Gamma-ray strength functions using approximate shell model calculations

T3 “Taking the Temperature”
Workshop on Statistical Nuclear Physics for Astrophysics and Applications
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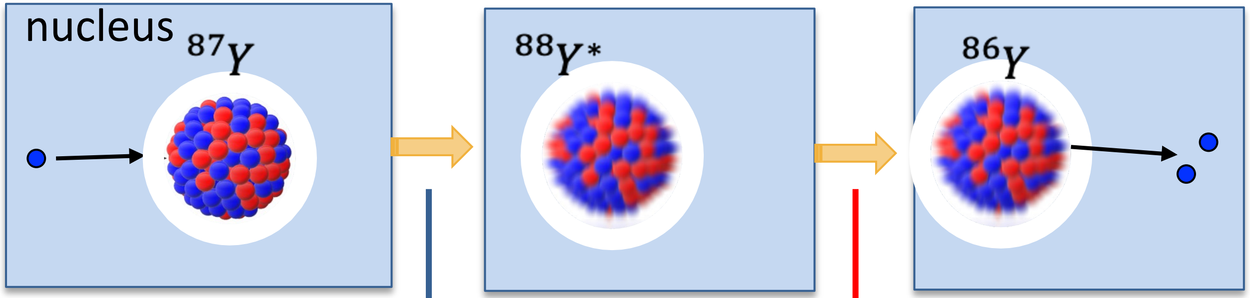
Compound nuclear (CN) reactions have two stages

Desired reaction

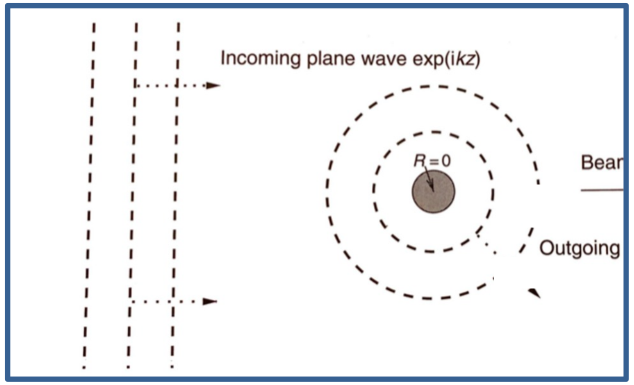
Target nucleus | Compound nucleus | Residual nucleus



CN cross section = (formation) x (decay)

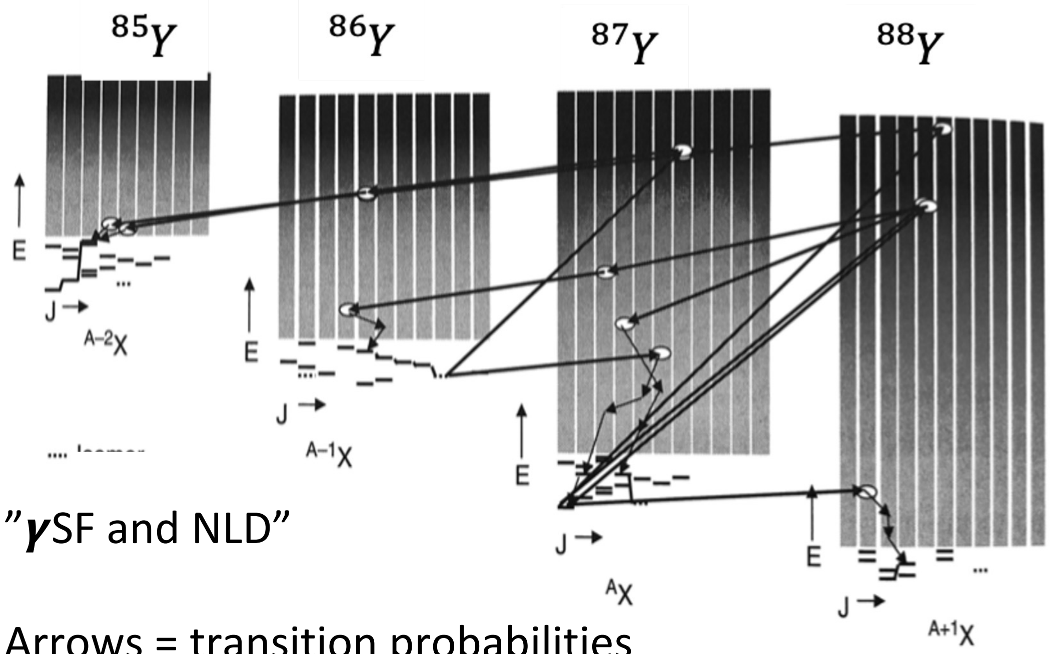
1. Formation

2. Decay



"Optical model"

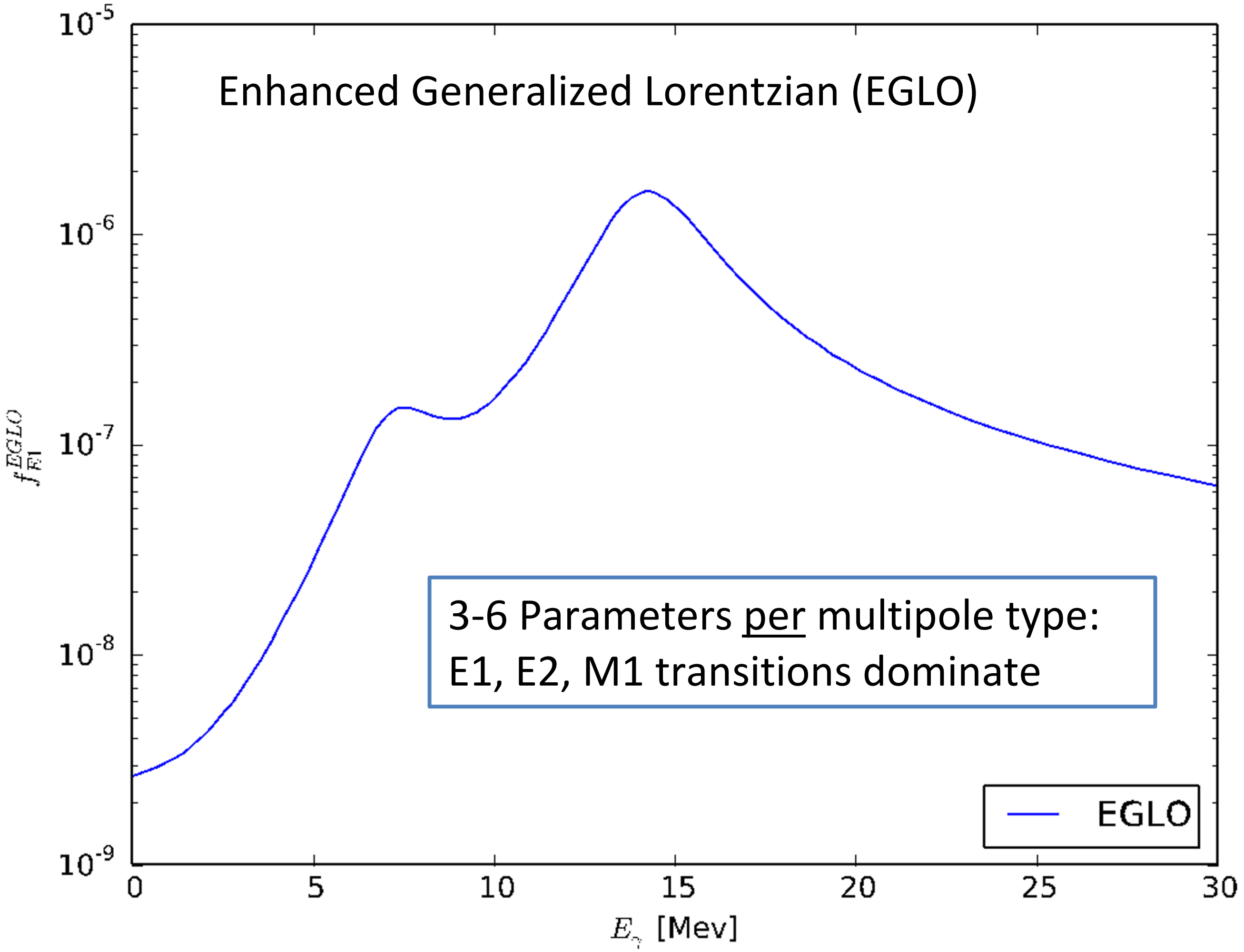
Figures from: "Nuclear Reactions for Astrophysics" Thompson and Nunes



"γSF and NLD"

Arrows = transition probabilities

Gamma-ray strength functions (gSF) approximate transition probabilities between (internal) states



Usage: CN is at some excitation energy, what is the probability to emit a gamma-ray of a particular energy?

How are Gamma ray strength functions measured or constrained?

- Direct methods: e.g. Photo absorption
- Indirect methods: e.g. Oslo methods, Surrogate methods

Photo-absorption cross section as overlapping gamma-widths

$$\langle \sigma_{\text{abs}}^{XL}(E_\gamma) \rangle = (2L+1)\frac{\pi^2}{k_\gamma^2}\frac{1}{\Delta E}\sum_{E_f=E_\gamma}^{E_\gamma+\Delta E} \Gamma_{0\to f}^{XL}$$

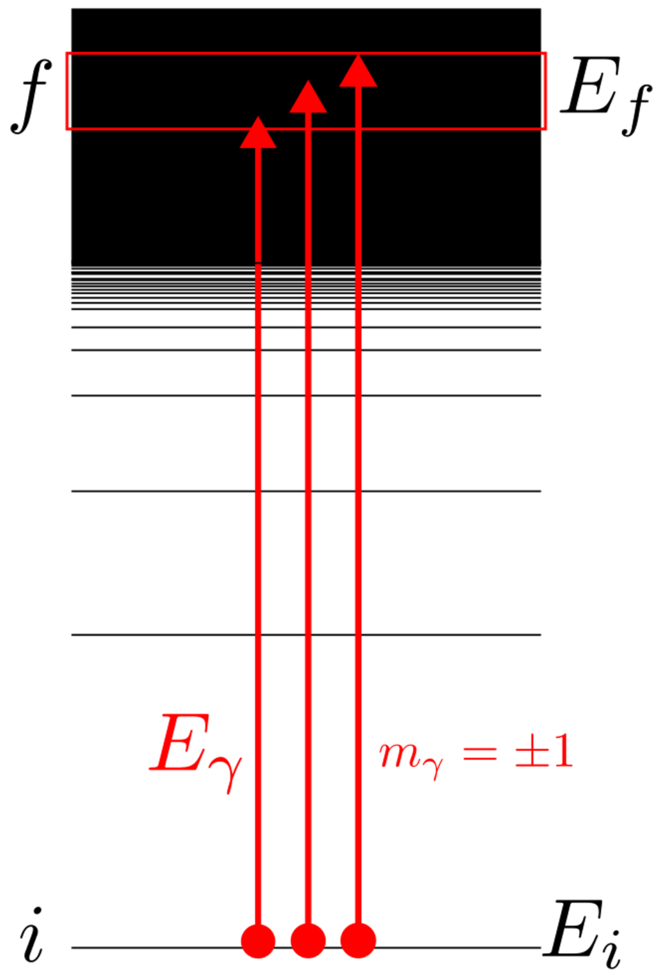


Photo-absorption cross section as overlapping gamma-widths

$$\langle \sigma_{\text{abs}}^{XL}(E_\gamma)\rangle = (2L+1)\frac{\pi^2}{k_\gamma^2}\frac{1}{\Delta E}\sum_{E_f=E_\gamma}^{E_\gamma+\Delta E}\Gamma_{0\to f}^{XL}$$

$$= (2L+1)\frac{\pi^2}{k_\gamma^2}\langle \Gamma_{0\to f}^{XL}\rangle_f\,\rho(E_f, J_f^\pi)$$

(Density of accessible states)

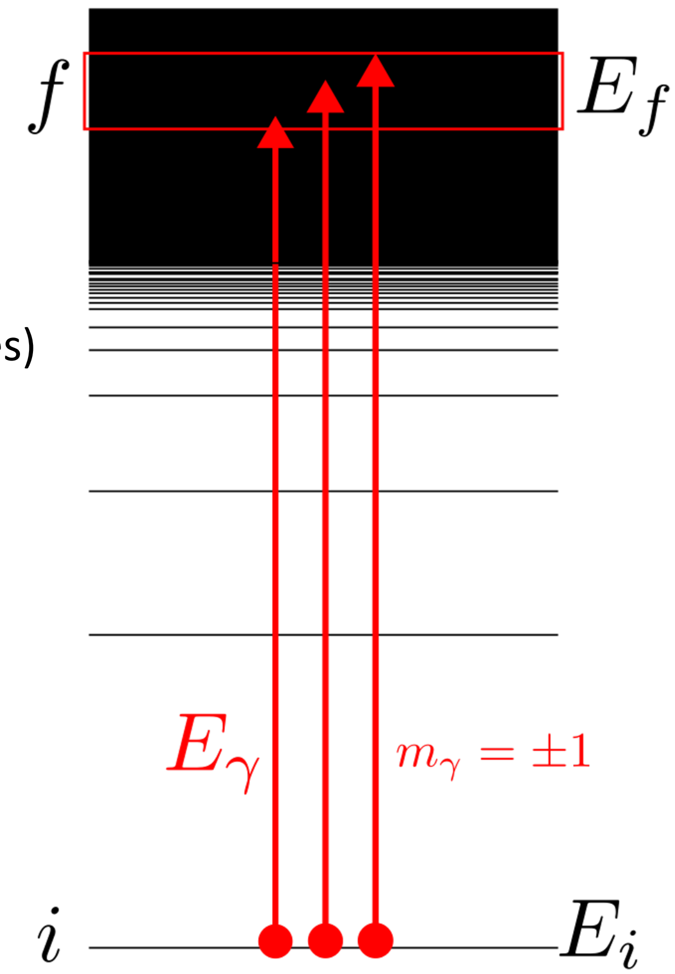


Photo-absorption cross section as overlapping gamma-widths

$$\langle\sigma^{XL}_{\text{abs}}(E_\gamma)\rangle = (2L+1)\frac{\pi^2}{k_\gamma^2}\frac{1}{\Delta E}\sum_{E_f=E_\gamma}^{E_\gamma+\Delta E}\Gamma^{XL}_{0\to f}$$

$$= (2L+1)\frac{\pi^2}{k_\gamma^2}\langle\Gamma^{XL}_{0\to f}\rangle_f\,\rho(E_f, J_f^\pi)$$

(Density of accessible states)

$$= (2L+1)\frac{\pi^2}{k_\gamma^2}E_\gamma^{2L+1}\overrightarrow{f}^{XL}(E_\gamma)$$

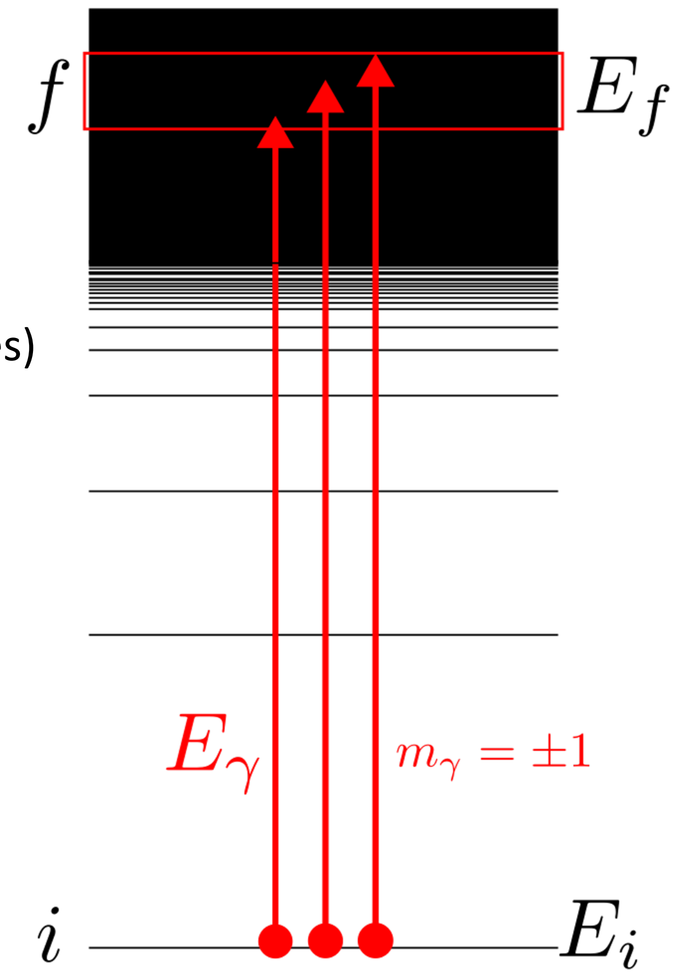


Photo-absorption cross section as overlapping gamma-widths

$$\langle \sigma_{\text{abs}}^{XL}(E_\gamma)\rangle = (2L+1)\frac{\pi^2}{k_\gamma^2}\frac{1}{\Delta E}\sum_{E_f=E_\gamma}^{E_\gamma+\Delta E}\Gamma_{0\to f}^{XL}$$

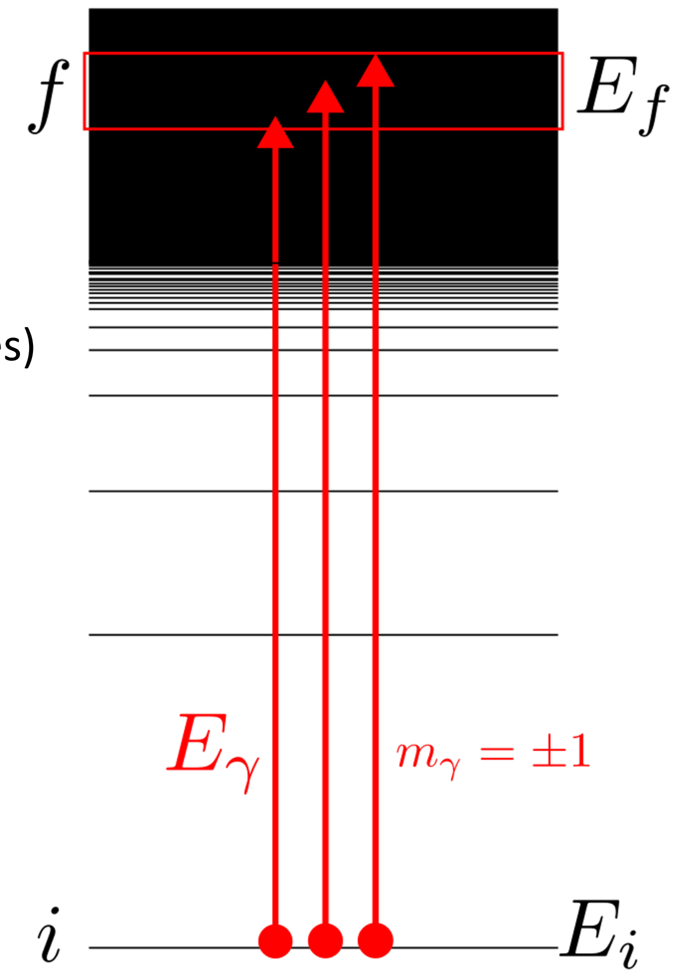
$$= (2L+1)\frac{\pi^2}{k_\gamma^2}\langle\Gamma_{0\to f}^{XL}\rangle_f \rho(E_f, J_f^\pi)$$

(Density of accessible states)

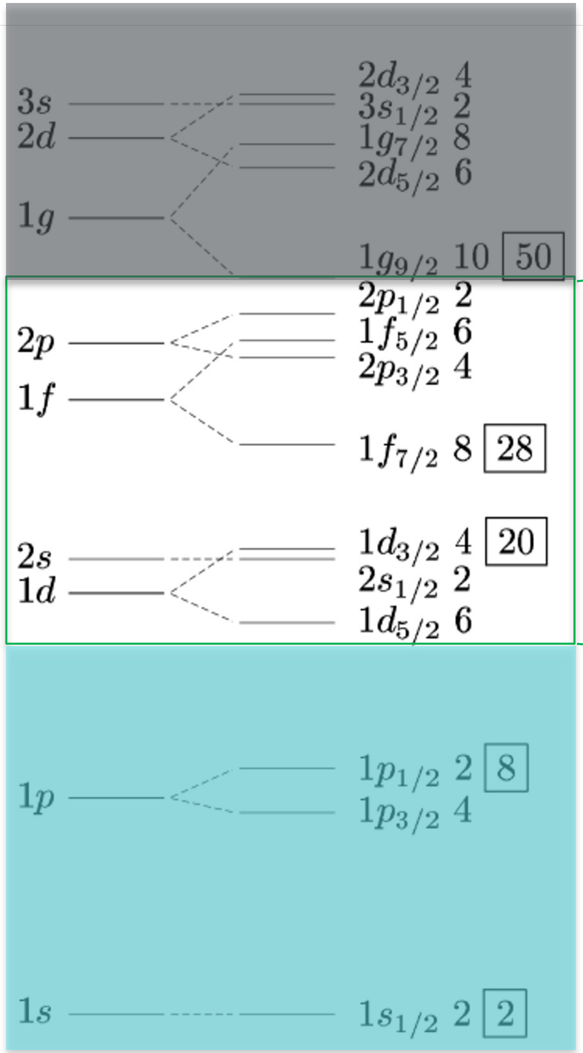
$$= (2L+1)\frac{\pi^2}{k_\gamma^2}E_\gamma^{2L+1}\overrightarrow{f}^{XL}(E_\gamma)$$

$$\overrightarrow{f}^{XL}(E_\gamma) = \frac{\langle\Gamma_{0\to f}^{XL}\rangle_f \rho(E_f, J_f^\pi)}{E_\gamma^{2L+1}}$$

“Bartholomew definition”



Shell Model takes all combinations of particle excitations in the valence space to capture many-body physics

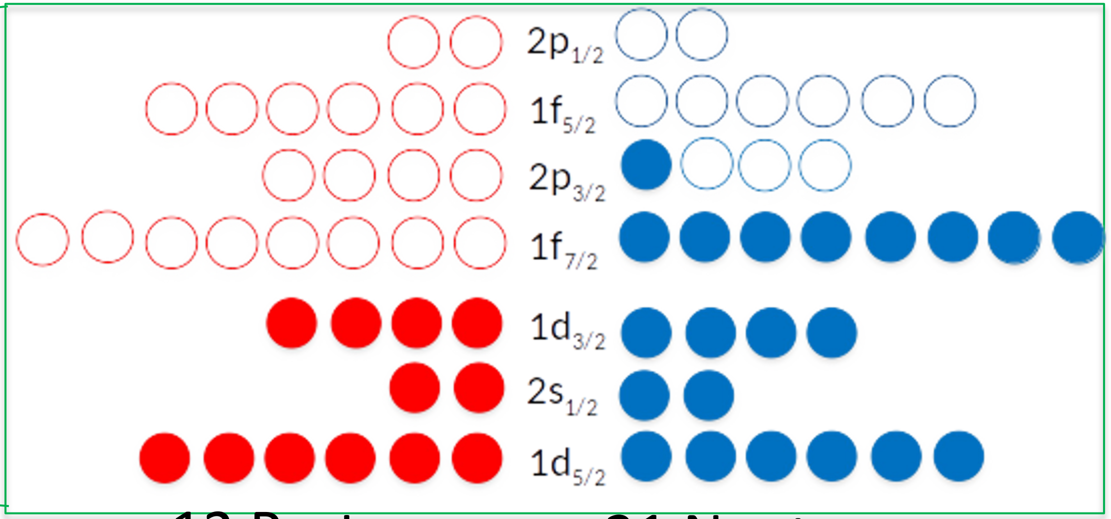


"∞" excluded states

Valence space

Frozen core

^{49}Ca in the sd-pf space



12 Protons

21 Neutrons

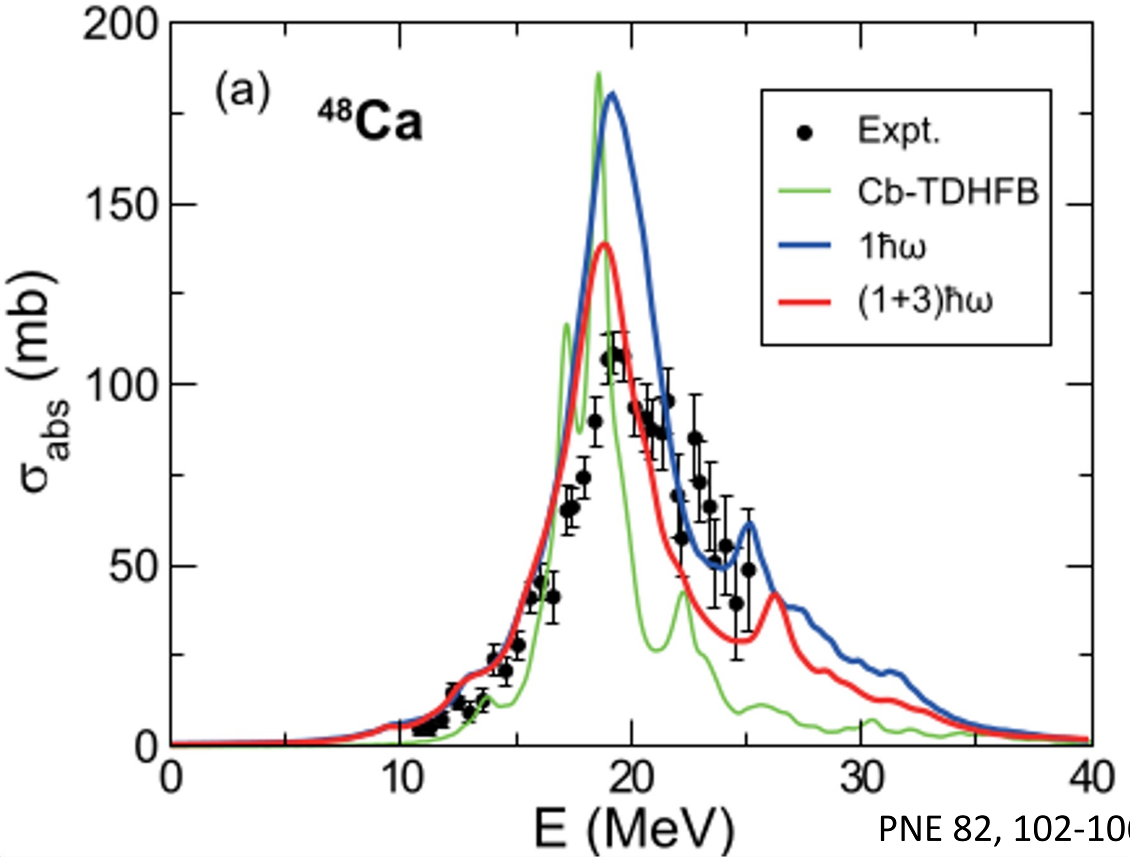
Configurations: 1×10^7

Configurations: 9×10^6

(Orders of magnitude smaller!)

Shell model can reproduce photoabsorption with a 1hw truncation

$$\overrightarrow{f}^{XL}(E_\gamma = E_f) = \frac{8\pi(L+1)}{(\hbar c)^{2L+1}L[(2L+1)!!]^2}\frac{1}{\Delta E}\sum_{E_f}^{E_f+\Delta E} B^{XL}_{0\to f}$$



PNE 82, 102-106 (2015)

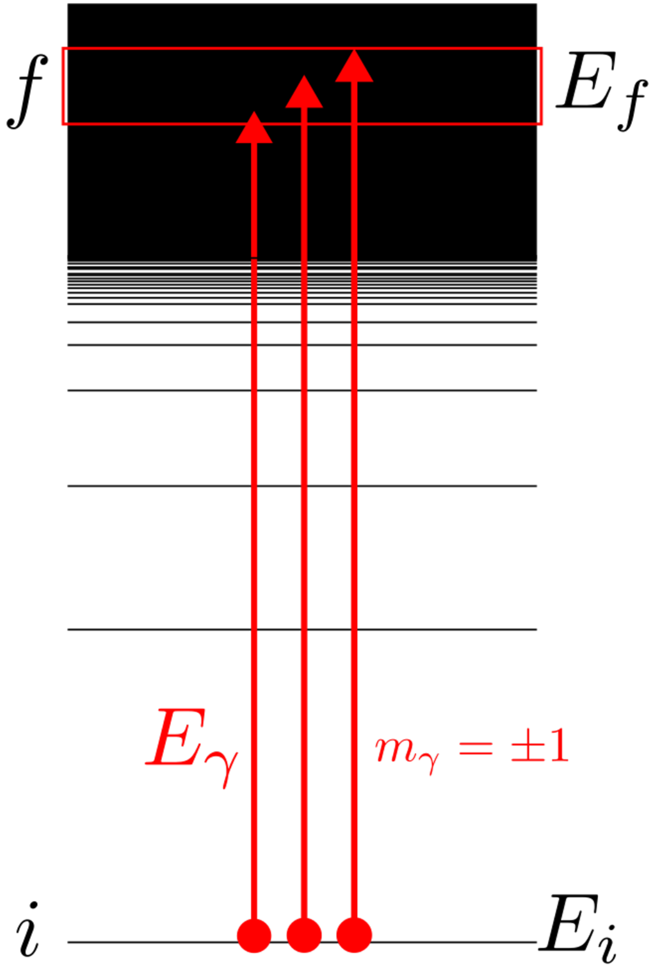


Photo de-excitation "downward" to *specific* isolated states

"Swap" initial and final states:

$$\overleftarrow{f}^{XL}(E_\gamma = E_i - E_f, E_f) = \frac{\langle \Gamma^{XL}_{i\to f}\rangle_i \rho(E_i, J_i^\pi)}{E_\gamma^{2L+1}}$$

$$= \frac{8\pi(L+1)}{(\hbar c)^{2L+1} L[(2L+1)!!]^2} \langle B^{XL}_{i\to f}\rangle_i \rho(E_i, J_i^\pi)$$

$\rho(E_i, J_i^\pi)$: Density of initial states which can transition to *specific* final state f

Brink-Axel hypothesis:

$$\overleftarrow{f^{XL}}(E_\gamma = E_i - E_f, E_f) \approx \overleftarrow{f^{XL}}(E_\gamma = E_i, 0)$$

ELBAH (Energy localized Brink-Axel hypothesis):

$$\overleftarrow{f^{XL}}(E_\gamma, E_f) \approx \overleftarrow{f^{XL}}(E_\gamma, E_f + \delta)$$

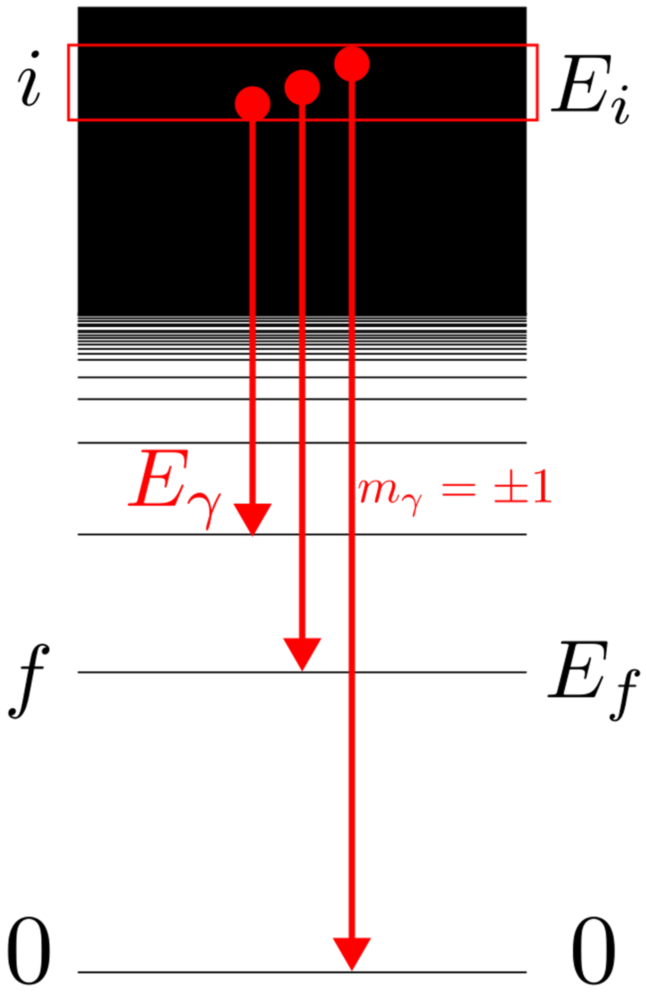


Photo de-excitation “downward” to another energy bin

- Low energy enhancement, “upbend”

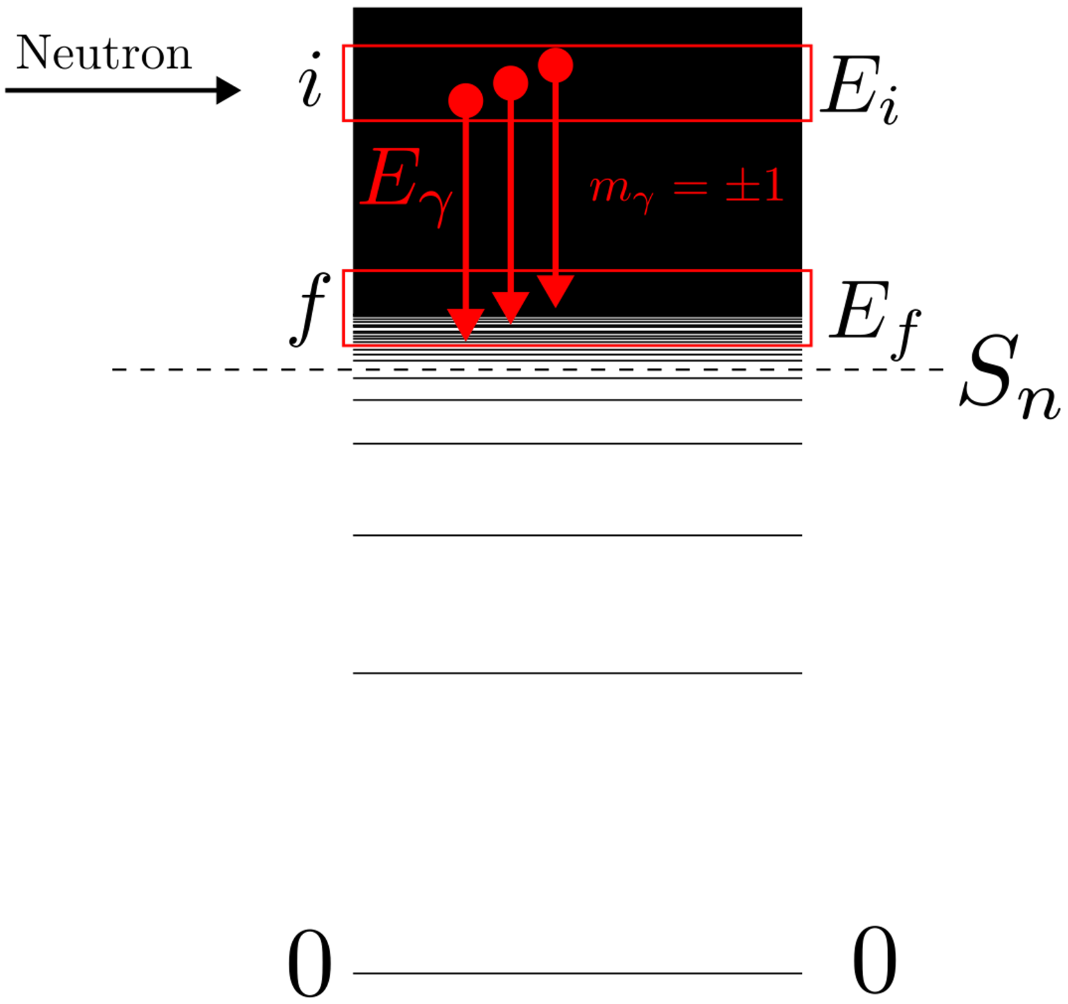


Photo de-excitation “downward” to another energy bin

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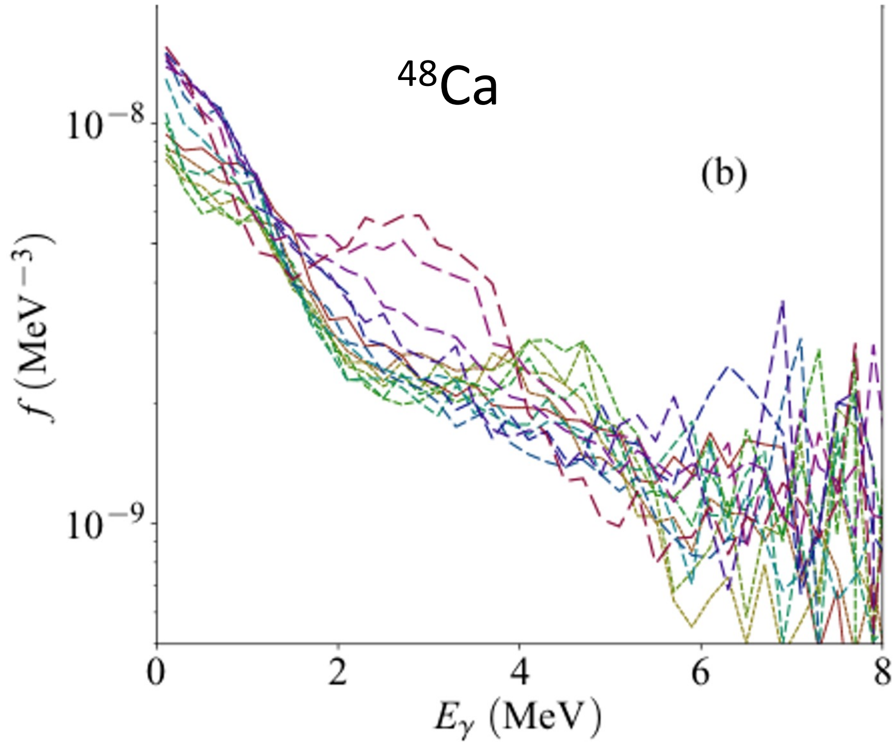
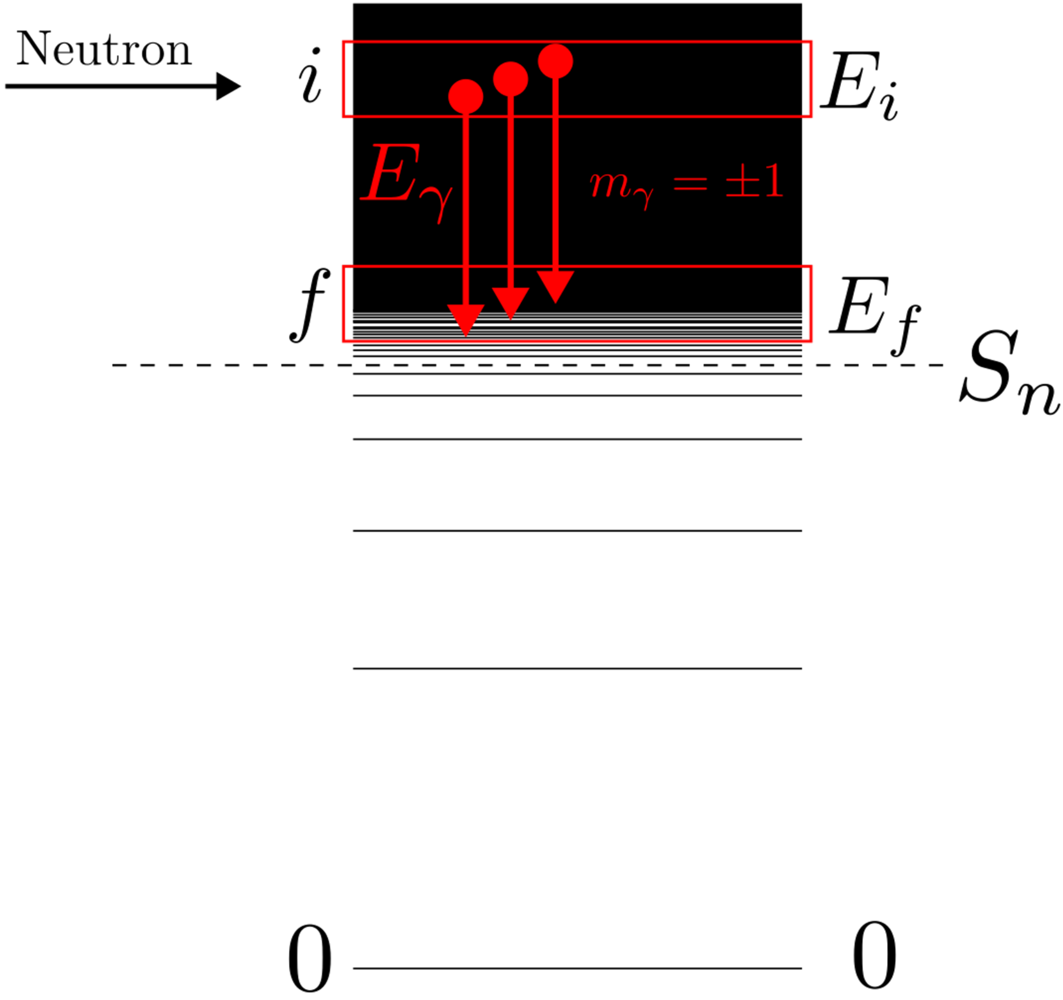


FIG. 4. γ-ray strength functions of isotopic chains of Ni calculated with ^{56}Ni (a) and ^{48}Ca (b) closed cores, respectively. See text for details.

PRC 98, 064321 (2018)



Definition of the “level density" is subtle

$$\overleftarrow{f}^{XL}(E_\gamma = E_i - E_f, E_f) = \frac{\langle \Gamma^{XL}_{i\to f}\rangle_i \rho(E_i, J_i^\pi)}{E_\gamma^{2L+1}}$$

$$= \frac{8\pi(L+1)}{(\hbar c)^{2L+1} L[(2L+1)!!]^2} \langle\langle B^{XL}_{i\to f}\rangle_i \rho(E_i, J_i^\pi)\rangle$$

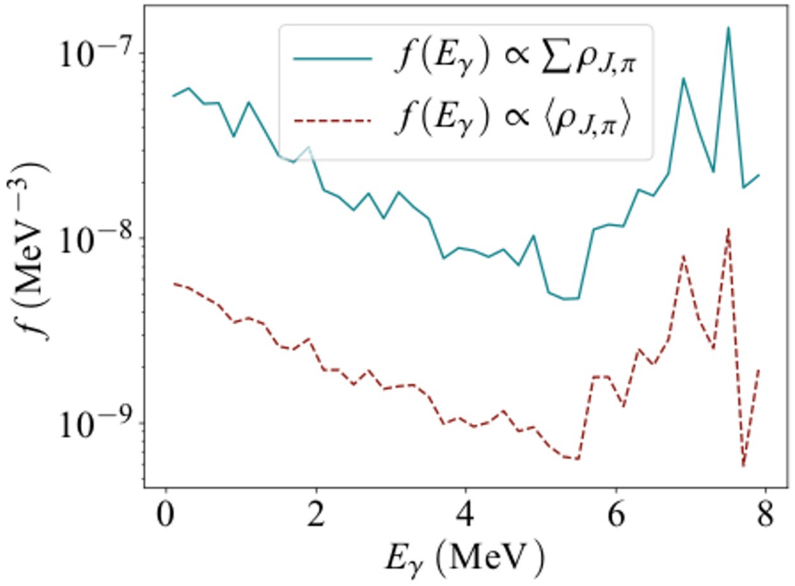
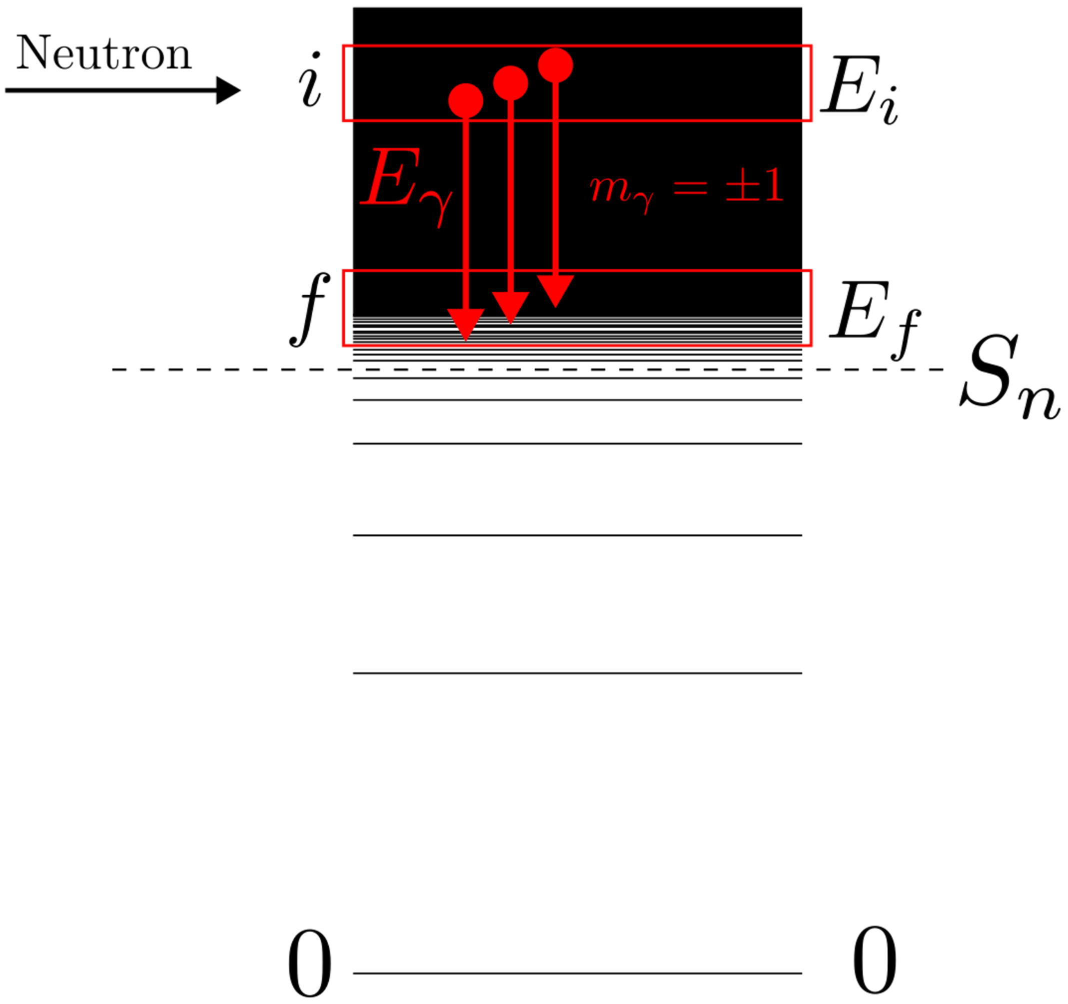


FIG. 13. Comparison of γ-ray strength functions for ^{56}Fe from shell-model calculations extracted using two different methods. See text for details.

PRC 98, 064321 (2018)



A simpler formula avoids a common mistake

$$\overleftarrow{f}^{XL}(E_\gamma = E_i - E_f) = \frac{8\pi(L+1)}{(\hbar c)^{2L+1}L[(2L+1)!!]^2}\langle \frac{1}{\Delta E}\sum_{E_i}^{E_i+\Delta E} B^{XL}_{i\to f}\rangle$$

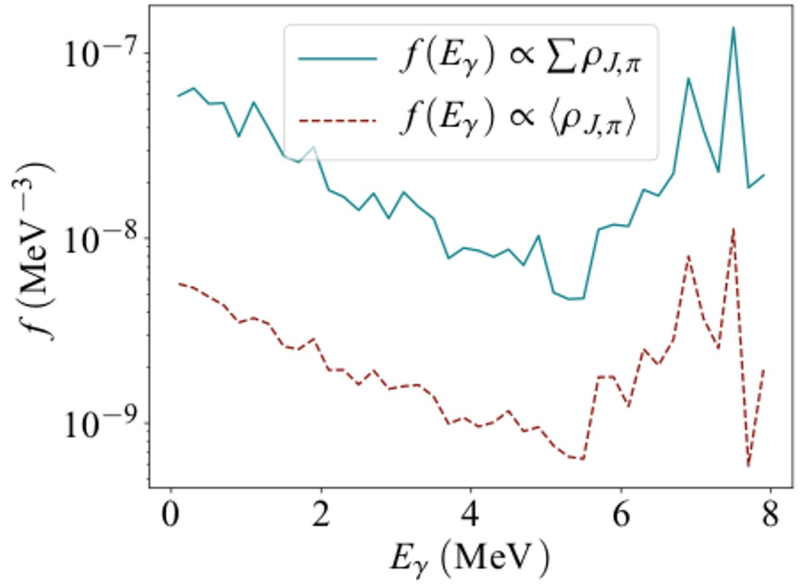


FIG. 13. Comparison of γ-ray strength functions for ^{56}Fe from shell-model calculations extracted using two different methods. See text for details.

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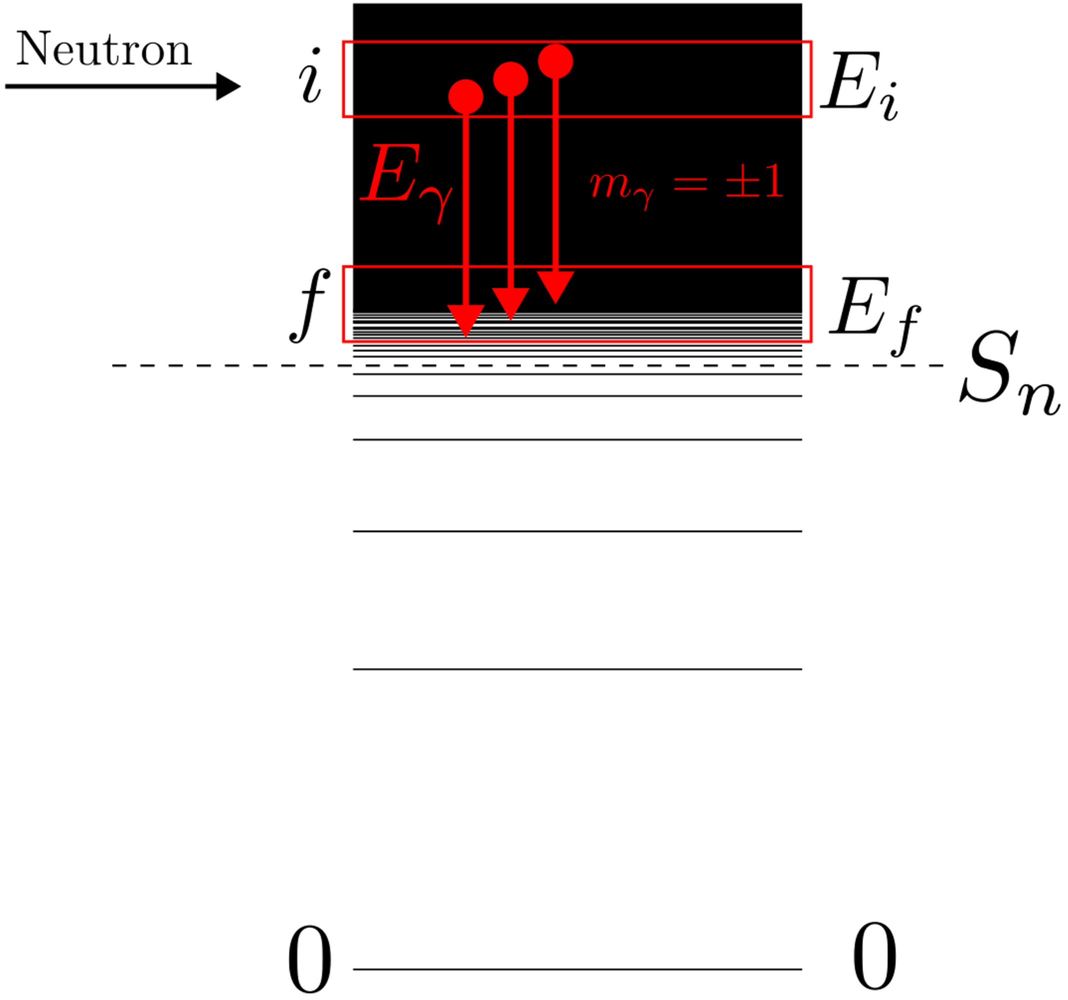
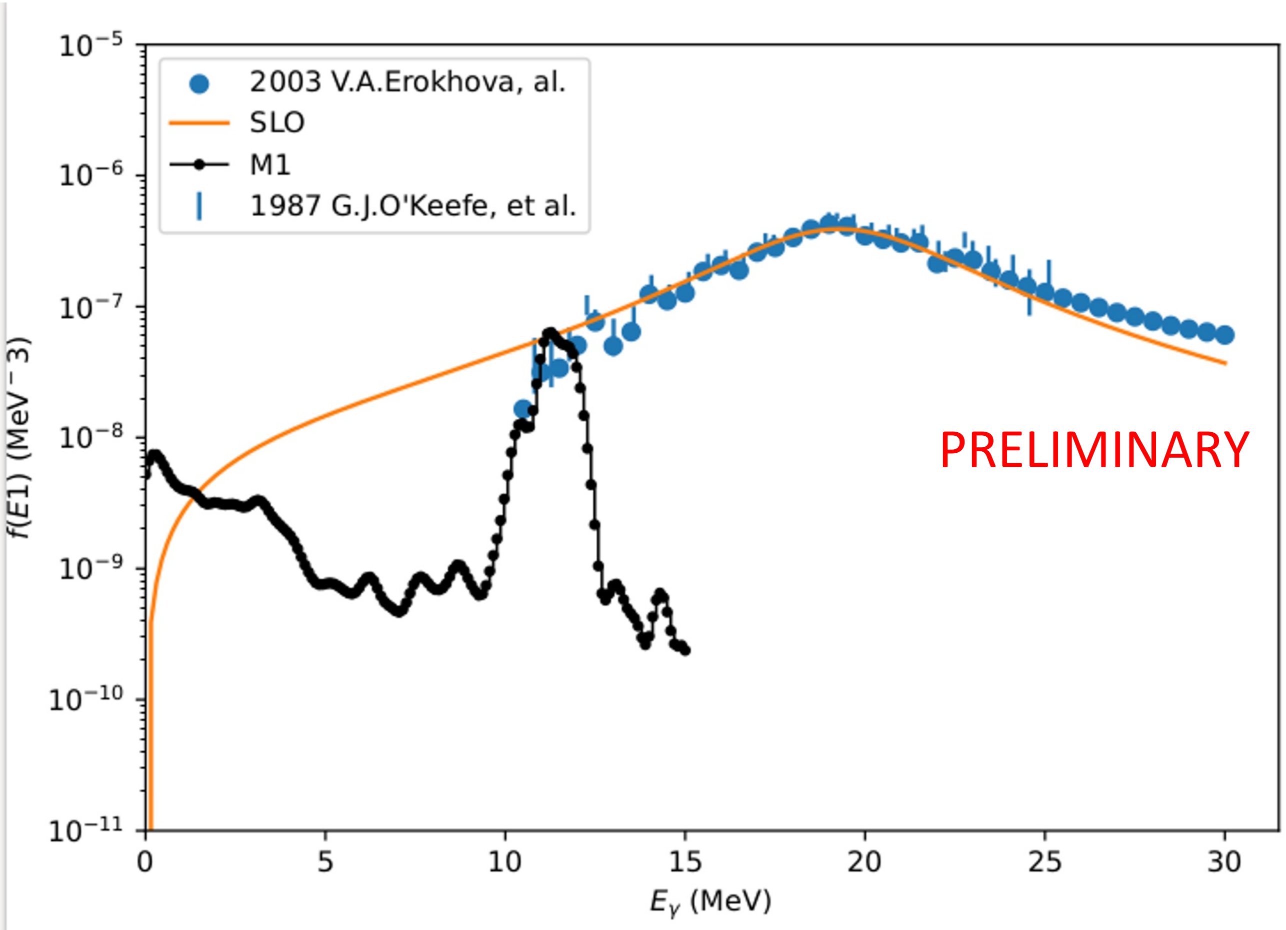


Ca-49 in the sdpf space with an Nmax 1 truncation

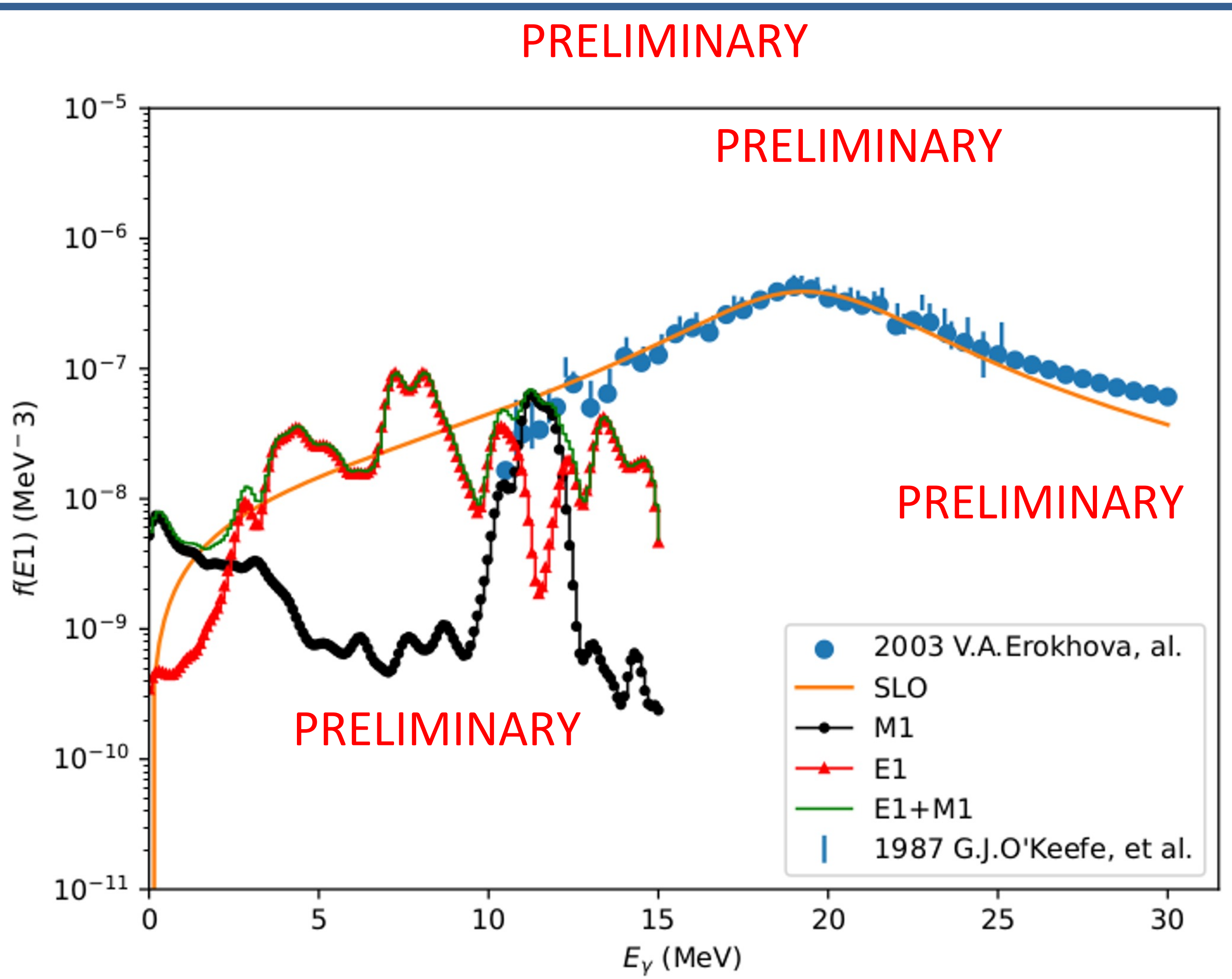
PRELIMINARY



Only 2 major shells (sd and pf)

1 hbar-omega truncation
M-scheme dimension 3 million
500 lowest states
Transitions between all states (downward)
Simple smoothing

Ca-49 in the sdpf space with an Nmax 1 truncation



Only 2 major shells (sd and pf)

- Missing states -> strength concentrated

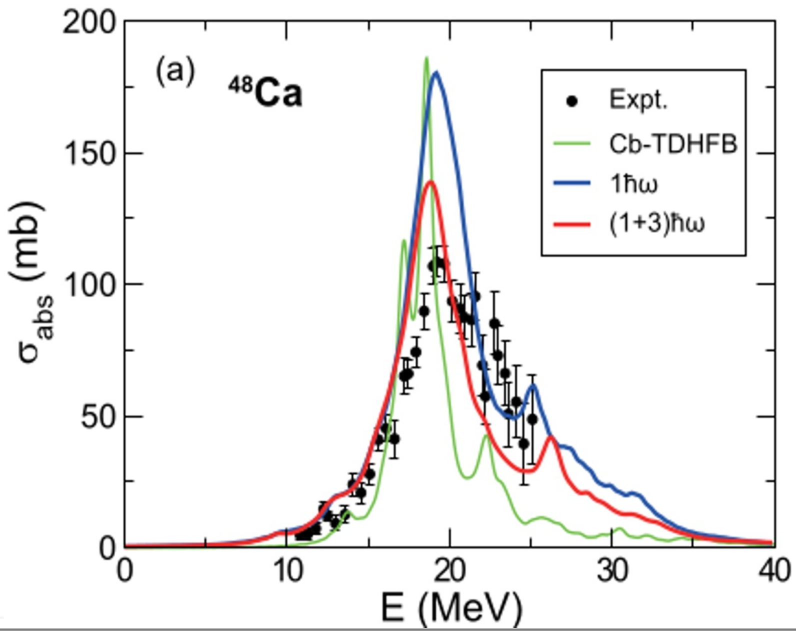
1 hbar-omega truncation

M-scheme dimension 3 million

500 lowest states

Transitions between all states (downward)

Simple smoothing



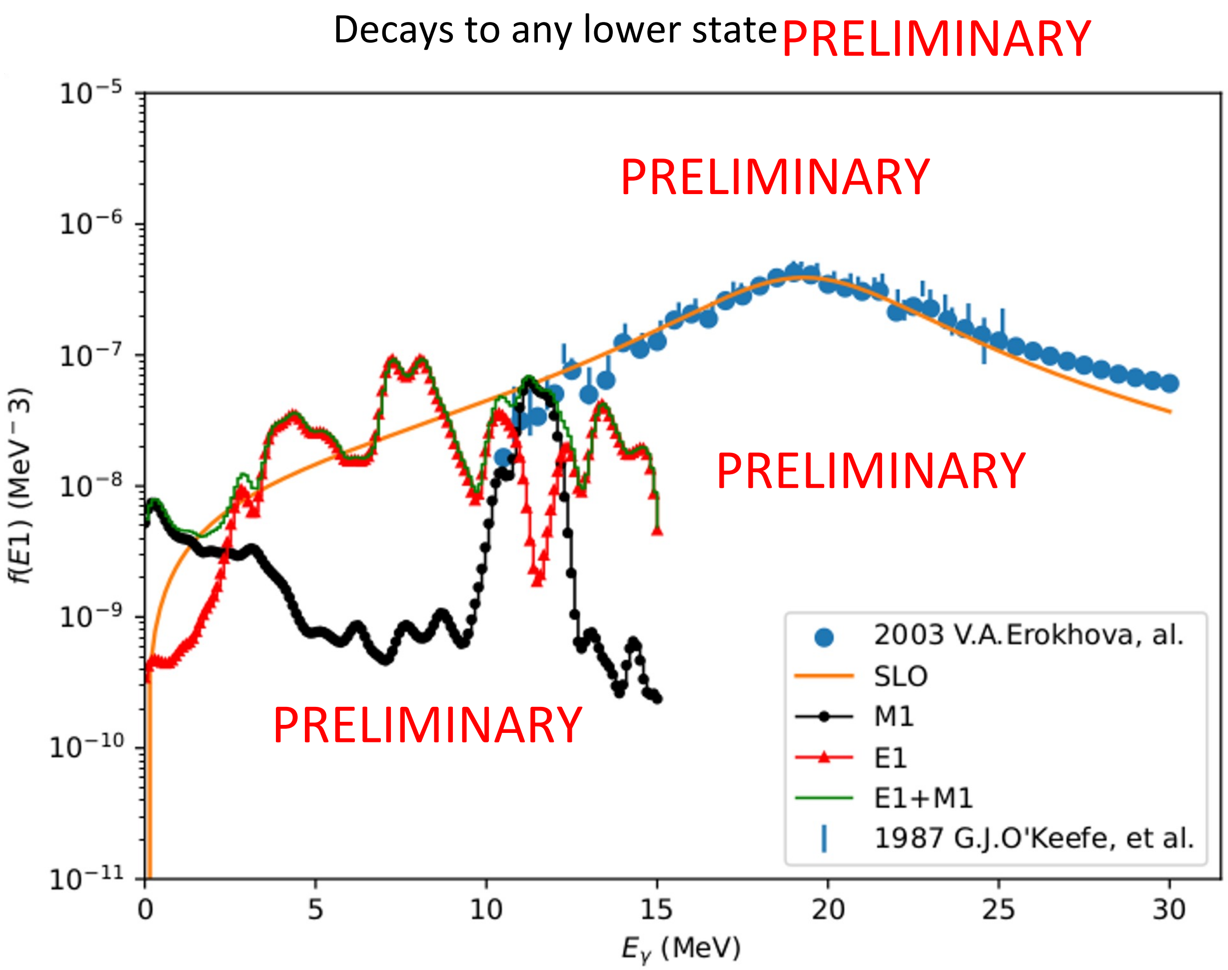
PNE 82, 102-106 (2015)

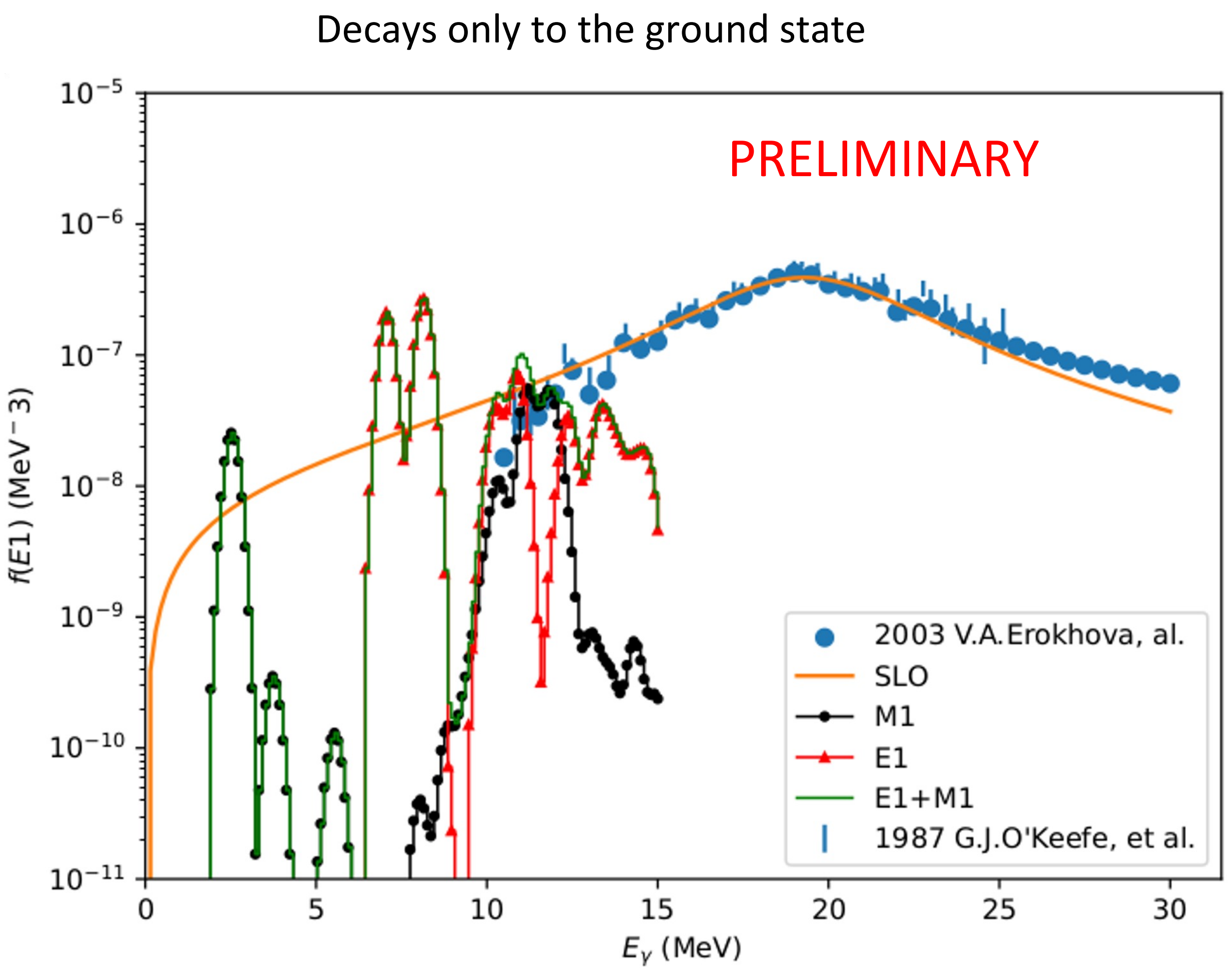
3 Major Shells

1hw, (1+3)hw

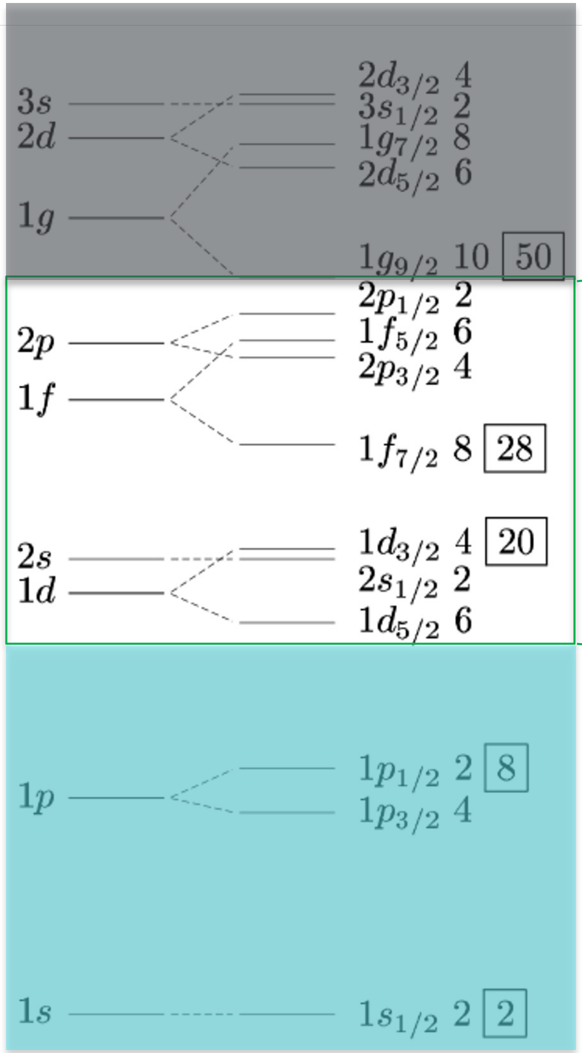
Up from the g.s.

Modeling GSF from the photoabsorption perspective





Shell Model takes all combinations of particle excitations in the valence space to capture many-body physics

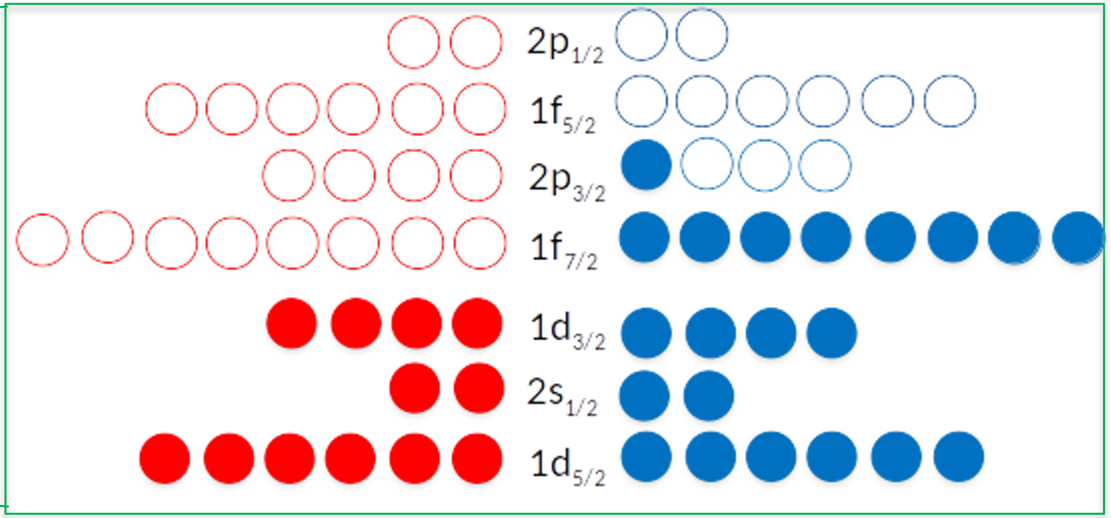


"∞" excluded states

Valence space

Frozen core

^{49}Ca in the sd-pf space



12 Protons

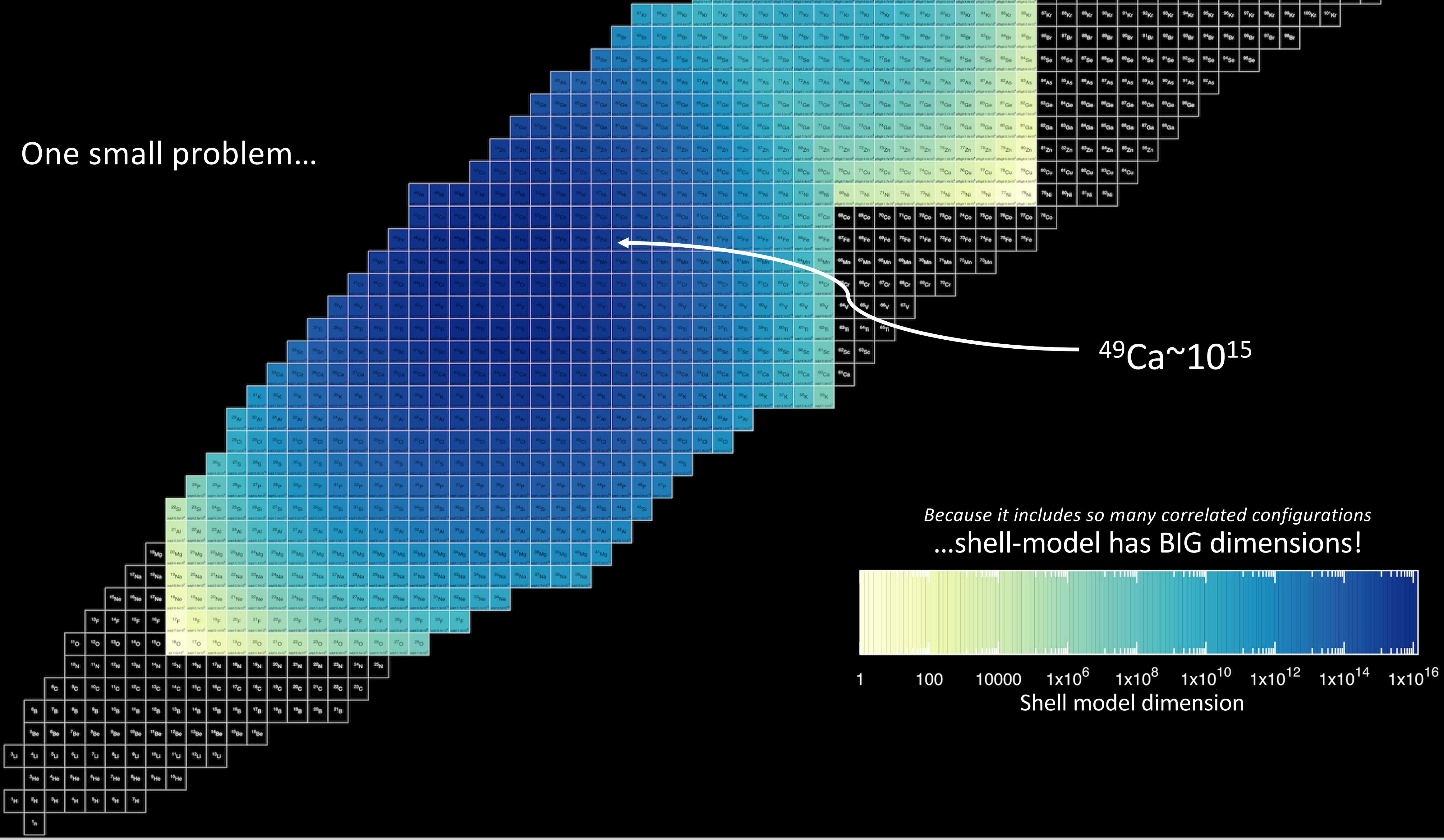
Configurations: 1 x 10^7

21 Neutrons

Configurations: 9x 10^6

(Orders of magnitude smaller!)

One small problem…

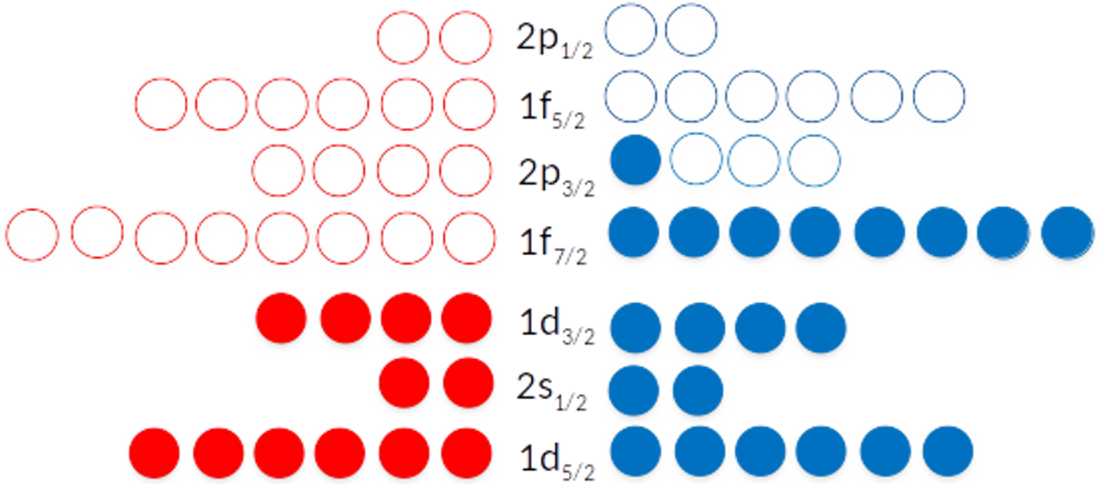


Because it includes so many correlated configurations

…shell-model has BIG dimensions!

A factorized basis can provide efficient representations

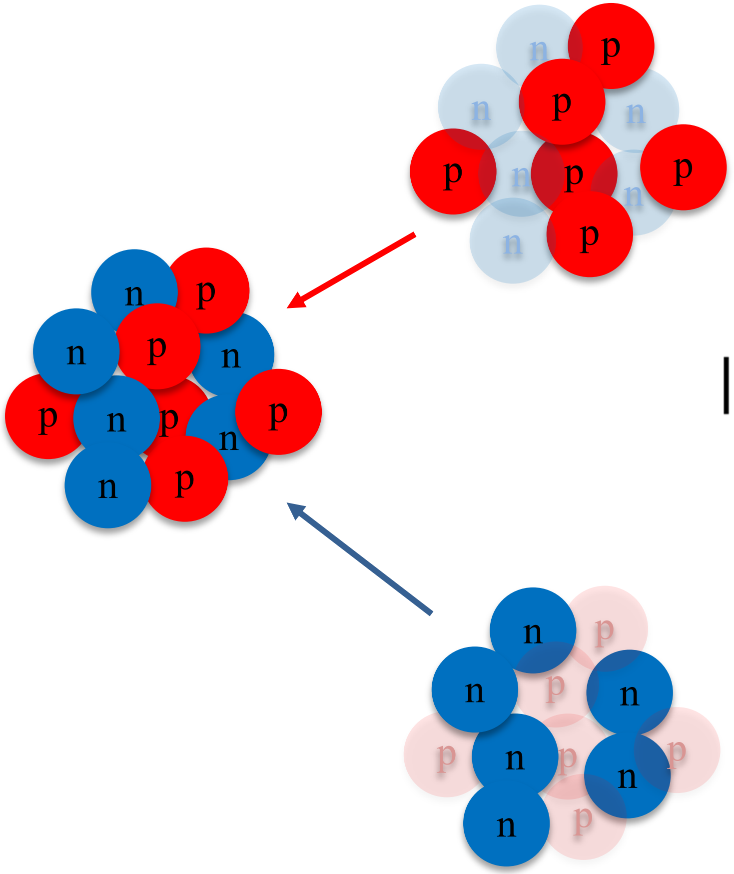
^{49}Ca in the sd-pf space



12 Protons

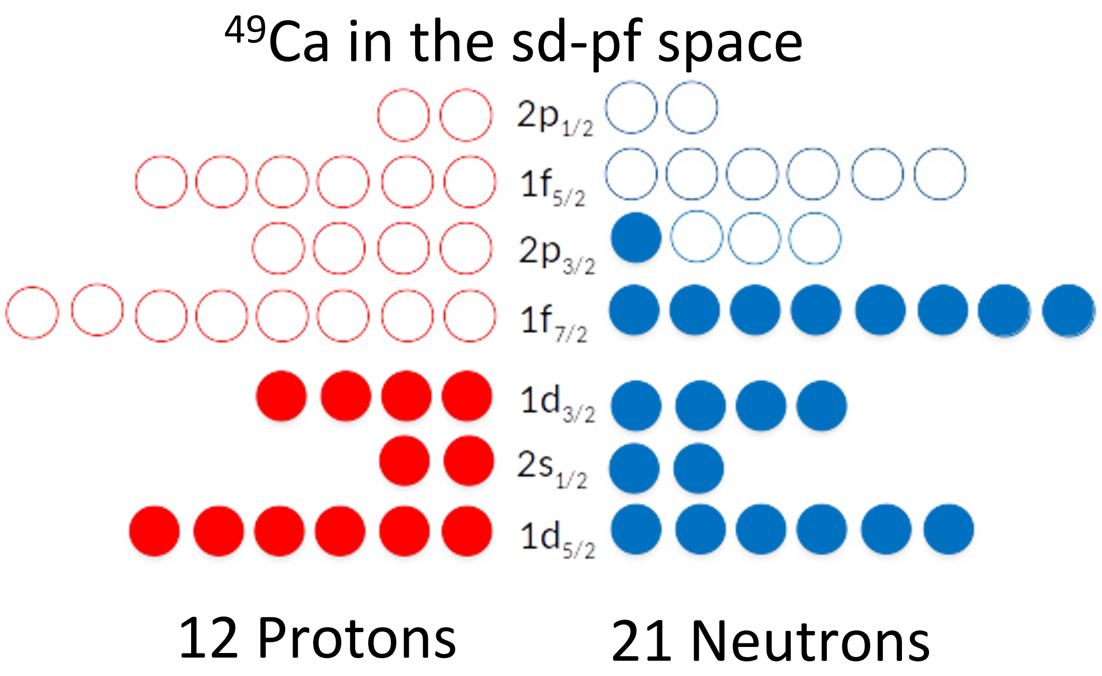
21 Neutrons

Bipartite Factorization



$$|\Psi\rangle = \sum_{ab} \psi_{ab} |p_a\rangle |n_b\rangle$$

Singular value decomposition of factorized amplitudes yields optimized basis



Factorized representation:

$$|\Psi\rangle = \sum_{ab} \psi_{ab} |p_a\rangle |n_b\rangle$$

Singular value decomposition (SVD):

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

SVD provides an optimized representation:

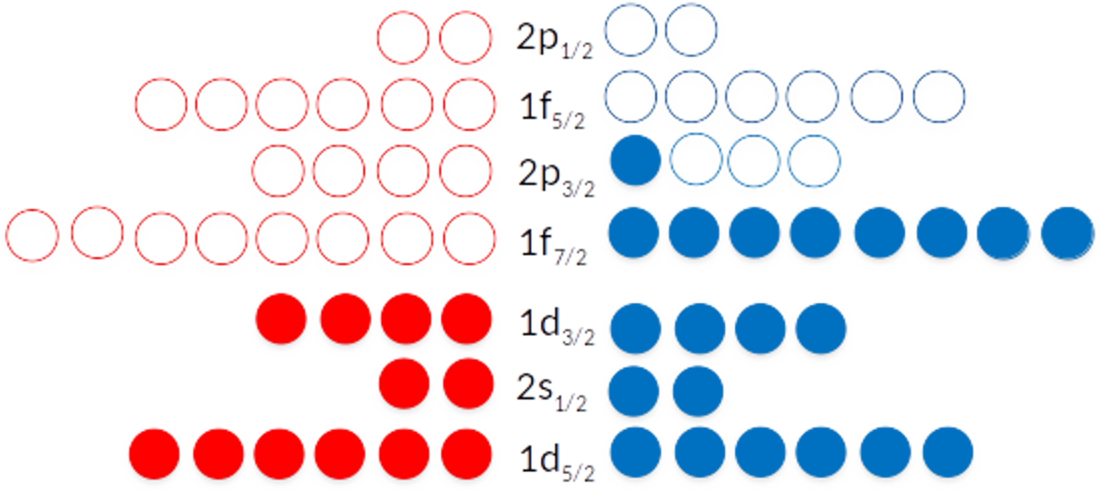
$$|\Psi\rangle = \sum_{c} s_c |p'_c\rangle |n'_c\rangle$$

One can iteratively solve for the optimal basis states, but this is challenging in practice (T. Papenbrock 2004, 2005)

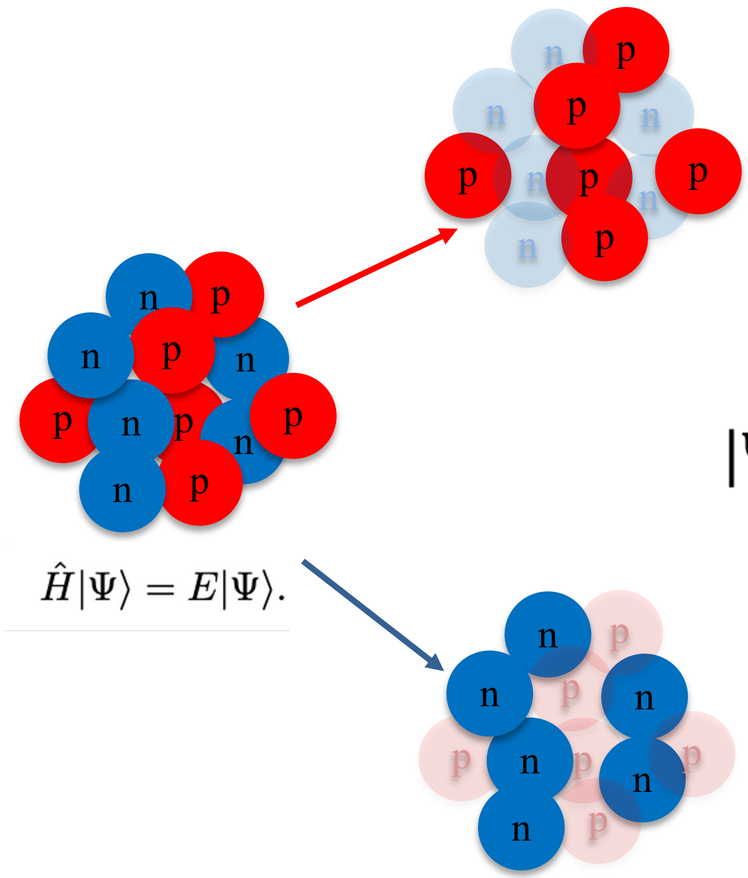
Our simplified approach: Approximately-optimize the basis with subspace diagonalization

Bipartite Factorization

^{49}Ca in the sd-pf space



12 Protons   21 Neutrons



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

Proton Hamiltonian

$$H_p|j_p\rangle = E_p|j_p\rangle$$

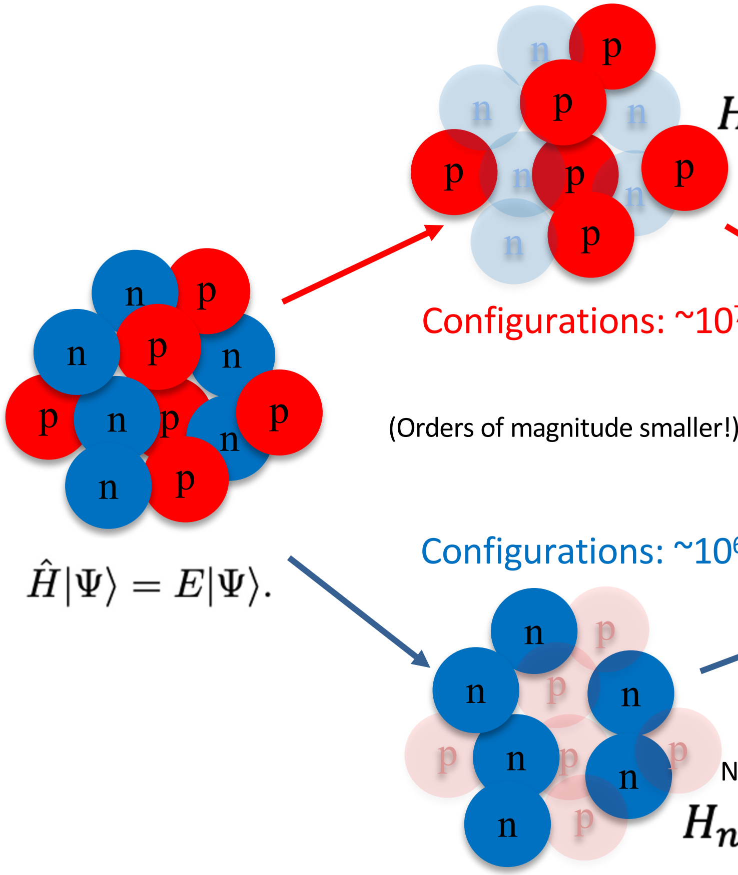
$$|\Psi\rangle = \sum_{ab} c_{ab}|j_p\rangle|j_n\rangle$$

Neutron Hamiltonian

$$H_n|j_n\rangle = E_n|j_n\rangle$$

We had evidence that this would work; especially[1] for Z > N

Bipartite Factorization



Proton Hamiltonian

$$H_p|j_p\rangle = E_p|j_p\rangle$$

Configurations: ~10^7

(Orders of magnitude smaller!)

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

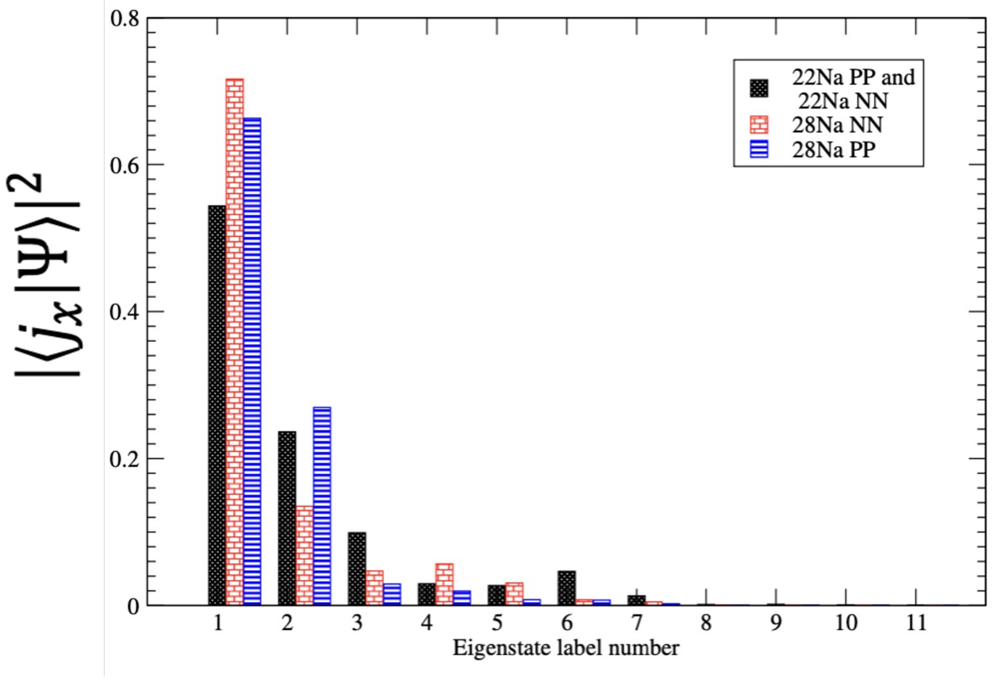
$$|\Psi\rangle = \sum_{ab} c_{ab}|j_p\rangle|j_n\rangle$$

Configurations: ~10^6

Neutron Hamiltonian

$$H_n|j_n\rangle = E_n|j_n\rangle$$

Exact ground-state overlap with subspace eigenstates



$|j_p\rangle$ or $|j_n\rangle$

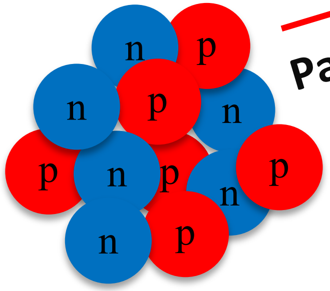
[1]Johnson & Gorton 2023 (J. Phys. G 50, 045110)

Proton and Neutron Approximate Shell Model (PANASH)

$$H = H_p + H_n + H_{pn}$$

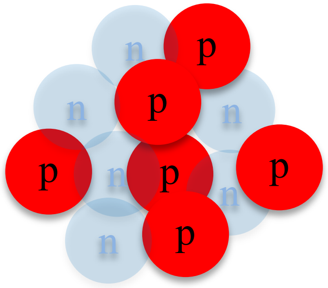
- Wave functions factorize into PN-partition eigenstates
- Coefficients decay exponentially
- Proton neutron entanglement decreases when N>Z (arxiv 2210.14338)

$$H|\Psi\rangle = E|\Psi\rangle$$



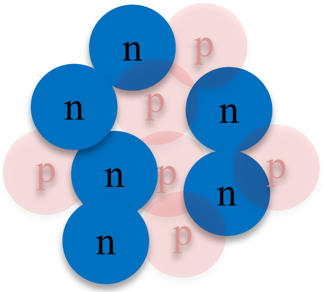
Partition

$$H_p|j_p\rangle = E_p|j_p\rangle$$



Solve

(Orders of magnitude smaller!)



$$H_n|j_n\rangle = E_n|j_n\rangle$$

Recouple

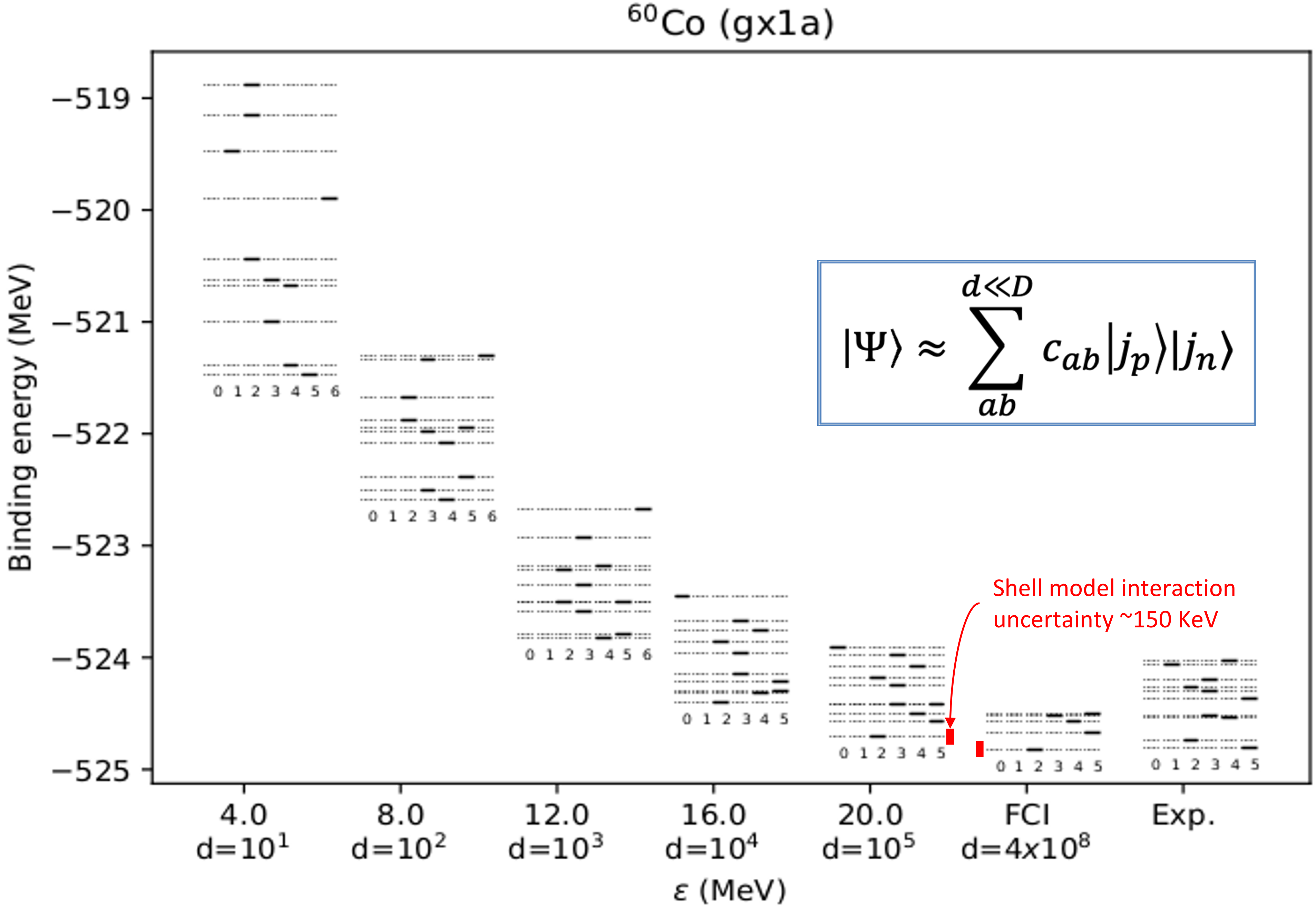
$$|j_p j_n; J\rangle = |j_p\rangle \otimes |j_n\rangle$$

Couple basis

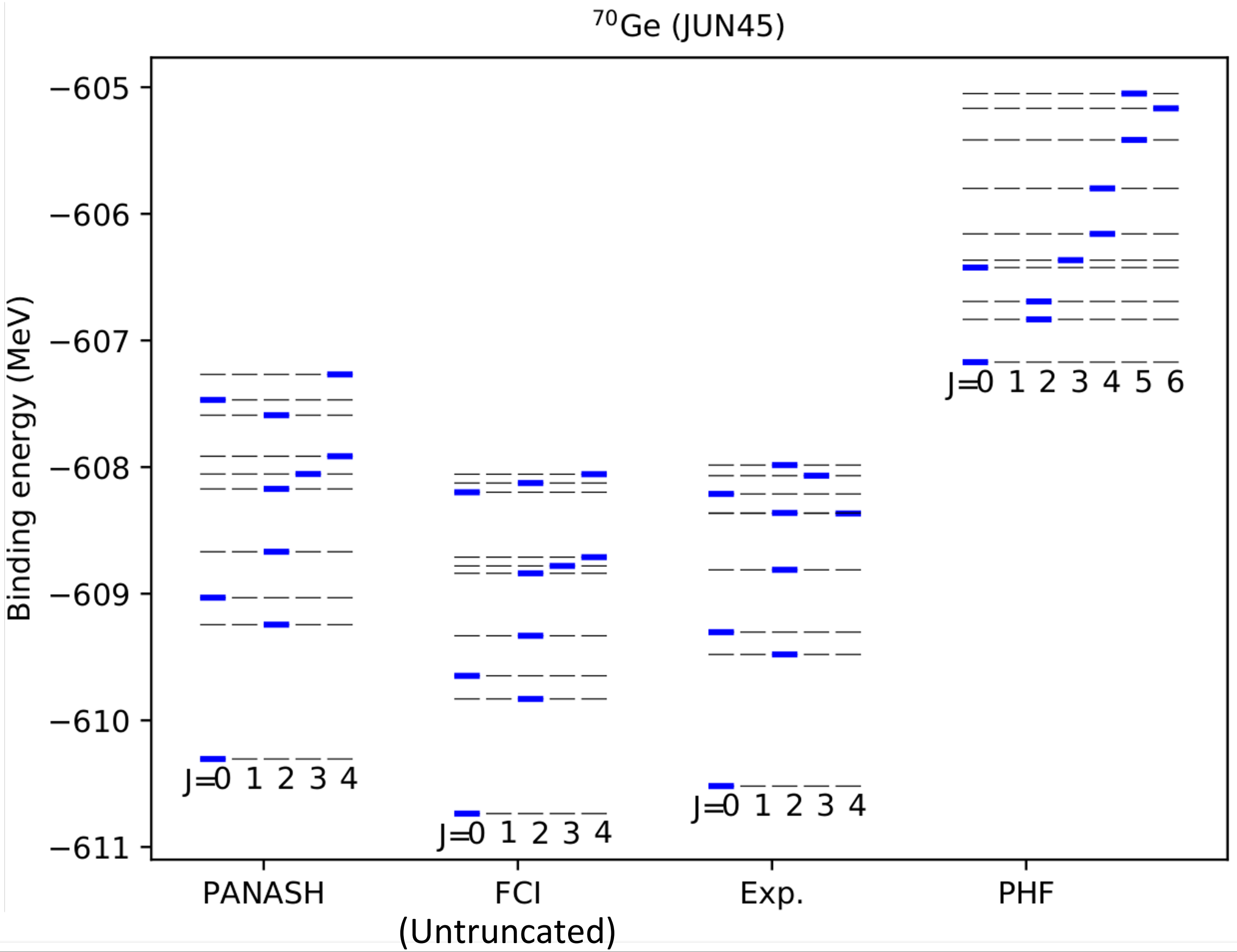
Truncate

$$\langle j'_p j'_n; J|H|j_p j_n; J\rangle = E_p + E_n + H_{pn}$$

Solve!


^{60}Co (gx1a)
Binding energy (MeV)
−519
−520
−521
−522
−523
−524
−525
0 1 2 3 4 5 6
0 1 2 3 4 5
4.0
d=10^1
8.0
d=10^2
12.0
d=10^3
16.0
d=10^4
20.0
d=10^5
FCI
d=4x10^8
Exp.
ε (MeV)
$$|\Psi\rangle \approx \sum_{ab}^{d \ll D} c_{ab} |j_p\rangle |j_n\rangle$$
Shell model interaction uncertainty ~150 KeV

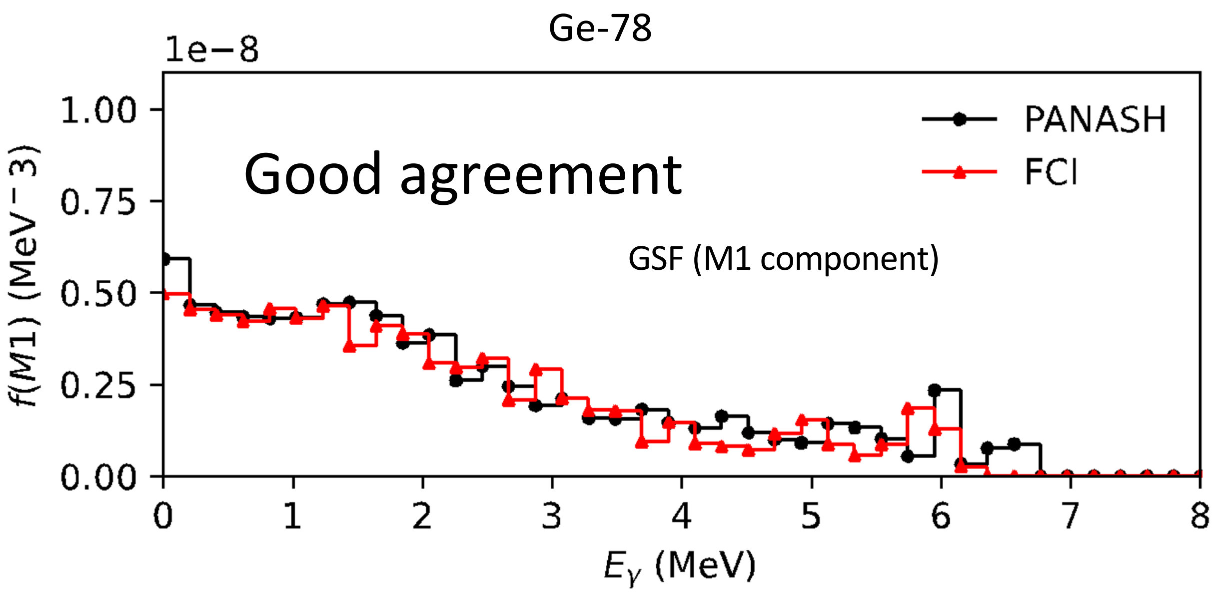
Convergence of spectra (preliminary)

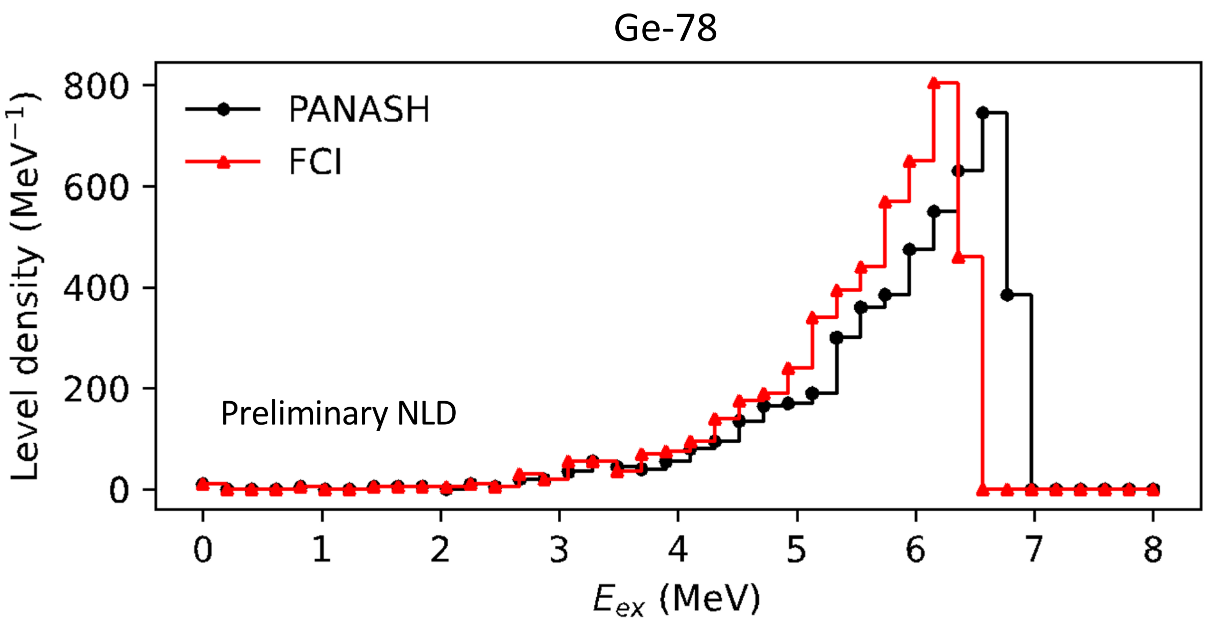


<u>Ge70 is a complicated nucleus!</u>

M-scheme untruncated dimension: 10^8
PANASH (this work) dimension: 10^4

We can easily calculate M1 strength functions (1 major shell)



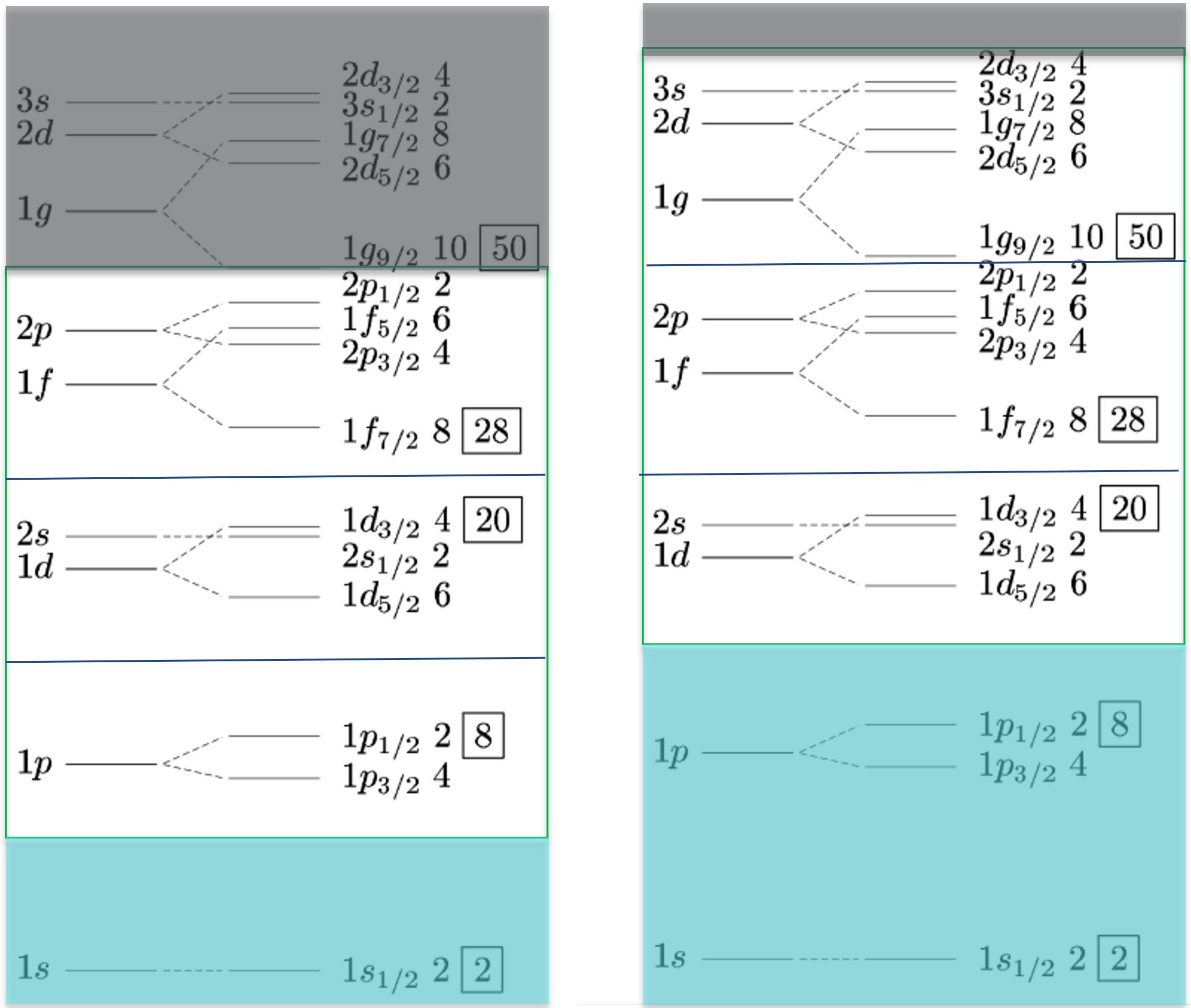


PANASH (this work): used 30% of proton/neutron eigenstate components: 34x basis reduction

Agreement with results of Frauendorf & Schwengner (PRC 105, 034335, 2022) w/ similar interaction

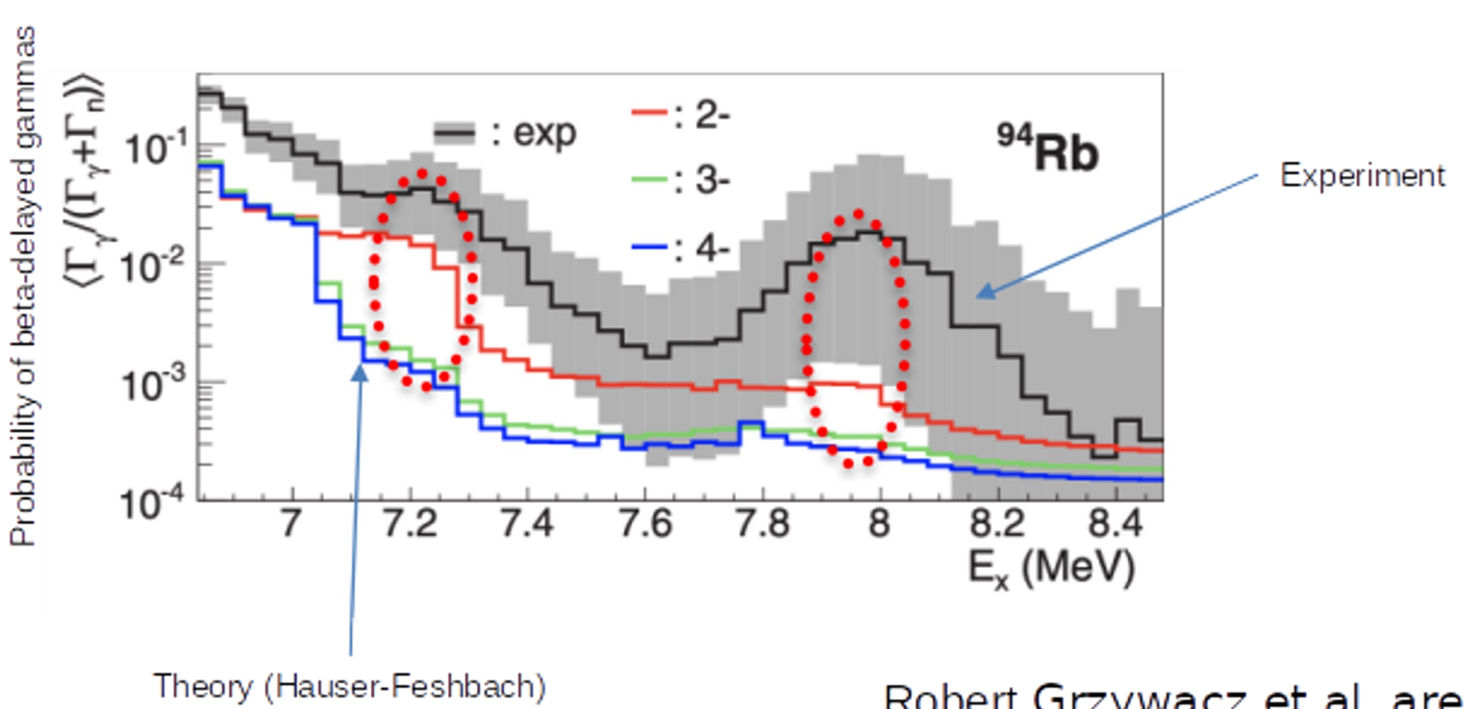
Our next ambition: E1 strength functions with 3 major shells

- No-core shell model
- Truncations within major shell will be required for heavier nuclei



What's going on with beta-delayed neutron emission?

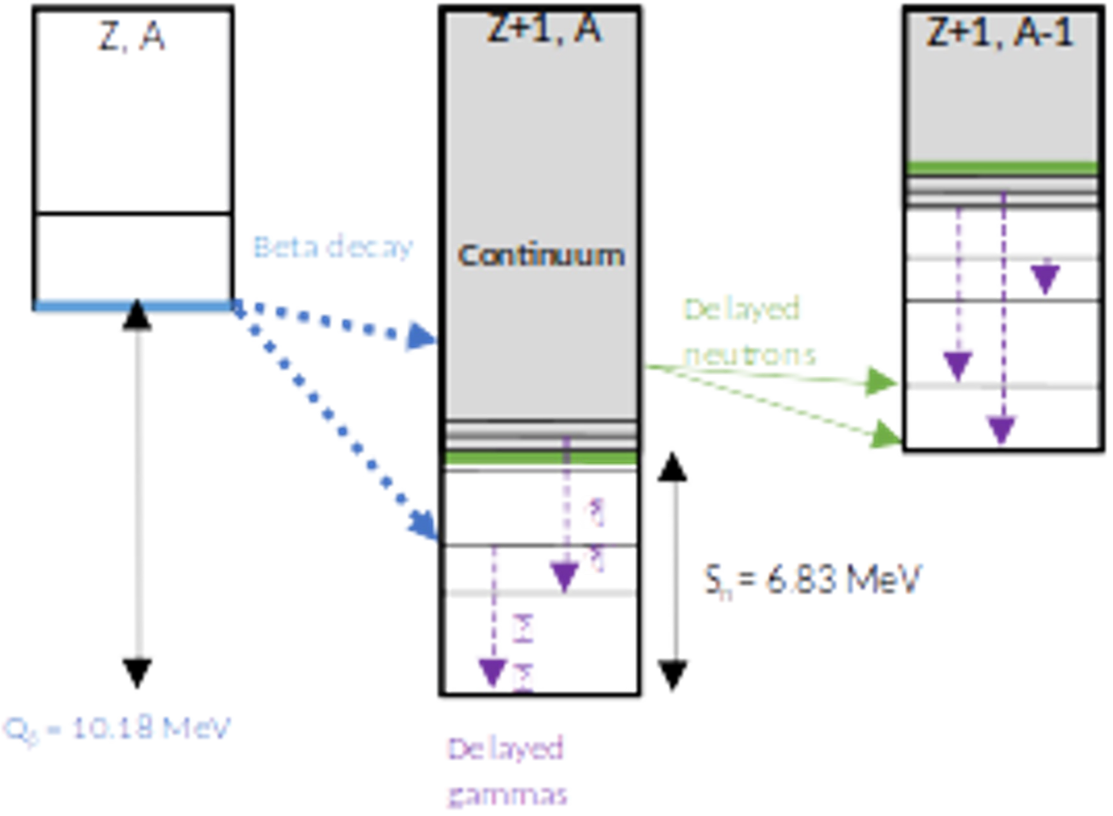
- Non statistical decay?
- Enhanced gamma-ray strength function?
- Forbidden decay contributions?



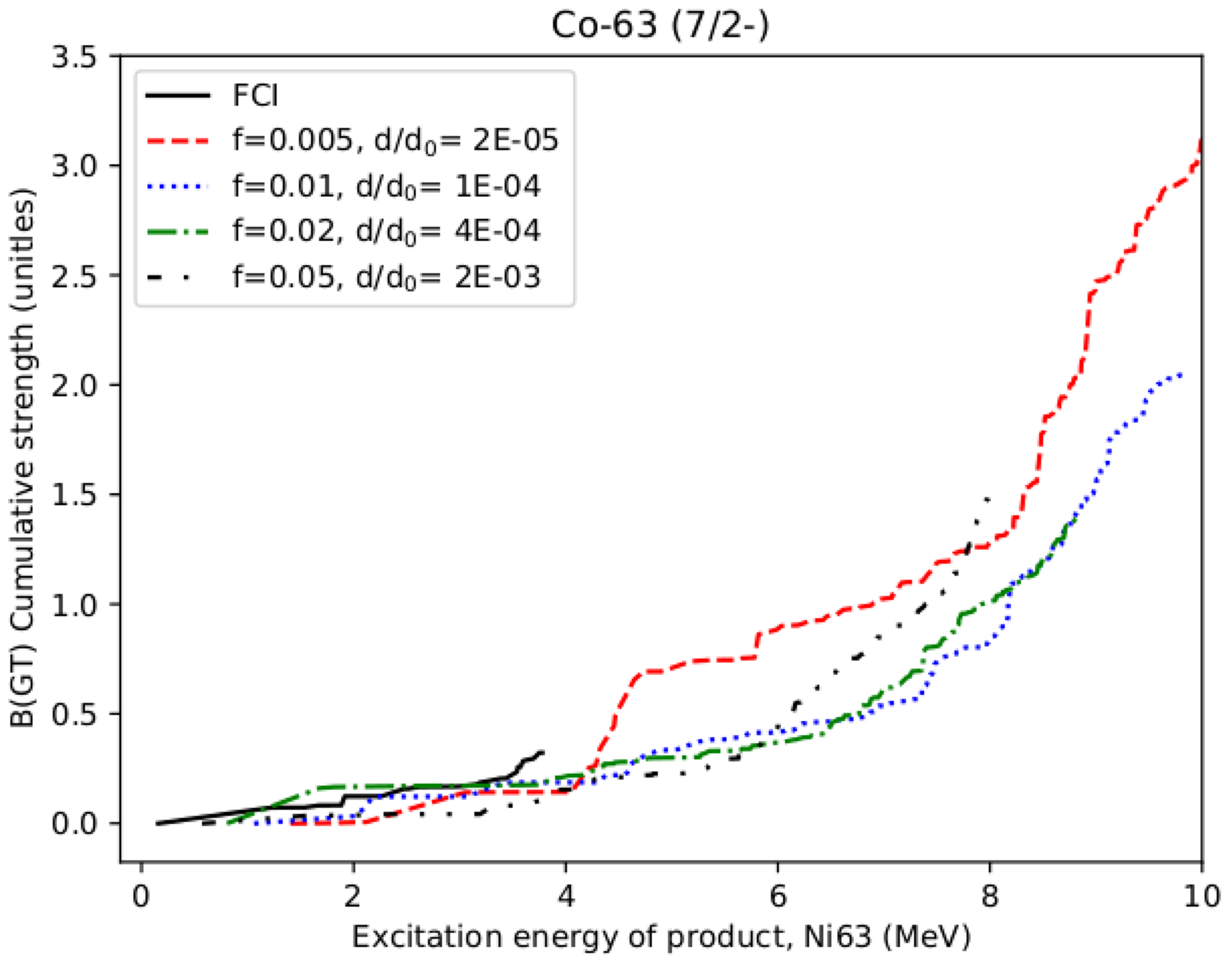
Robert Grzywacz et al. are also investigating the nonstatistical nature of neutron emission near Sn-134!

Valencia, et al., 2017 https://link.aps.org/doi/10.1103/PhysRevC.95.024320

Application of approximate shell model for statistical reactions



PANASH truncation can approximate Gamow-Teller distributions



M-scheme dim: 141 million

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Abstract

The nuclear shell model is an under-utilized source of statistical nuclear properties such as nuclear level densities and gamma-ray strength functions, both of which are fundamental to statistical nuclear reaction models used in nuclear data evaluations. In part, this is because accurate calculations for nuclei of astrophysical interest often require model spaces exceeding our computational resources. The large numbers of states required for statistical analysis compounds with the larger model spaces typically needed to include excitations of both parities, a pre-requisite for E1 gamma-ray strength functions. To address this, we have applied our proton-neutron shell model truncation scheme to approximate the wave functions typical shell model calculations cannot handle. In our benchmark cases, we find that this is an effective way to estimate the gamma-ray strength functions, while better methods already exist for nuclear level densities.