = 8$ dim 500 million

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

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

Largest (?) known calculation, ^{12}Be, $N_{max}=12$, 35 billion (McCoy *et al*, with MFDn)

Some typical M-scheme basis dimensions....



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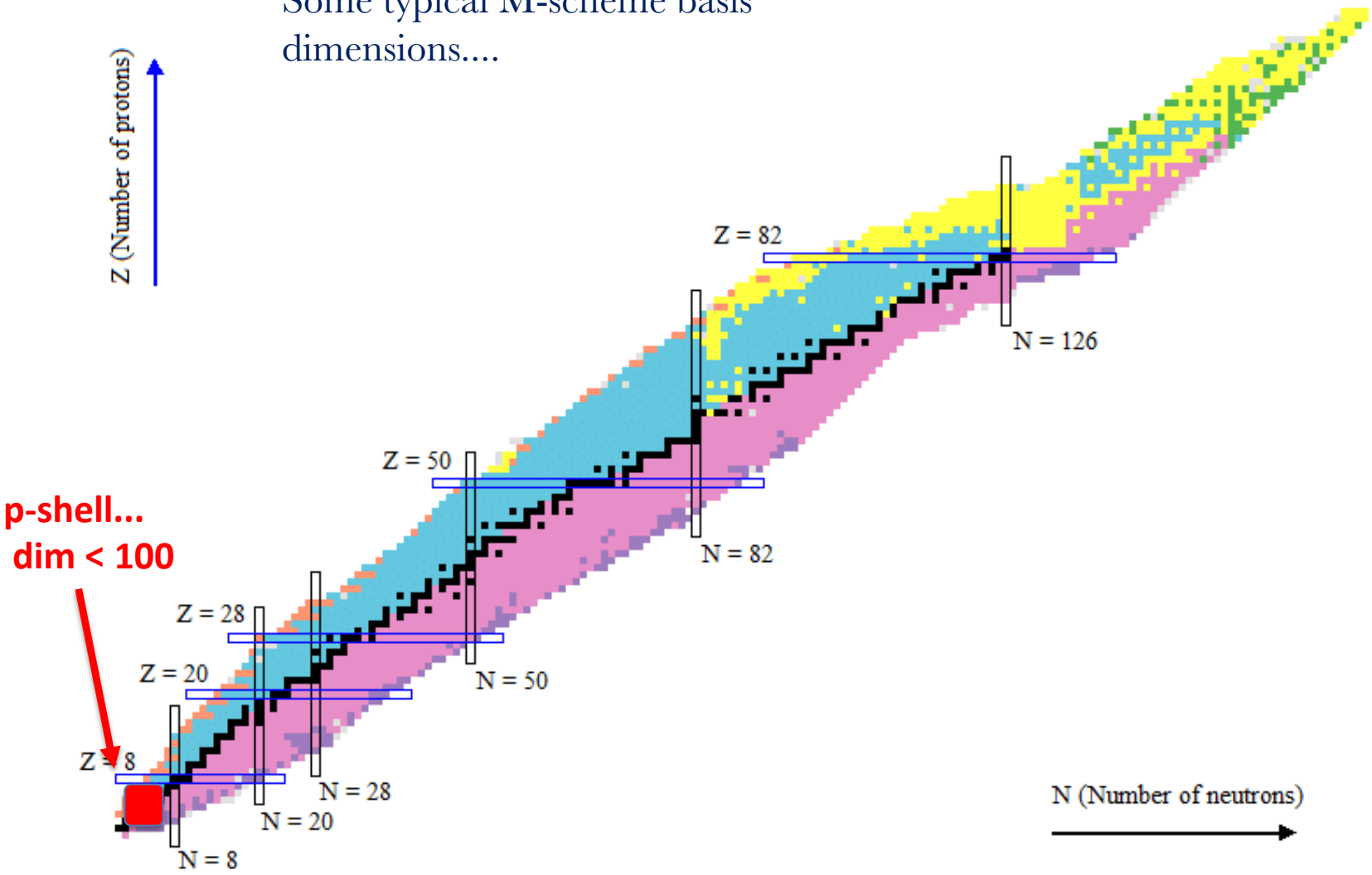

p-shell...
dim < 100

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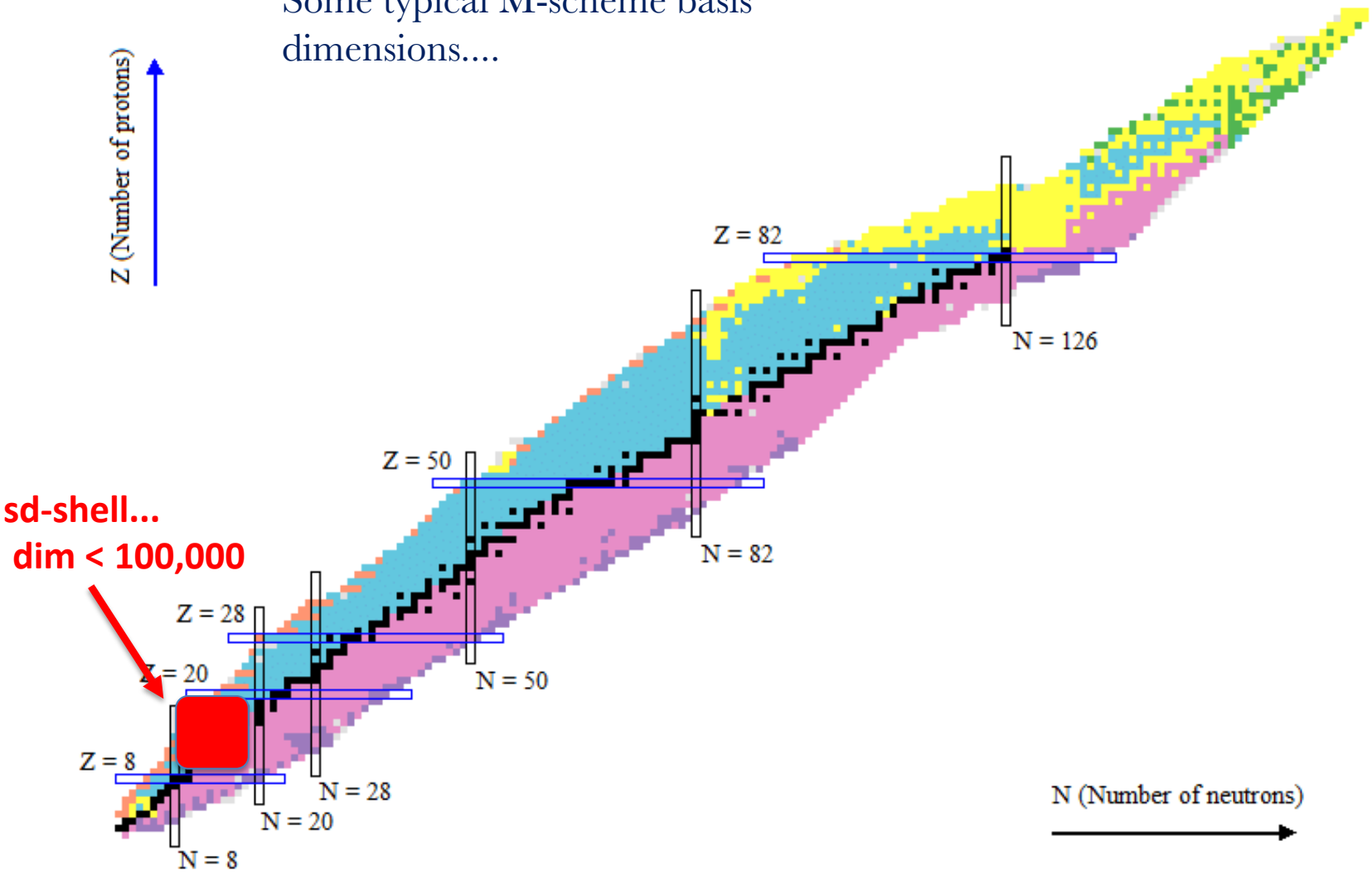
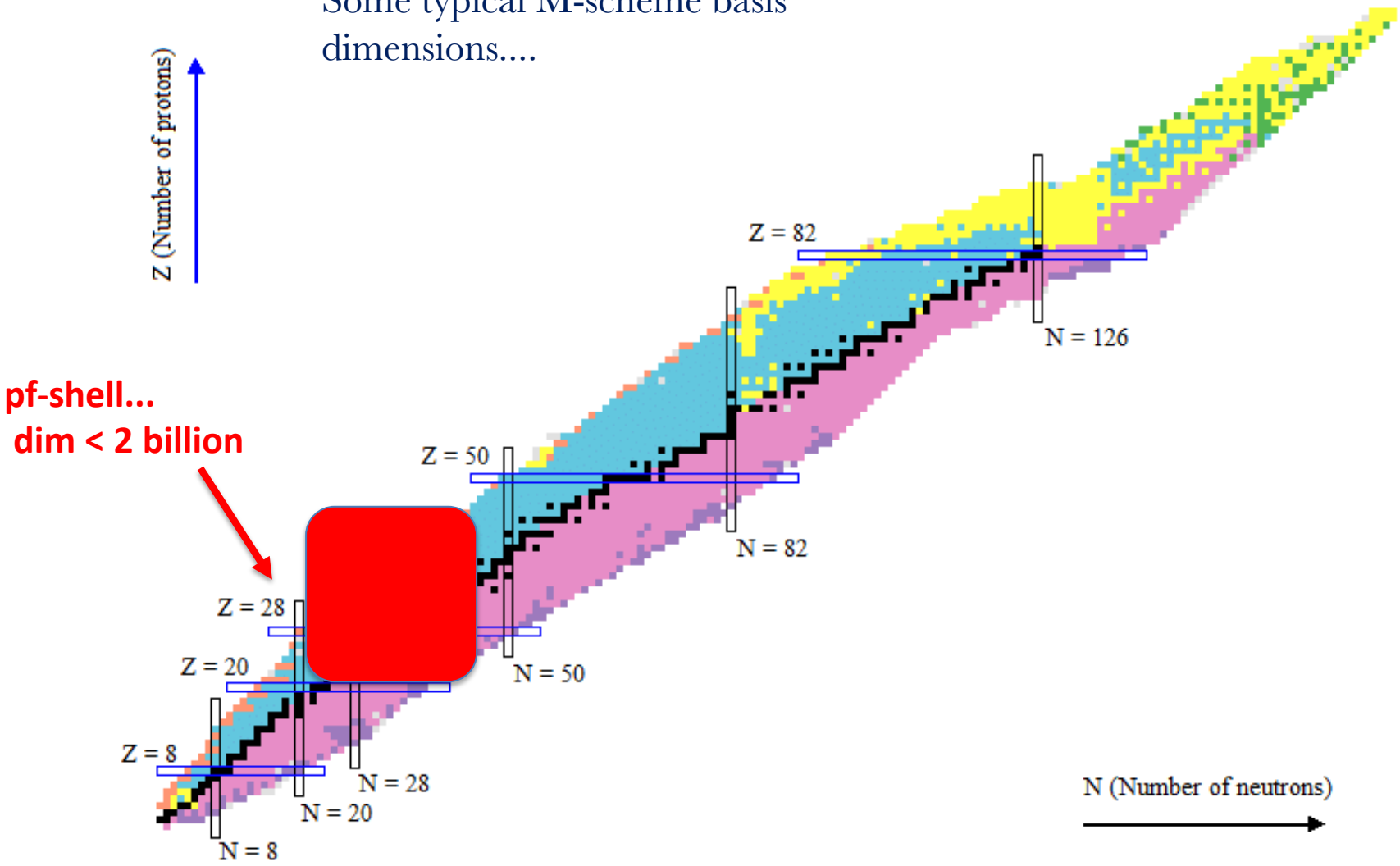
Some typical M-scheme basis dimensions....



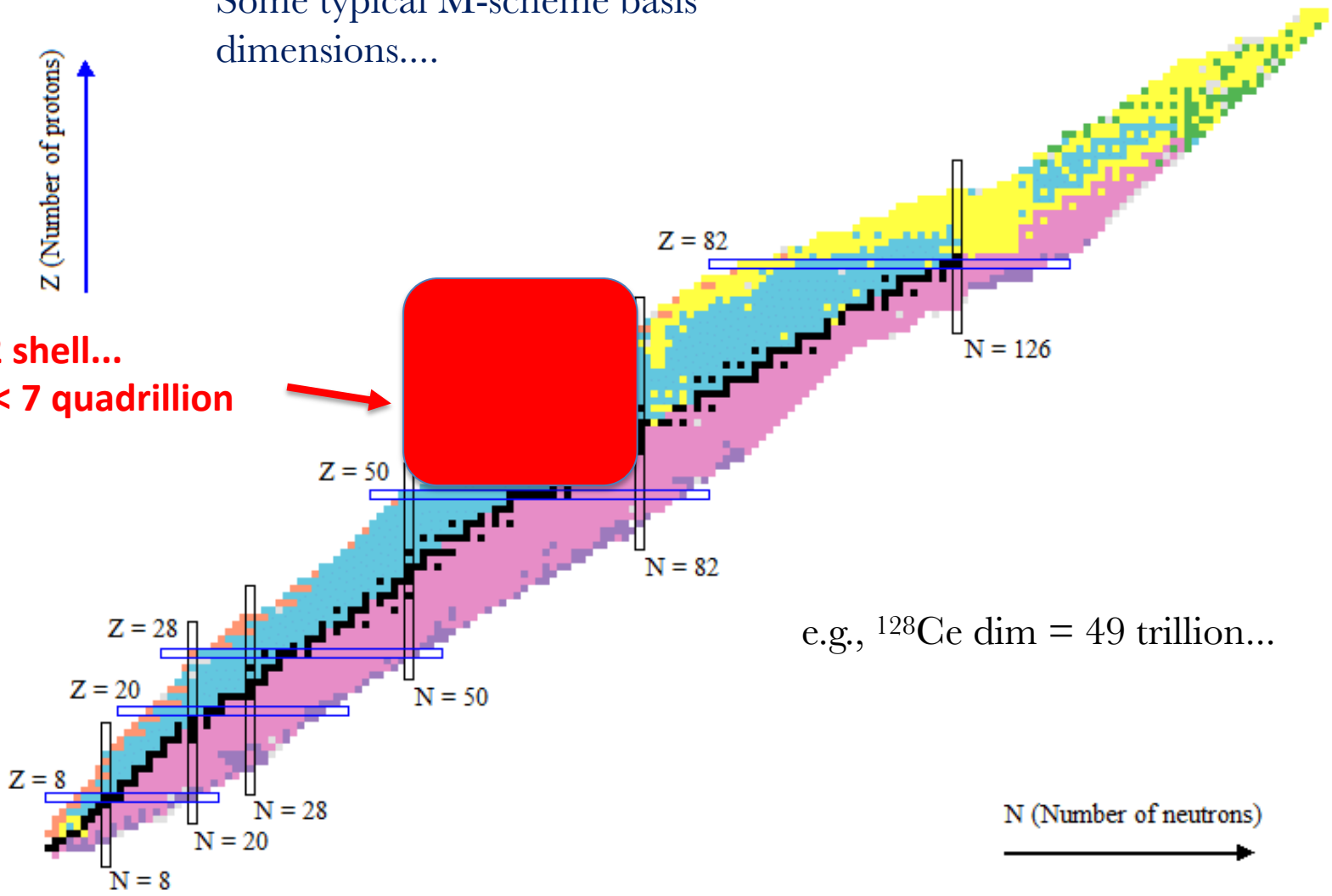
sd-shell...
dim < 100,000

Some typical M-scheme basis dimensions....



pf-shell...
dim < 2 billion

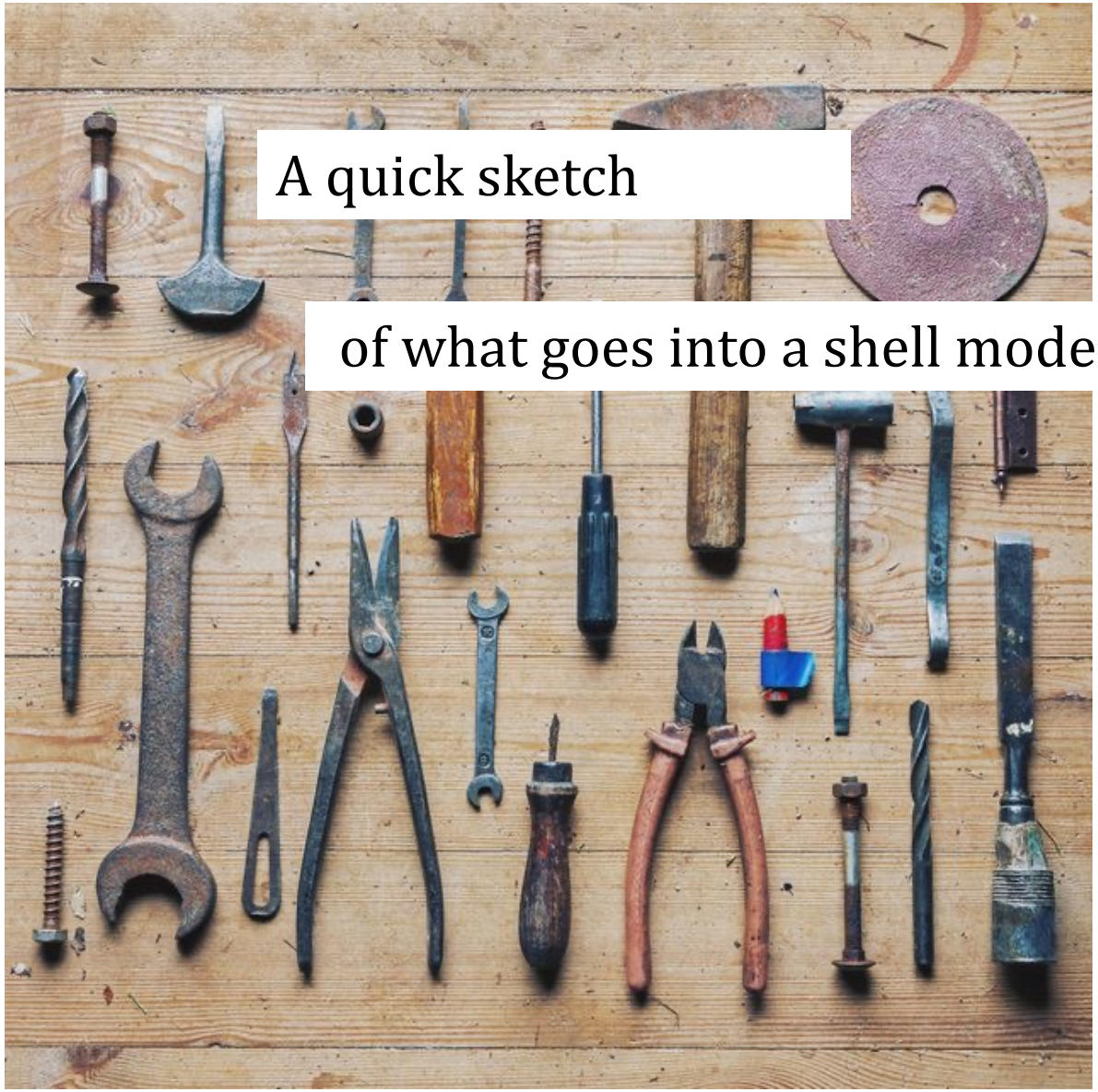
Some typical M-scheme basis dimensions....



50-82 shell...
dim < 7 quadrillion

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

PART II



A quick sketch

of what goes into a shell model calculation

What goes into a shell model calculation

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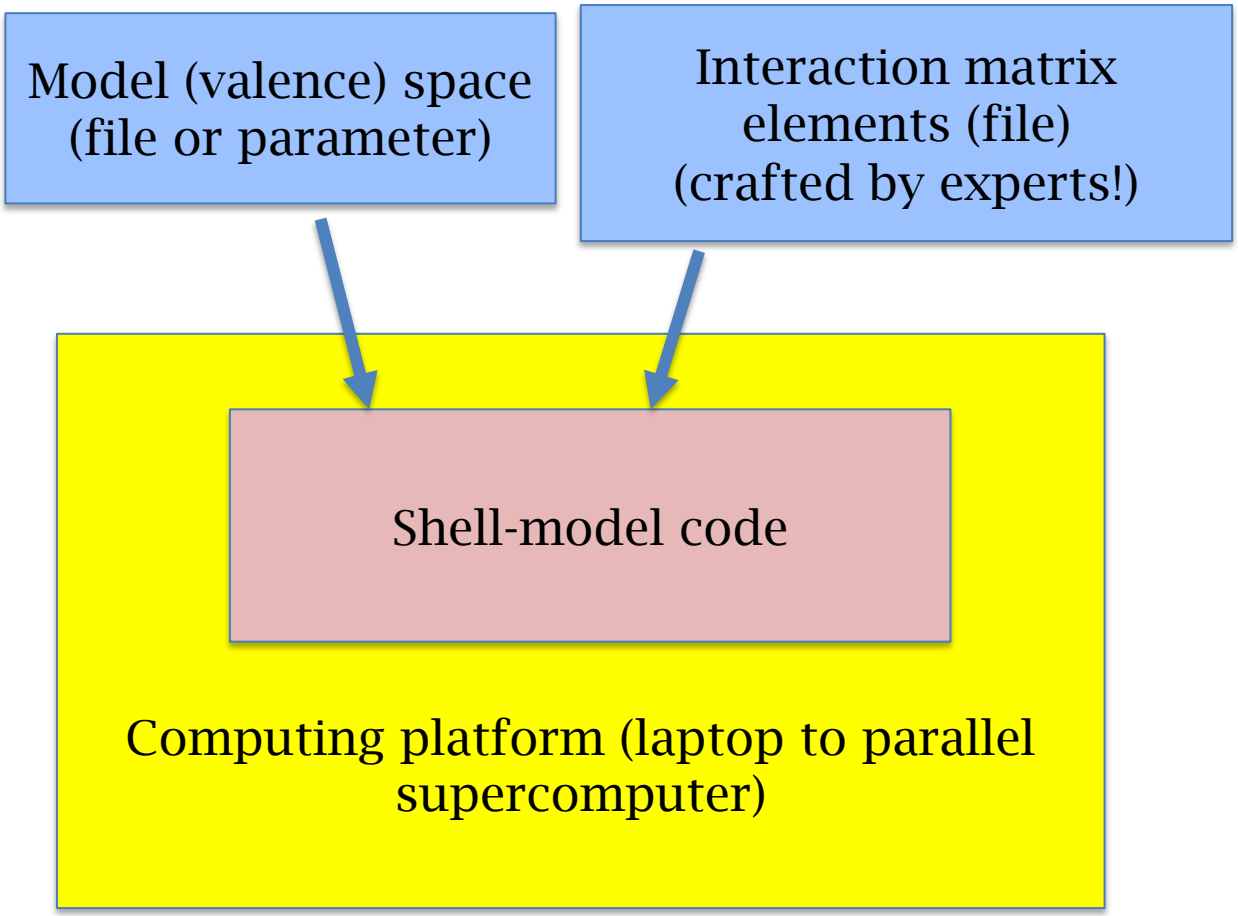
What goes into a shell model calculation

San Diego State University

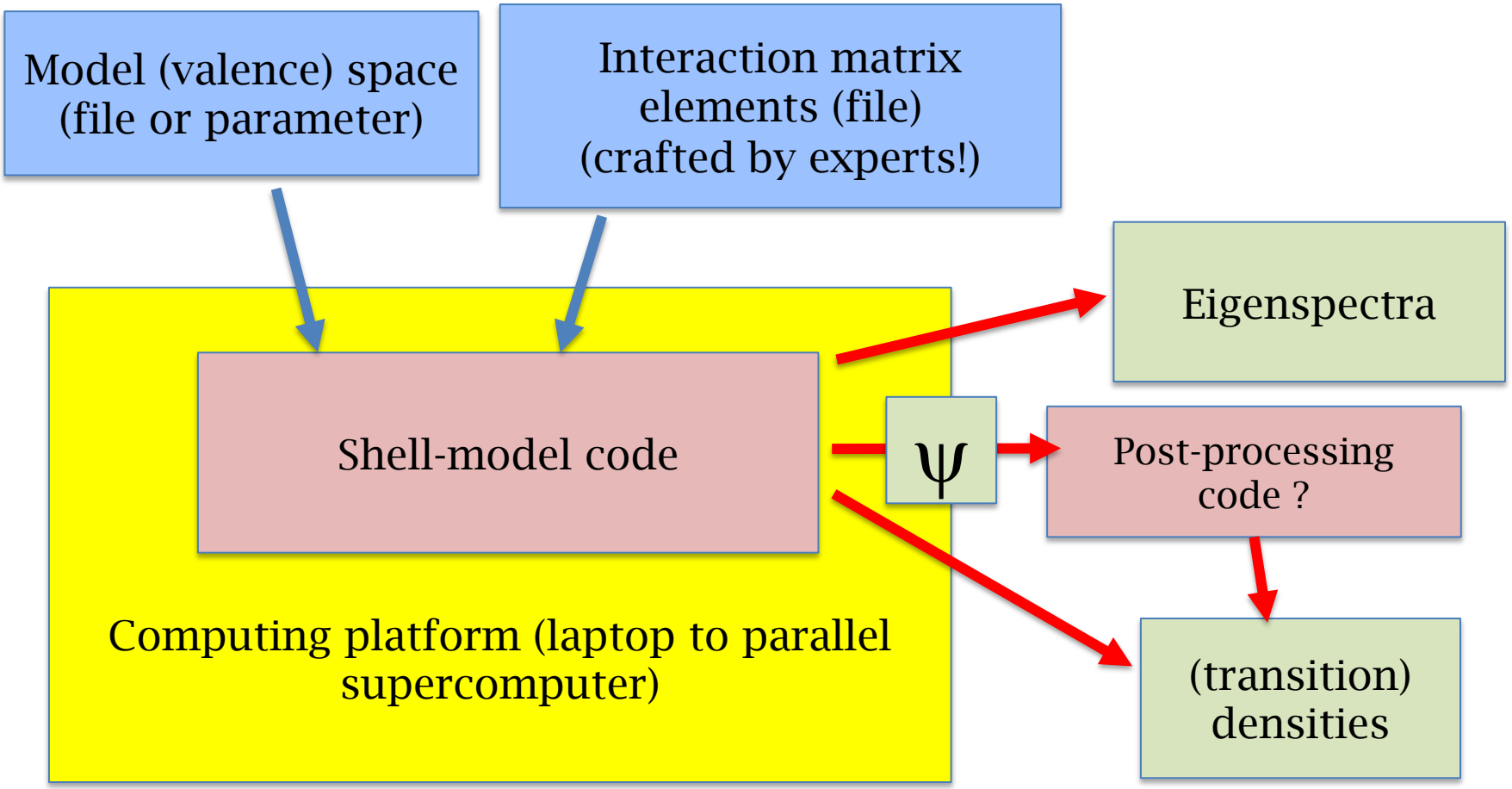
Model (valence) space
(file or parameter)

Interaction matrix
elements (file)
(crafted by experts!)

What goes into a shell model calculation



What goes into a shell model calculation



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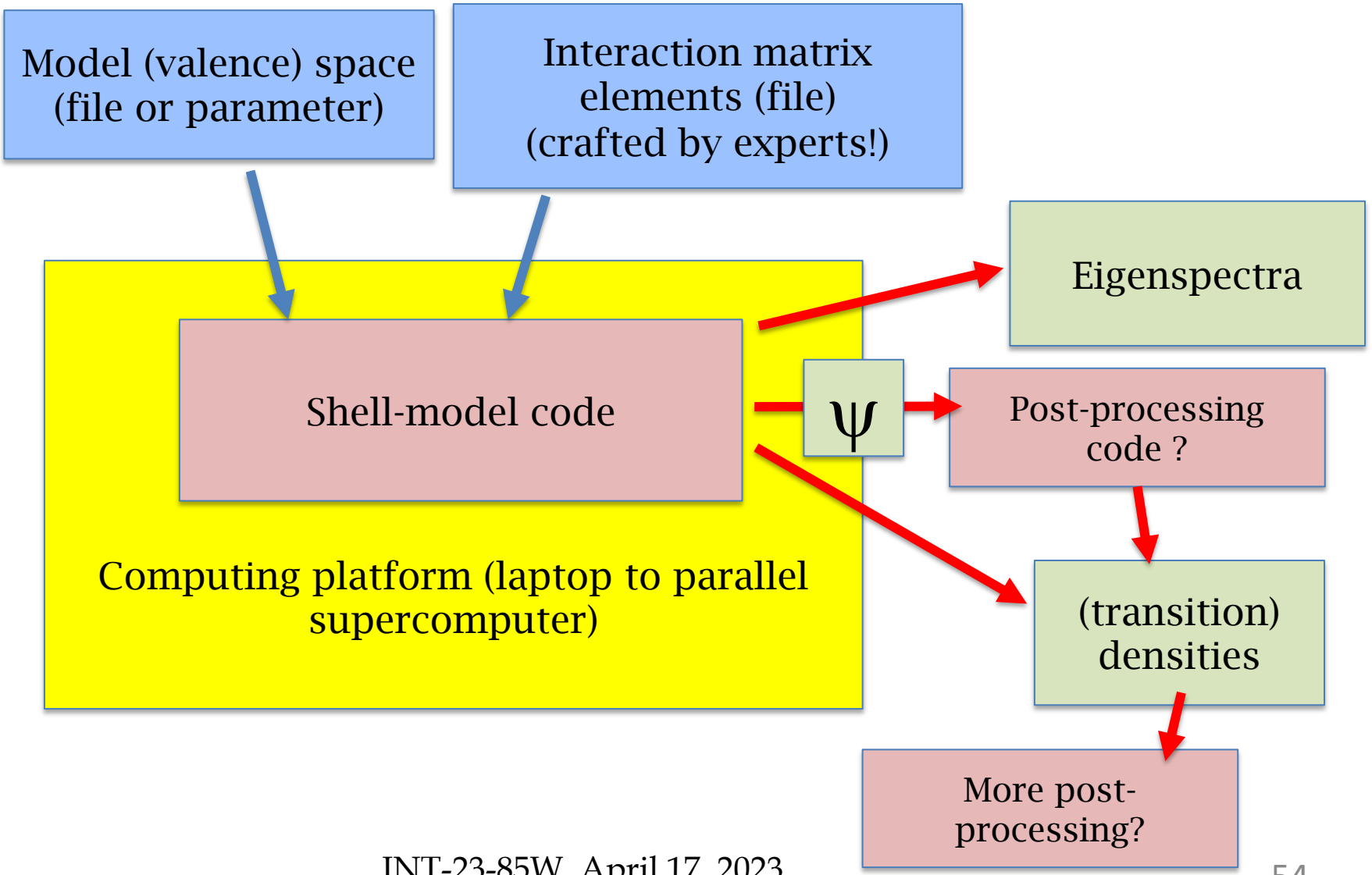

What can a shell model code calculate?

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- Hamiltonian eigenspectra and wave functions
- Matrix elements of one- and two-body (etc) operators between wave functions
- Spectroscopic factors (one-body easiest)

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+

- Strength functions of transition operators
- Group-theoretic decompositions
- Application of many-body Green's function

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San Diego State University

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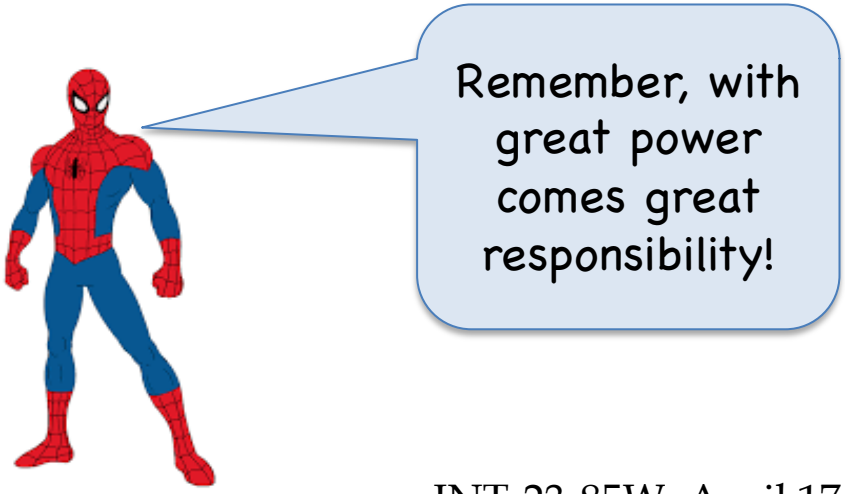

What's difficult for a shell model code?

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- 3- and 4-body forces and densities
- *Specific* highly excited states (if convergence required)

What's tricky for a shell model code?

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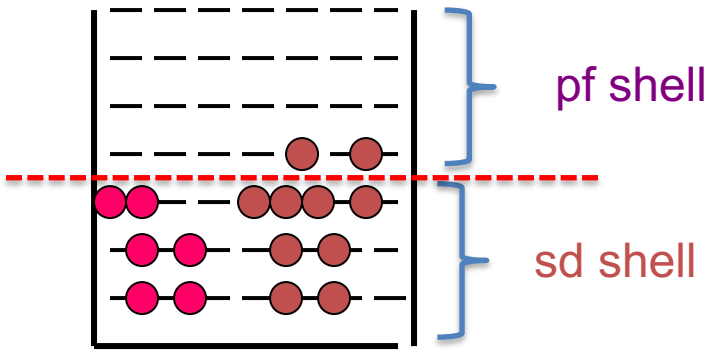
Cross-shell valence space calculations, e.g., *p*-*sd* or *sd*-pf

- Interactions are usually fitted to a very specific truncation; even if the code can handle a larger space, the results may not be valid
- One has to pay attention to spurious center-of-mass excitations

full M-scheme dimension

^{40}Mg: 286 billion

^{40}Ar: 927 trillion!



What's tricky for a shell model code?

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Cross-shell valence space calculations, e.g., *p-sd* or *sd*-pf

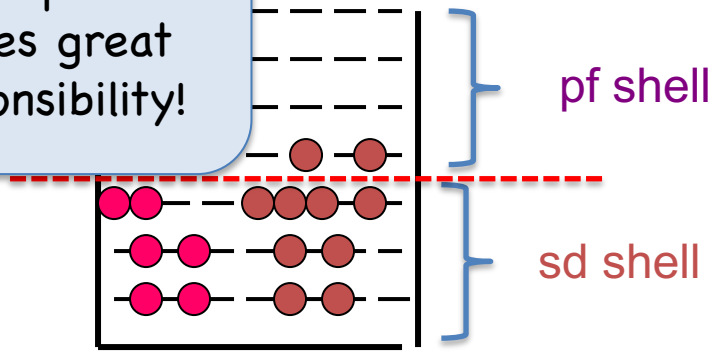
- Interactions are usually fitted to a very specific truncation; even if the code can handle a larger space, the results may not be valid
- One has to pay attention to spurious center-of-mass excitations

full M-sch…on

^{40}Mg:

^{40}Ar:

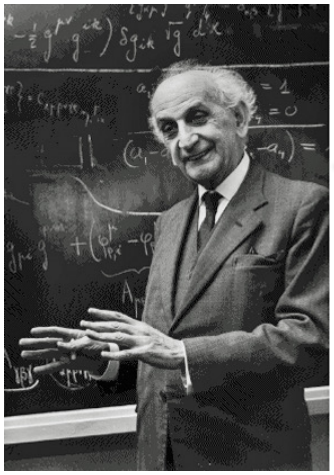
Remember, with great power comes great responsibility!



PART III

Some technical details

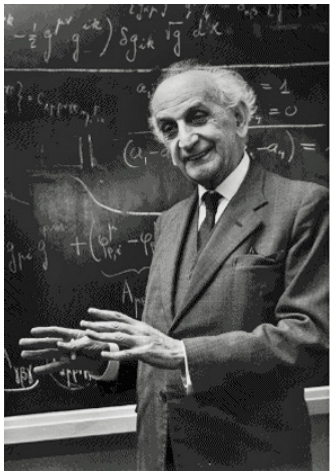
on the success of the shell model



(Cornelius Lanczos)

How do we solve such large matrices?

The Lanczos Algorithm!

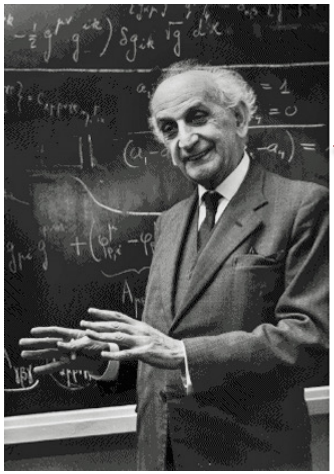


(Cornelius Lanczos)

$$\mathbf{A}\vec{v}_1 = \alpha_1\vec{v}_1 + \beta_1\vec{v}_2$$
$$\mathbf{A}\vec{v}_2 = \beta_1\vec{v}_1 + \alpha_2\vec{v}_2 + \beta_2\vec{v}_3$$
$$\mathbf{A}\vec{v}_3 = \beta_2\vec{v}_2 + \alpha_3\vec{v}_3 + \beta_3\vec{v}_4$$
$$\mathbf{A}\vec{v}_4 = \beta_3\vec{v}_3 + \alpha_4\vec{v}_4 + \beta_4\vec{v}_5$$

Starting from some initial vector (the "pivot") v_1 ,
the Lanczos algorithm iteratively creates
a new basis (a "Krylov space").

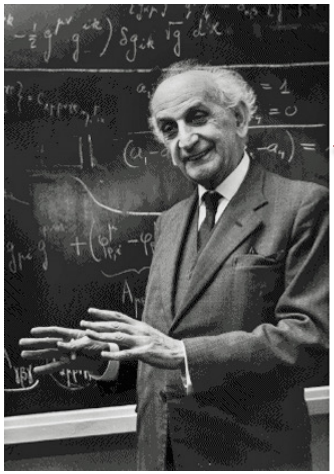
Lanczos is a special case of Arnoldi methods



(Cornelius Lanczos)

This transforms the matrix A into a new basis, in which A is now tridiagonal

$$H \rightarrow \hat{H} = \begin{pmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & \alpha_3 & \beta_3 & \\ & & \ddots & \ddots & \ddots \end{pmatrix}$$



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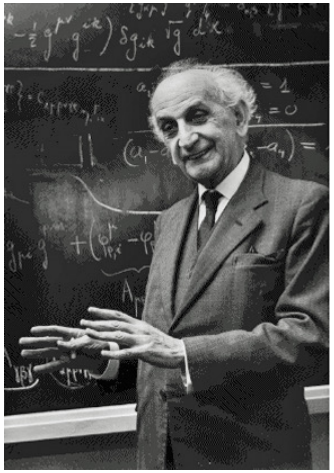
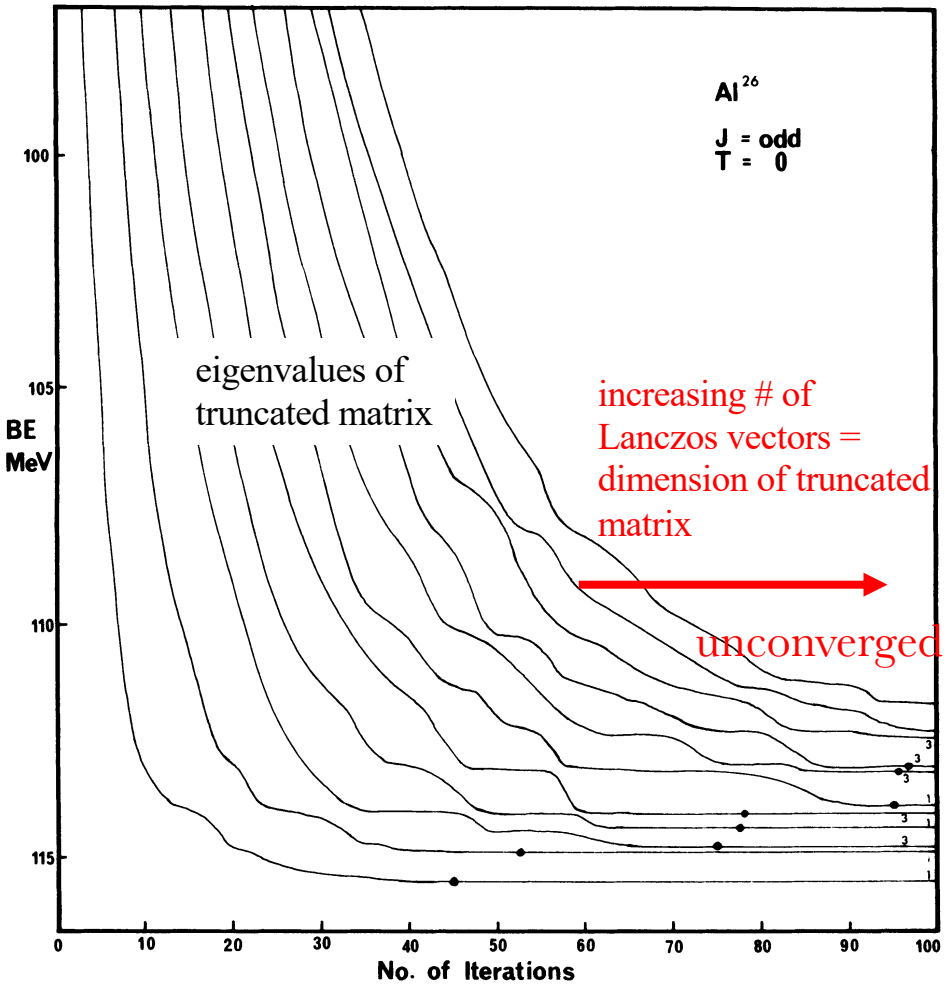
This is like Householder…except one does not fully transform the matrix.

The extremal eigenvalues of the transformed, truncated matrix quickly converge to the extremal eigenvalues of the original matrix!



(Cornelius Lanczos)



Whitehead, R. R., et al.
Advances in nuclear physics.
(1977) 123-176.

The one drawback of Lanczos is, due to round-off error, one must explicitly enforce orthogonality of Lanczos vectors

("reorthogonalization")

Consider three ways to compute the strength function:

1. Transitions between individual initial and final states (using transition densities):

requires converged initial, final states

2. Transition from a converged initial state to unconverged final states using "Lanczos trick"

difficult to get converged initial state at high energy

3. (NEW) Transitions from semi-converged initial state to unconverged final states using "Lanczos trick"

requires a local approximation to Brink-Axel

The *naïve* way to compute strength functions is between individual, converged states, both initial and final states

$$\langle f|\hat{O}|i\rangle = \sum_{a,b} \langle a|\hat{O}|b\rangle \langle f|\hat{c}_a^+ \hat{c}_b|i\rangle$$

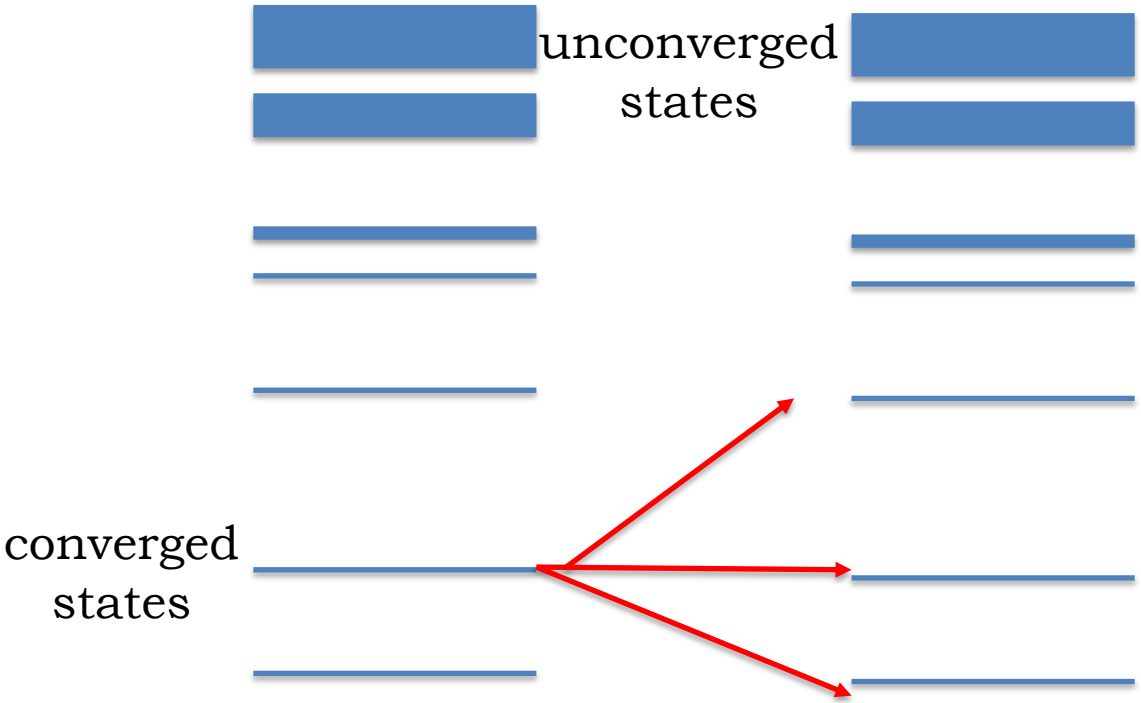
Many-body matrix element

One-body matrix element

One-body density matrix elements between many-body states

$$S(E_i, E_x) = \sum_f |\langle f|\hat{T}|i\rangle|^2 \delta(E_x - E_f + E_i)$$

The *naïve* way to compute strength functions is between individual, converged states, both initial and final states



But higher states take more Lanczos iterations to converge

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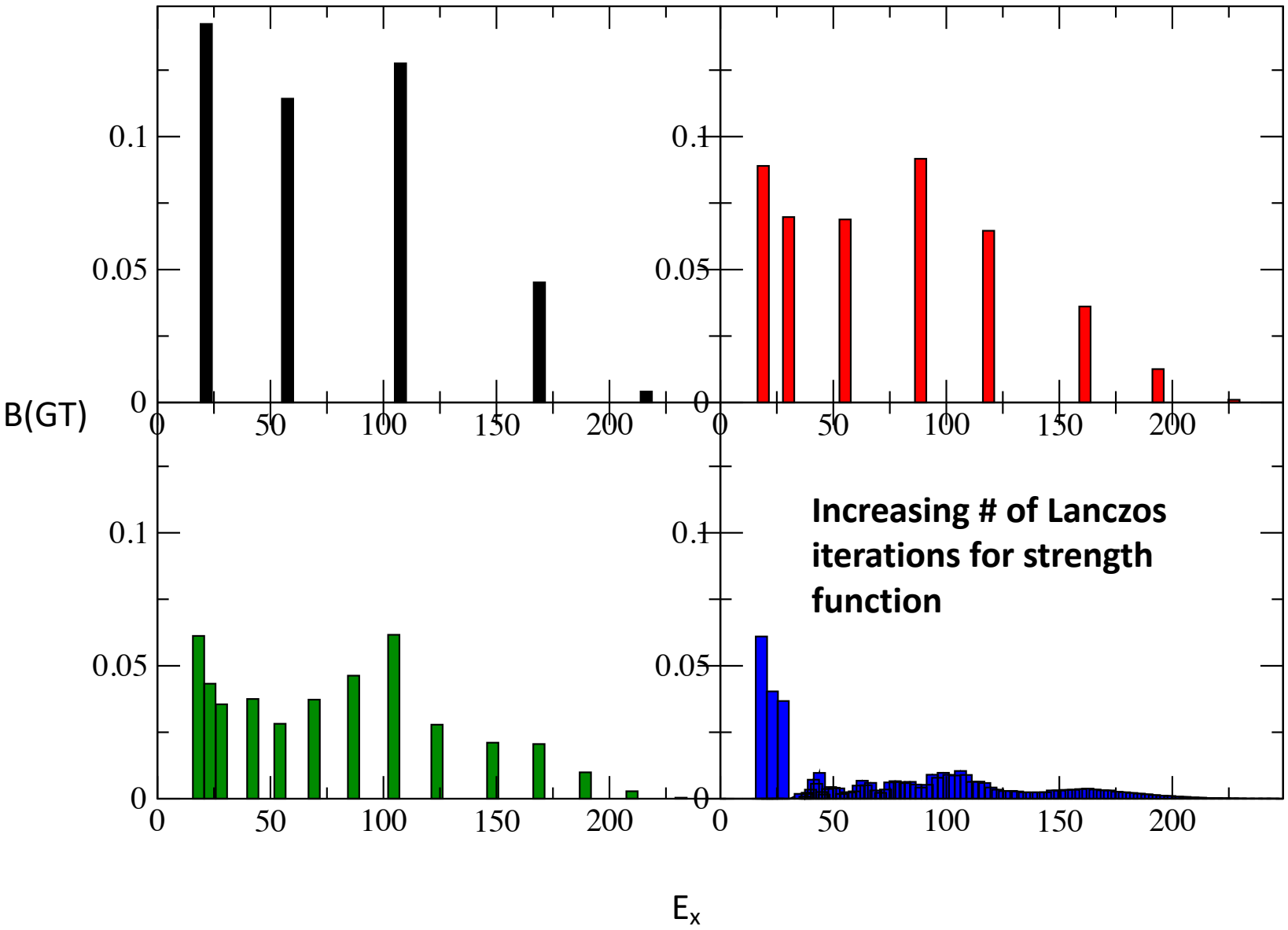
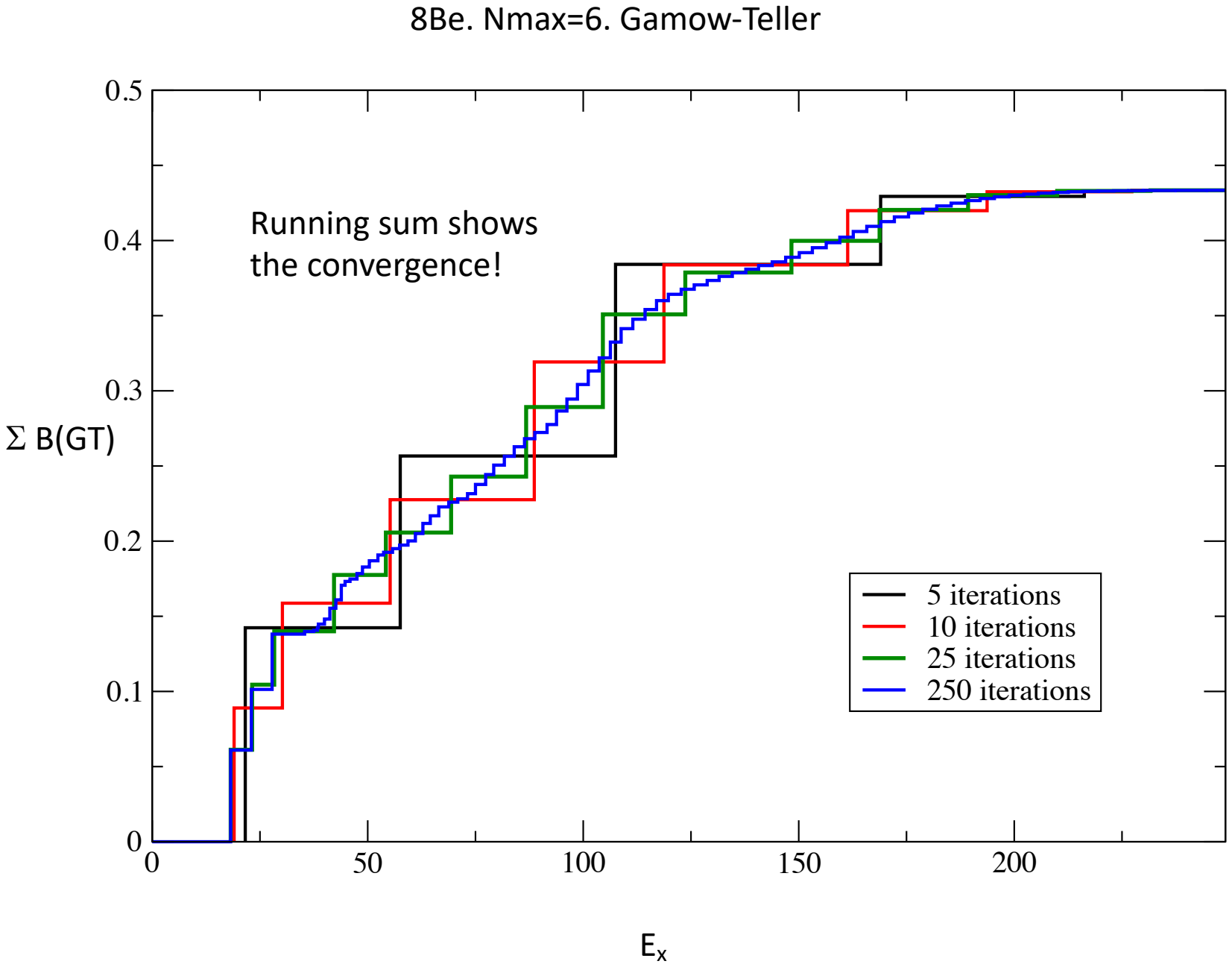
Do we need each individual transition?

There is a 'trick' for generating strength functions easily using Lanczos.

Whitehead and Watt *J Phys G* **4**, 835(1978)
Whitehead, Watt, and Kelvin. *Phys Lett* ***B*** **89**, 313 (1980)
Whitehead in *Theory and Applications of Moment Methods in Many-Fermion Systems,* 235 (1980)
Bloom, Prog. Part. Nucl. Phys **11**, 205 (1984)

8Be. Nmax=6. Gamow-Teller




8Be. Nmax=6. Gamow-Teller
Running sum shows
the convergence!
Σ B(GT)
E_x
0
0.1
0.2
0.3
0.4
0.5
0
50
100
150
200
5 iterations
10 iterations
25 iterations
250 iterations

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This works because Lanczos generates exact moments of the strength function (2n-1 for n iterations)

See e.g. Whitehead in *Theory and Applications of Moment Methods in Many-Fermion Systems*, 235 (1980)

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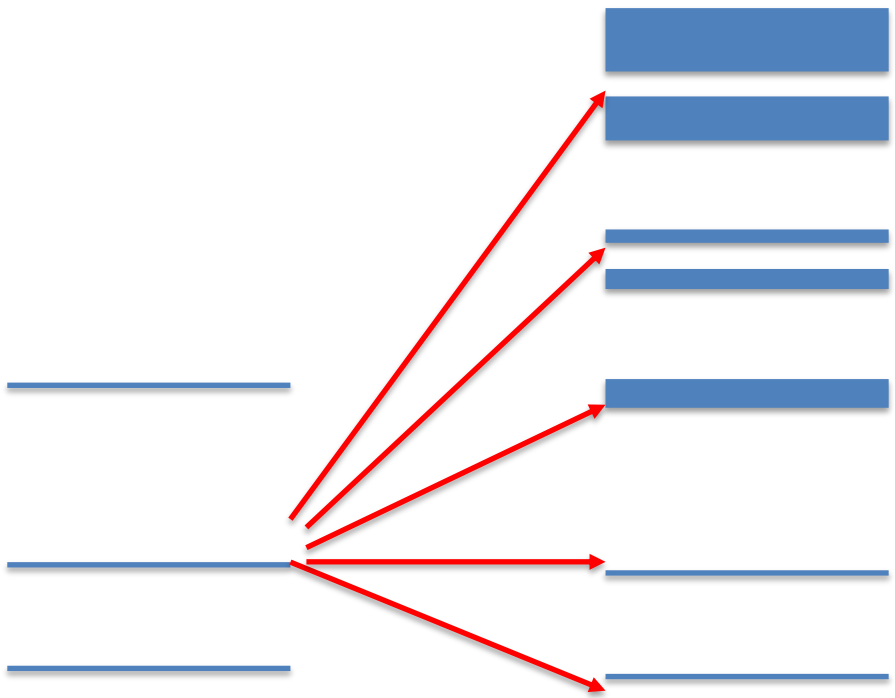
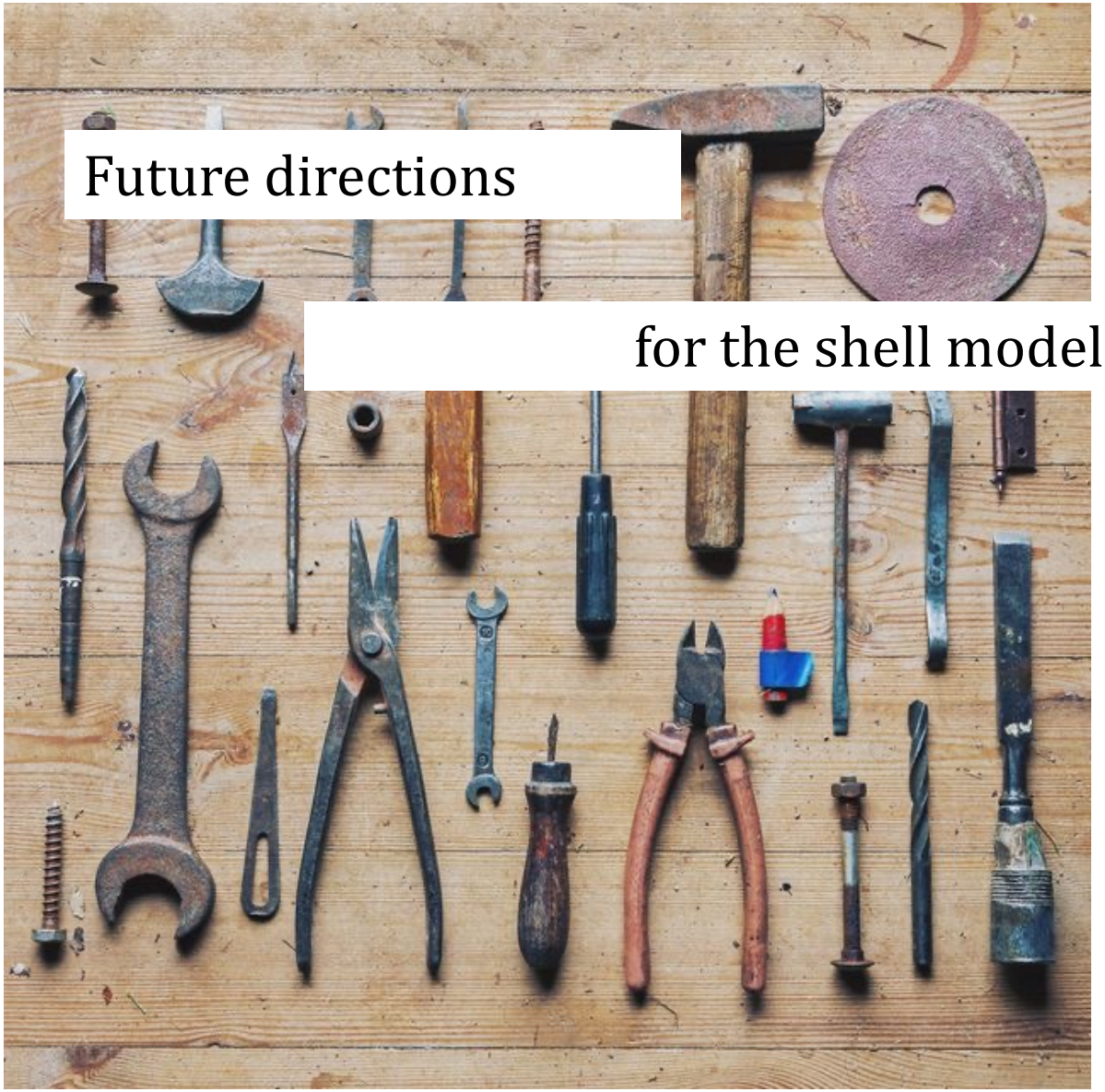
The *initial* state is converged, but final states *do not need to be converged*

(because moments)



PART IV



Future directions

for the shell model

FUTURE DIRECTIONS FOR SHELL MODEL CALCULATIONS

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- Coupling separate proton and neutron states
- Novel efficient truncation scheme
- Generator-coordinate-like approach
- Group-theoretical truncations

Future directions for shell model calculations

San Diego State University

- Coupling separate proton and neutron states
- Novel efficient truncation scheme
- Generator-coordinate-like approach
- Group-theoretical truncations

motivated by looking at proton-neutron 'entanglement entropy', CWJ & Gorton, J. Phys. G **50**, 045110 (2023).

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:

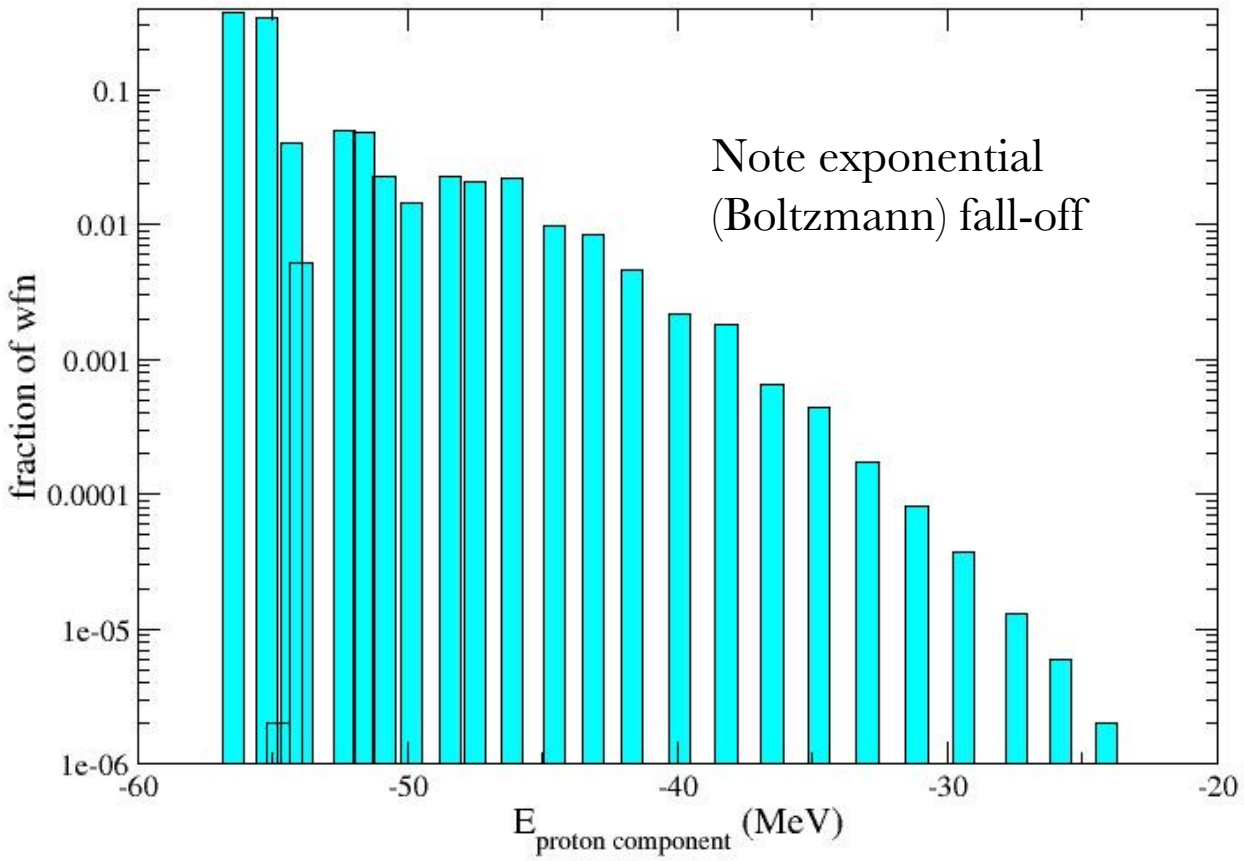
$$\left|\Psi_J\right\rangle = \sum_{ab} c_{ab} \left[\left|\Psi_p a, J_p\right\rangle \otimes \left|\Psi_n b, J_n\right\rangle\right]_J$$

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

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

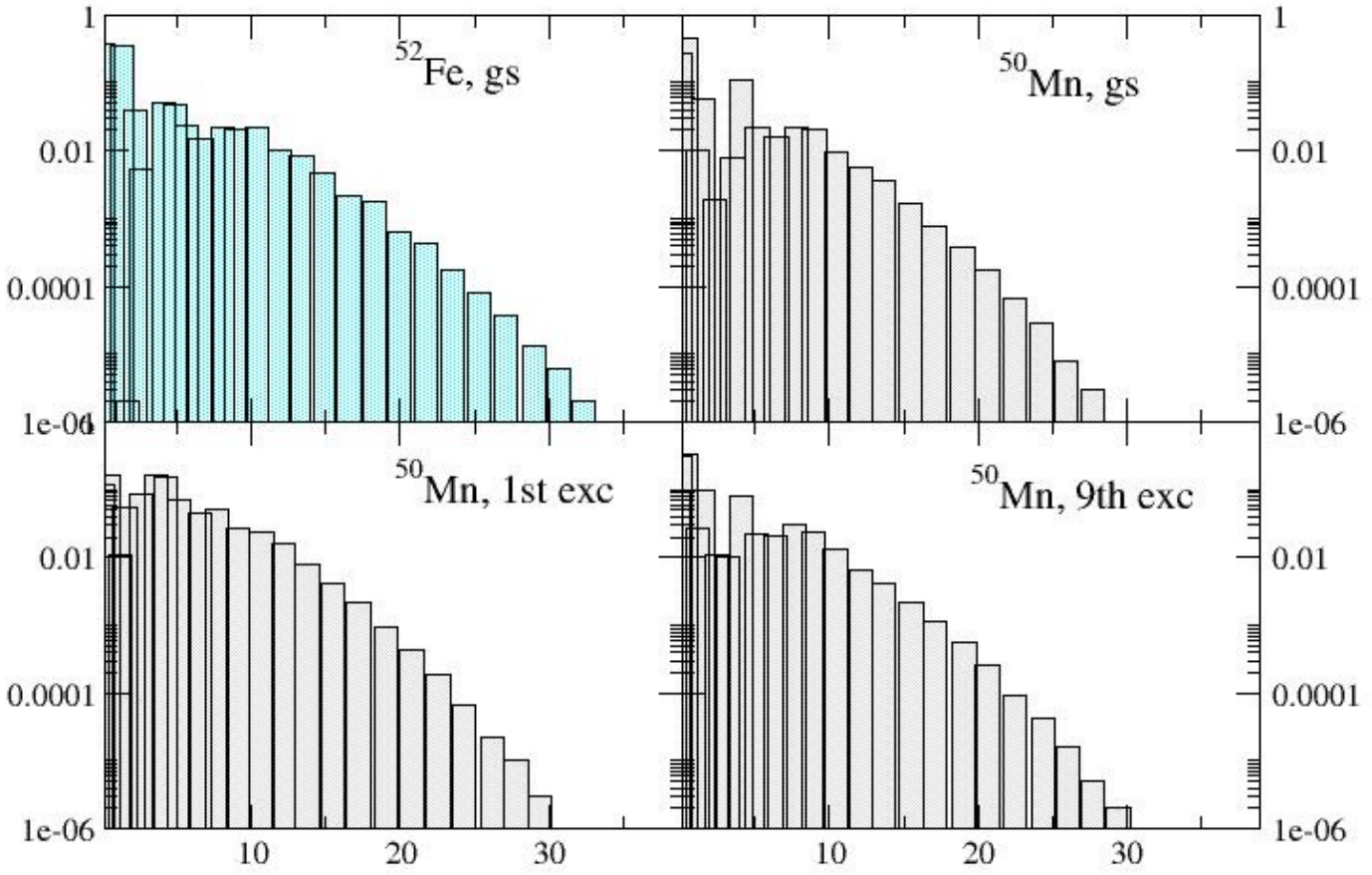
decomposition of g.s.



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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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

INT-23-85W, April 17, 2023

Oliver Gorton

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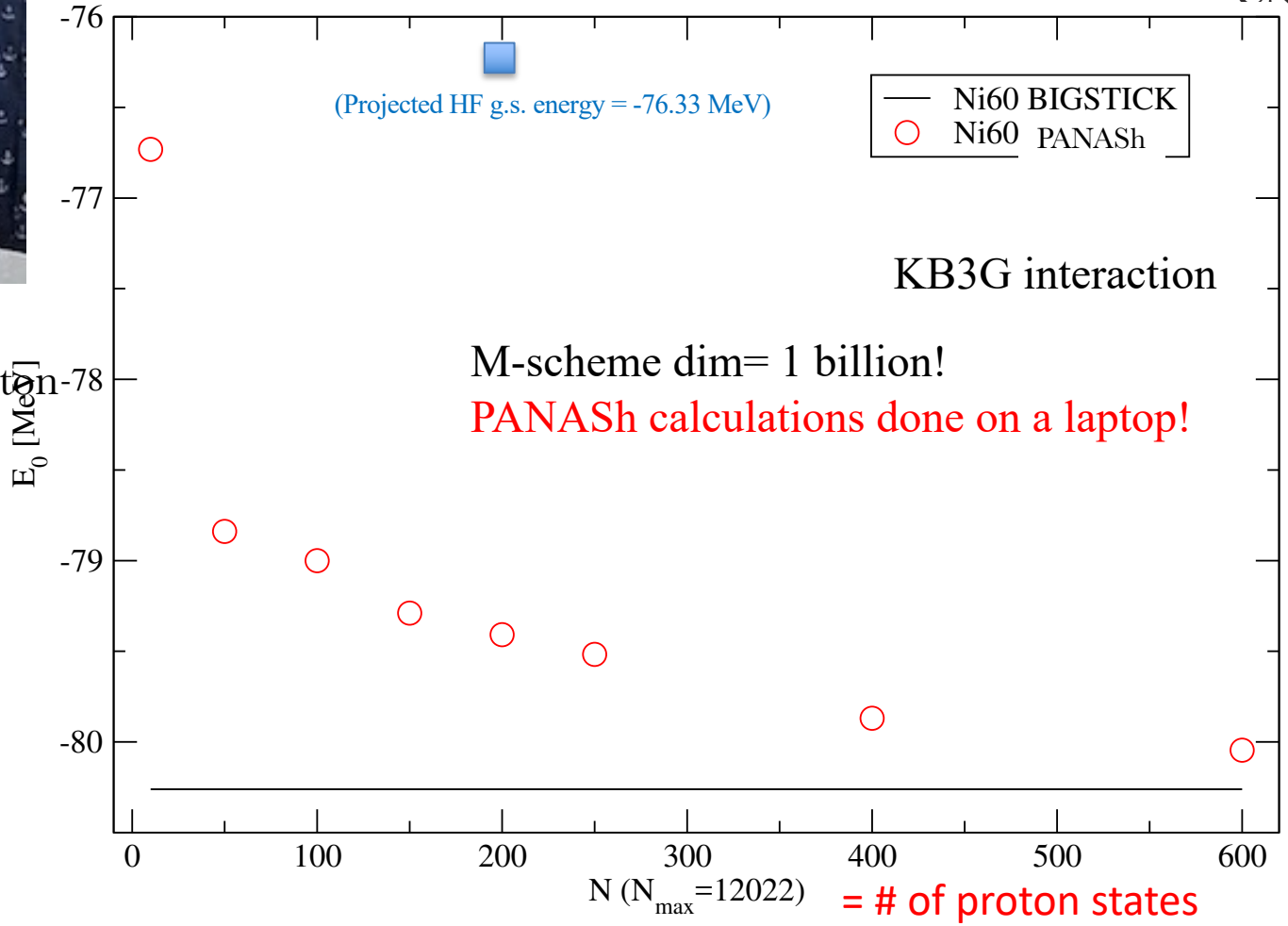
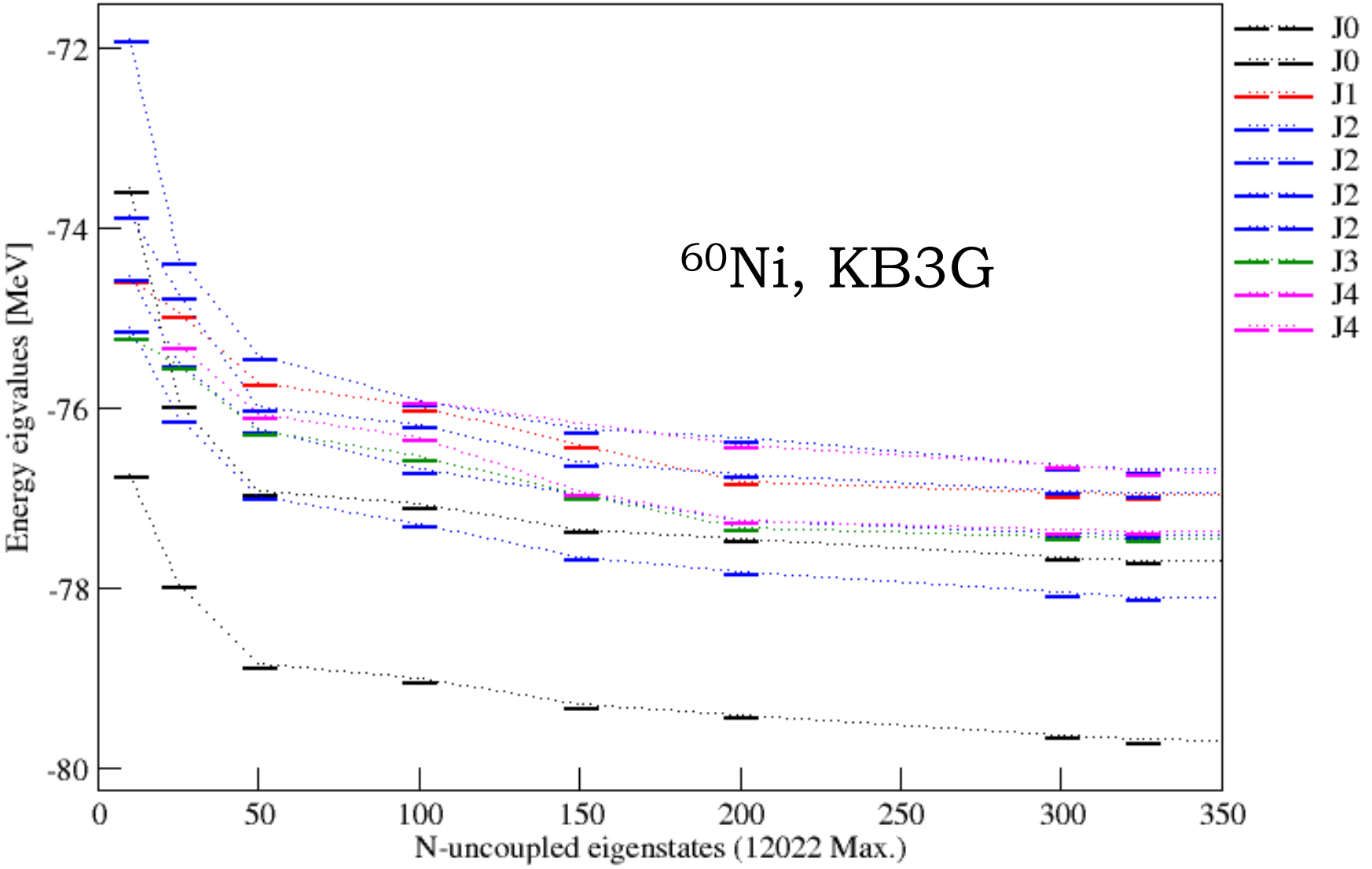
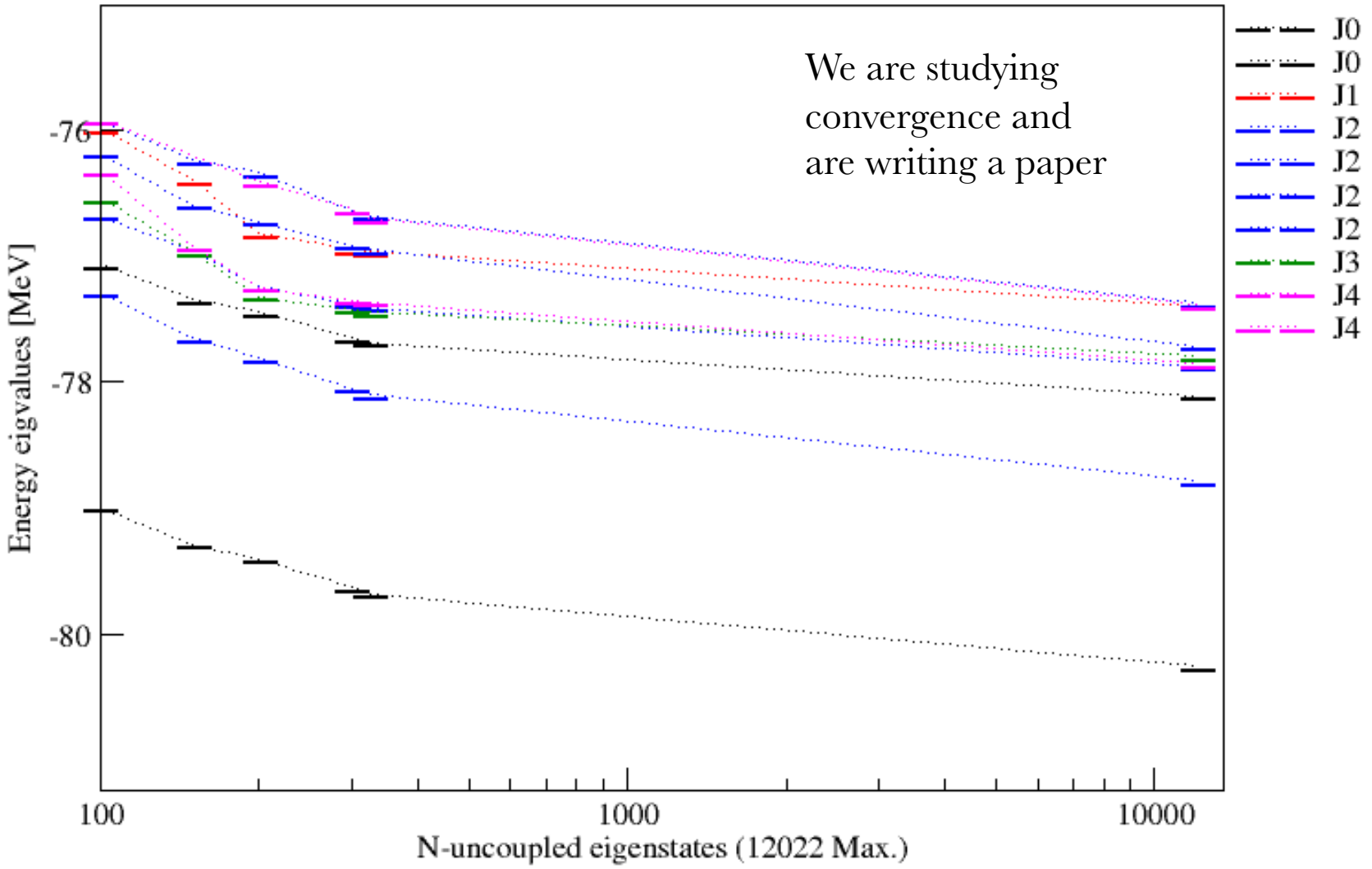



^{60}Ni, KB3G
Energy eigvalues [MeV]
-72
-74
-76
-78
-80
0
50
100
150
200
250
300
350
N-uncoupled eigenstates (12022 Max.)
J0
J0
J1
J2
J2
J2
J2
J3
J4
J4


We are studying
convergence and
are writing a paper
J0
J0
J1
J2
J2
J2
J2
J3
J4
J4
-76
-78
-80
Energy eigvalues [MeV]
100
1000
10000
N-uncoupled eigenstates (12022 Max.)

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Summary:

Modern nuclear structure physics is **modern** and a vigorous, rigorous discipline, **necessary** for many other fields (astrophysics, tests of fundamental symmetries, etc.)

One approach is **diagonalization of the Hamiltonian in a basis.** Modern techniques and computers can handle up to ~ 35 billion basis states (though that is is not the primarily measure of computational burden) and there are many promising techniques for extending the reach and accuracy of shell model calculations