Shell model for astrophysics and nuclear technologies

Nuclear Theory | NT-S4D3A1

Thursday, 26 June | Session 4 – Room Madrid 1

16:25 - 18:00

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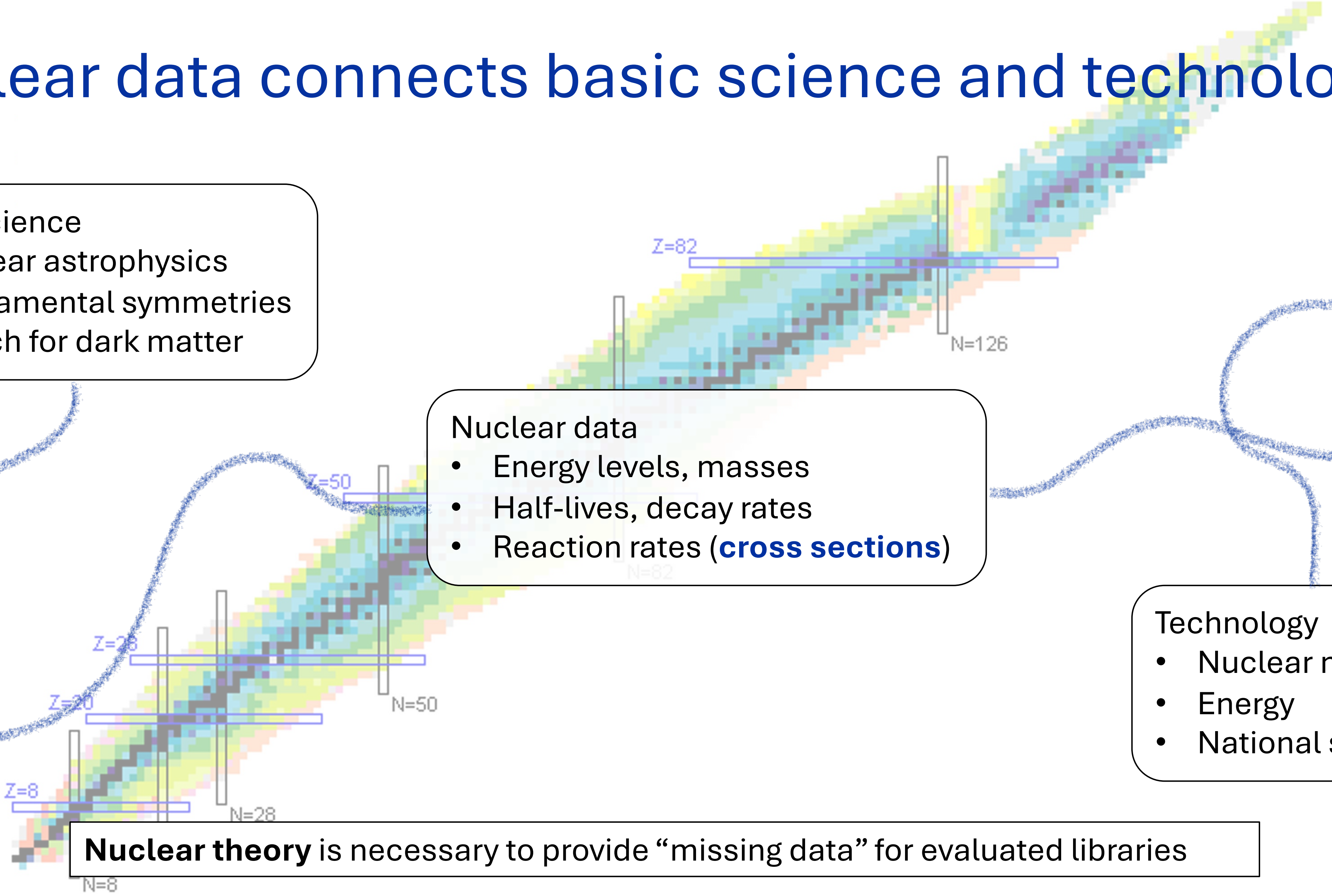
Nuclear data connects basic science and technology



Basic Science
- Nuclear astrophysics
- Fundamental symmetries
- Search for dark matter

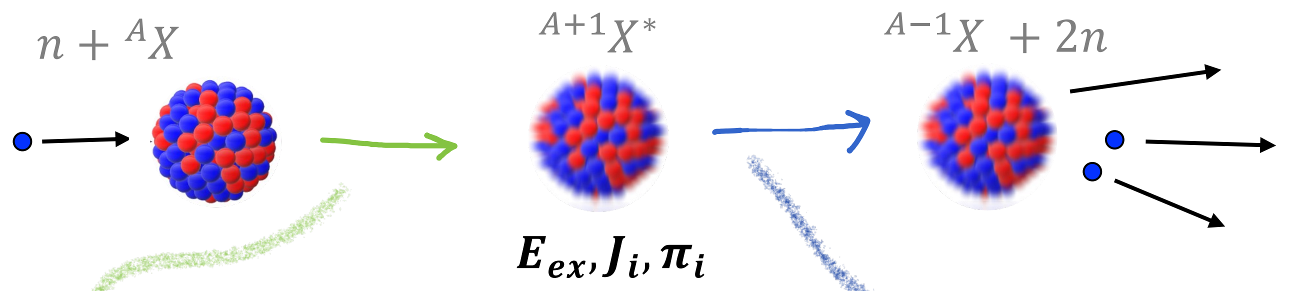
Nuclear data
- Energy levels, masses
- Half-lives, decay rates
- Reaction rates (**cross sections**)

Technology
- Nuclear medicine
- Energy
- National security

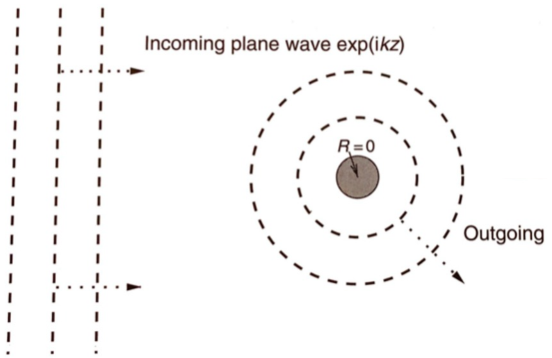
Nuclear theory is necessary to provide “missing data” for evaluated libraries

Hauser-Feshbach formalism: optical model + statistical decay

0.1 – 100 MeV



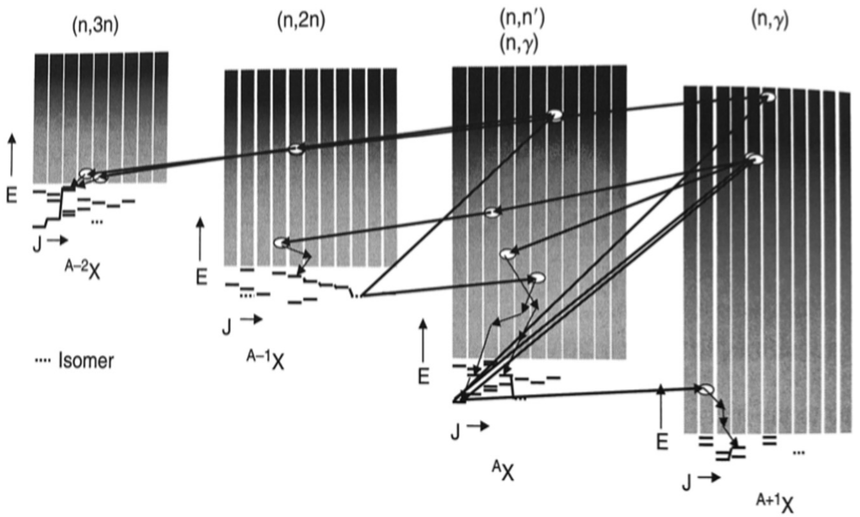
Optical model



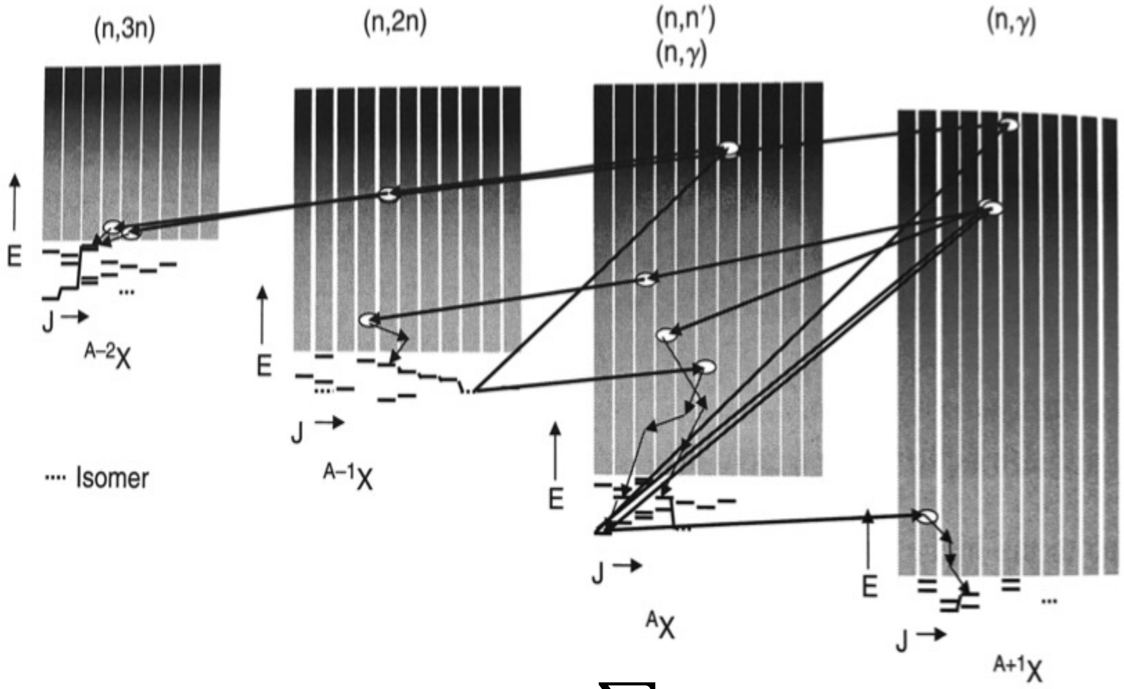
HF Codes

TALYS
EMPIRE
CoH
YAHFC
STAPRE

Statistical decay



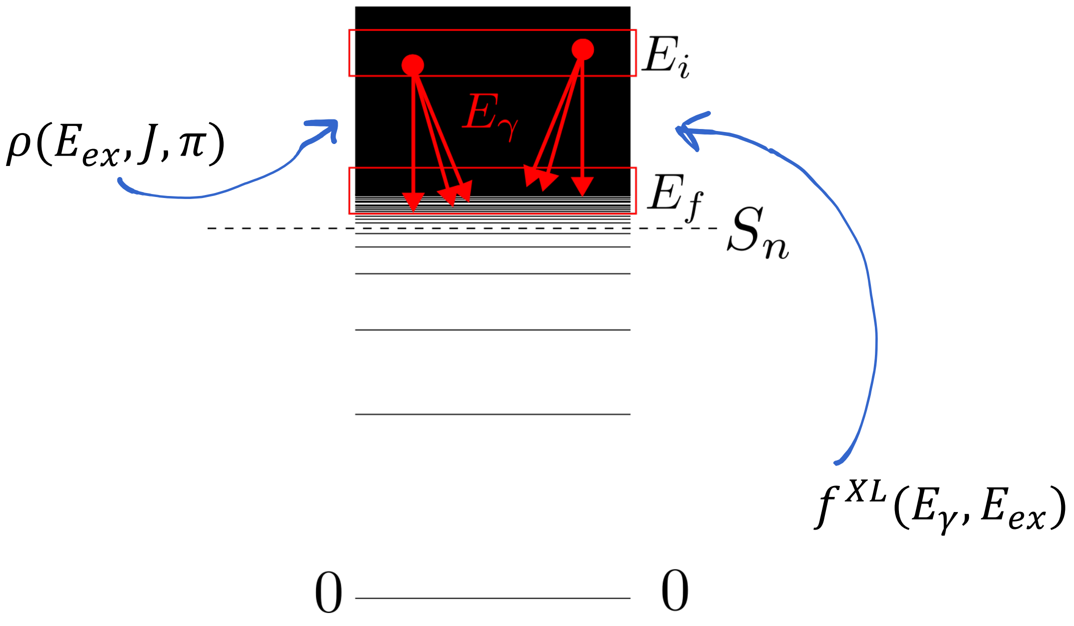
The decay of the compound state is a complicated many-body process



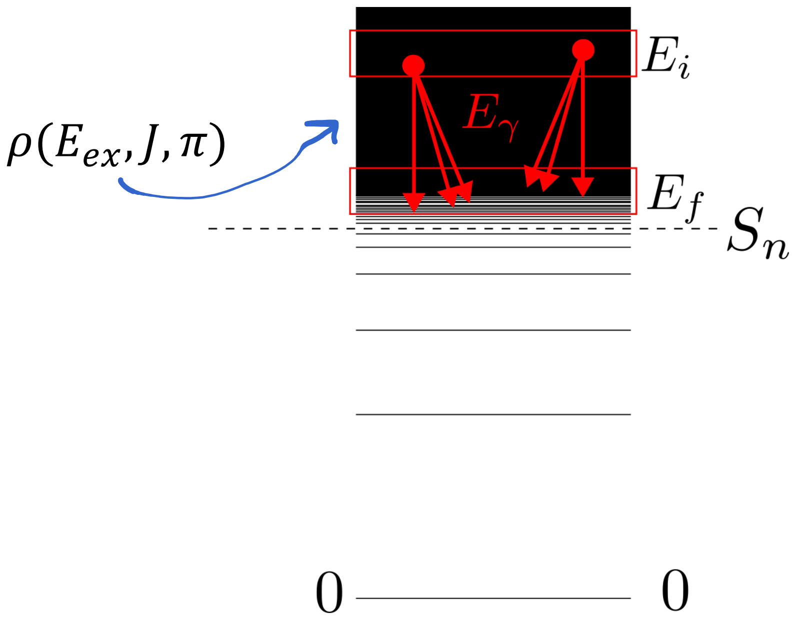
"*ab initio*" physics: $$P(n,2n) \propto \sum_{\Psi_f \hat{T} \Phi_i} \rho_{\Psi_f} \left|\langle \Psi_f(R) \middle| \hat{T} \middle| \Phi_i(CN) \rangle\right|^2 P(CN)$$

We are still years away from an *ab initio* description of reactions chart-wide

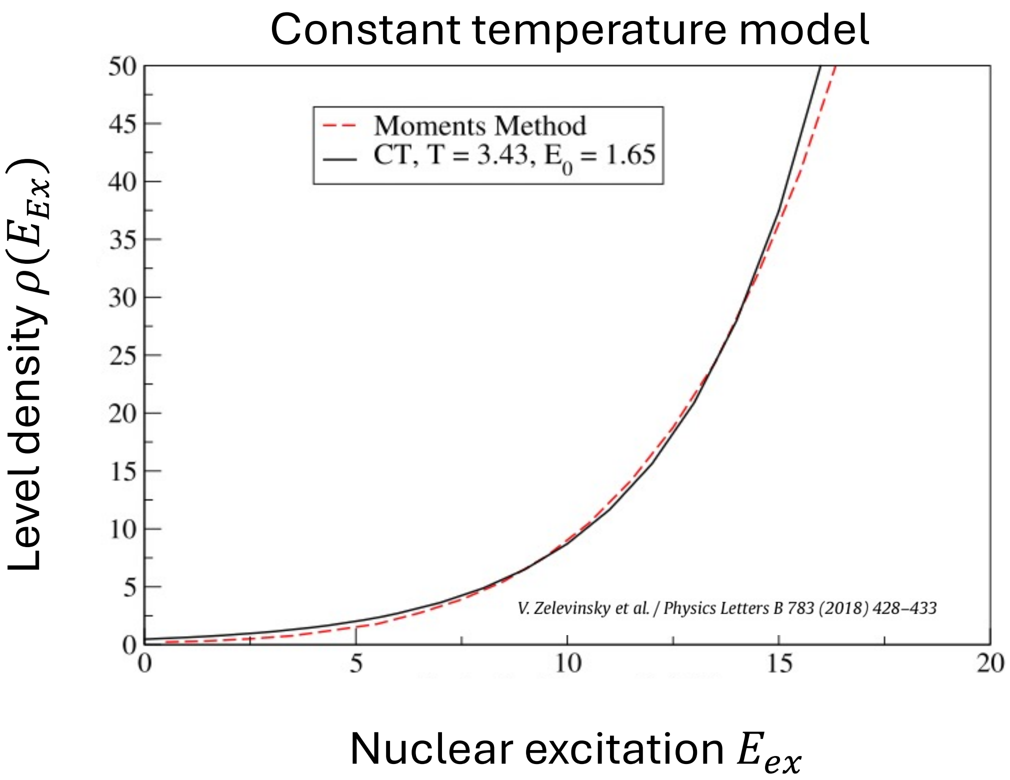
Gamma strength functions and nuclear level densities are still the evaluator's choice



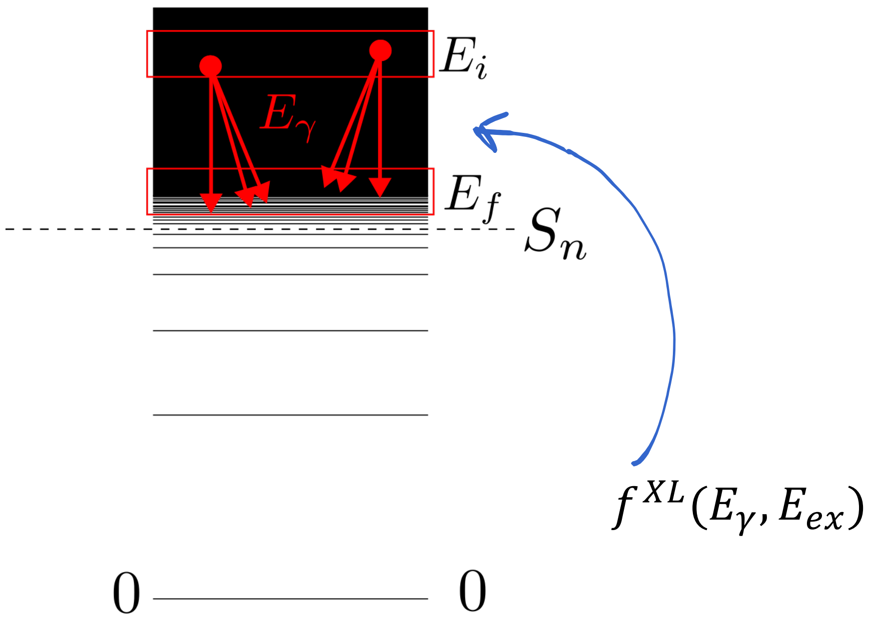
Nuclear level densities (NLD) approximate the availability of states



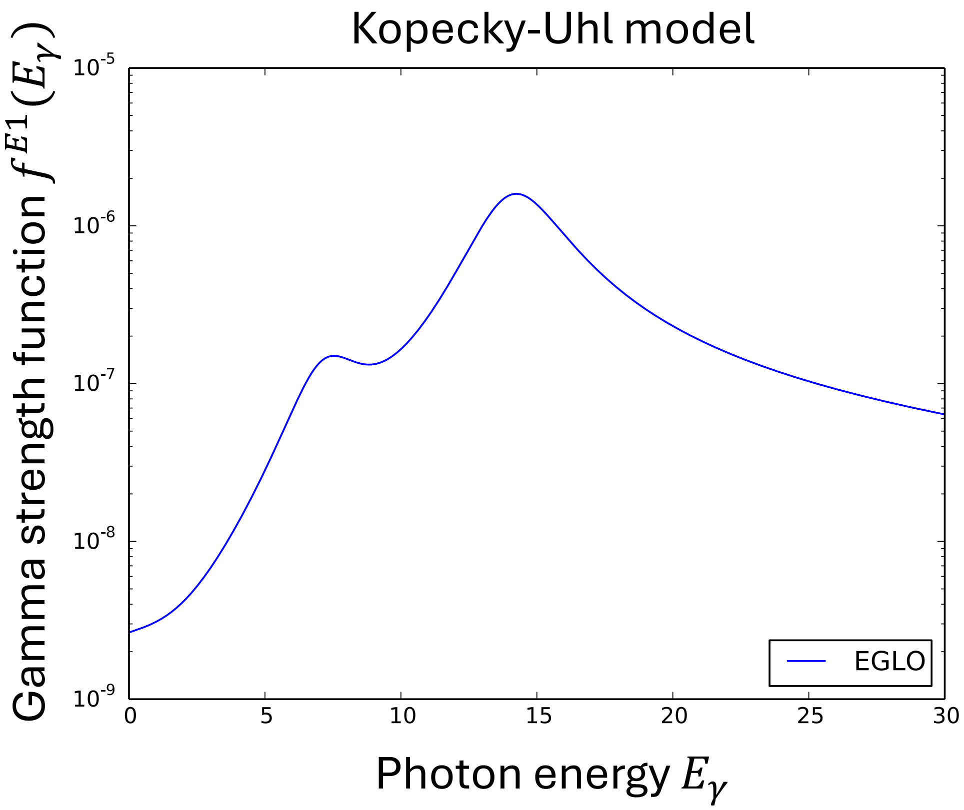
3 - 5 parameters per nucleus



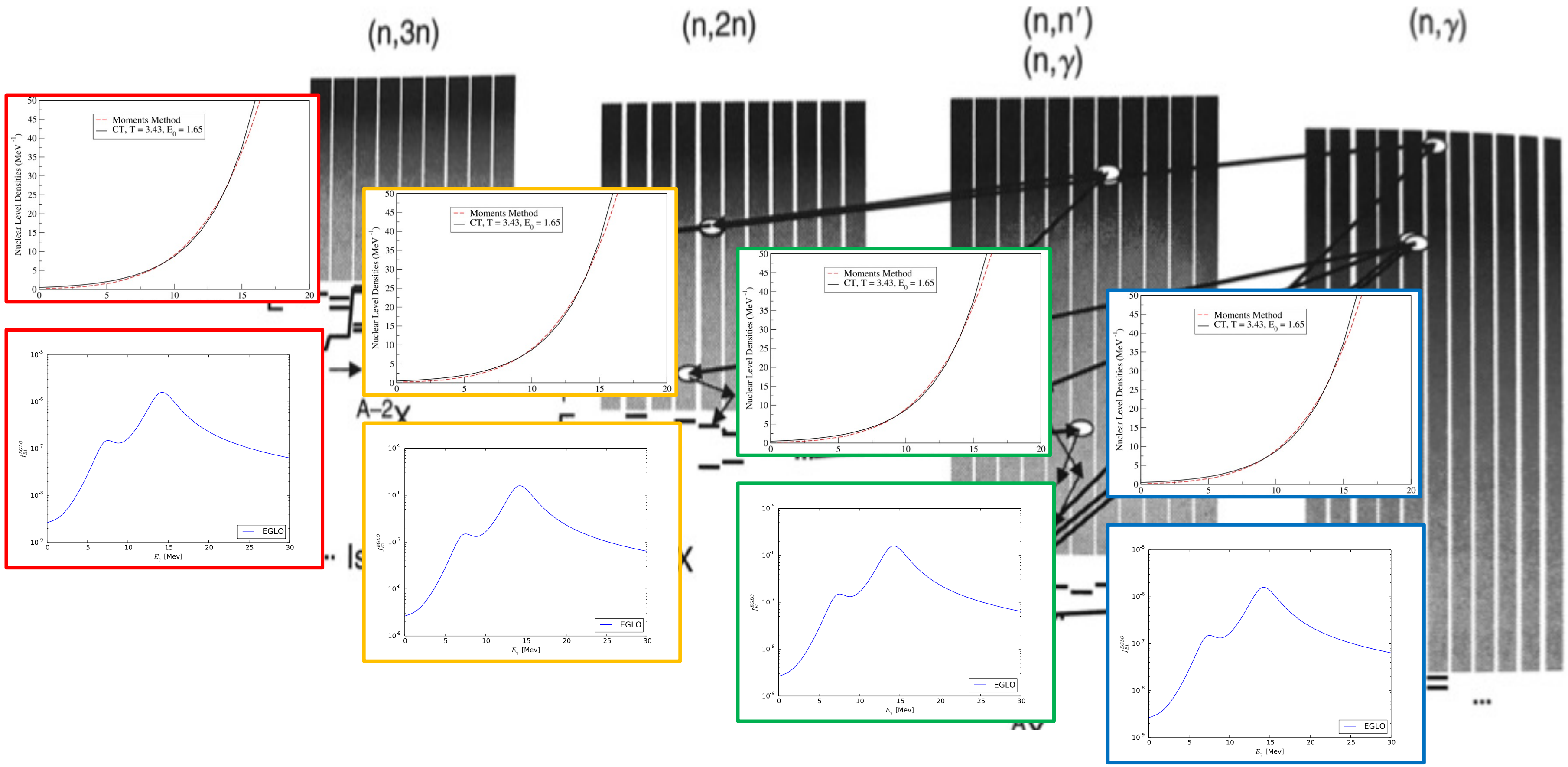
Gamma-ray strength functions (GSF) approximate transition probabilities between (internal) states



3 - 6 parameters per multipole type:
E1, E2, M1 transitions dominate

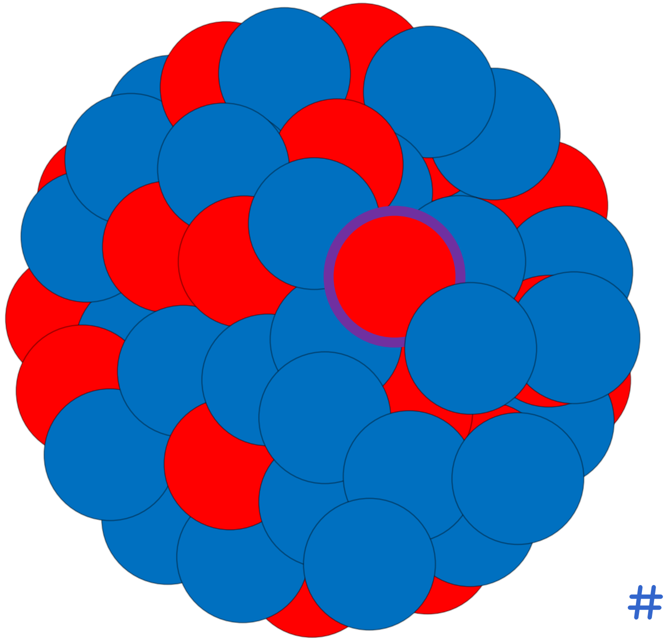


NLD, GSF are required for many nuclei at once. We want the best models available.



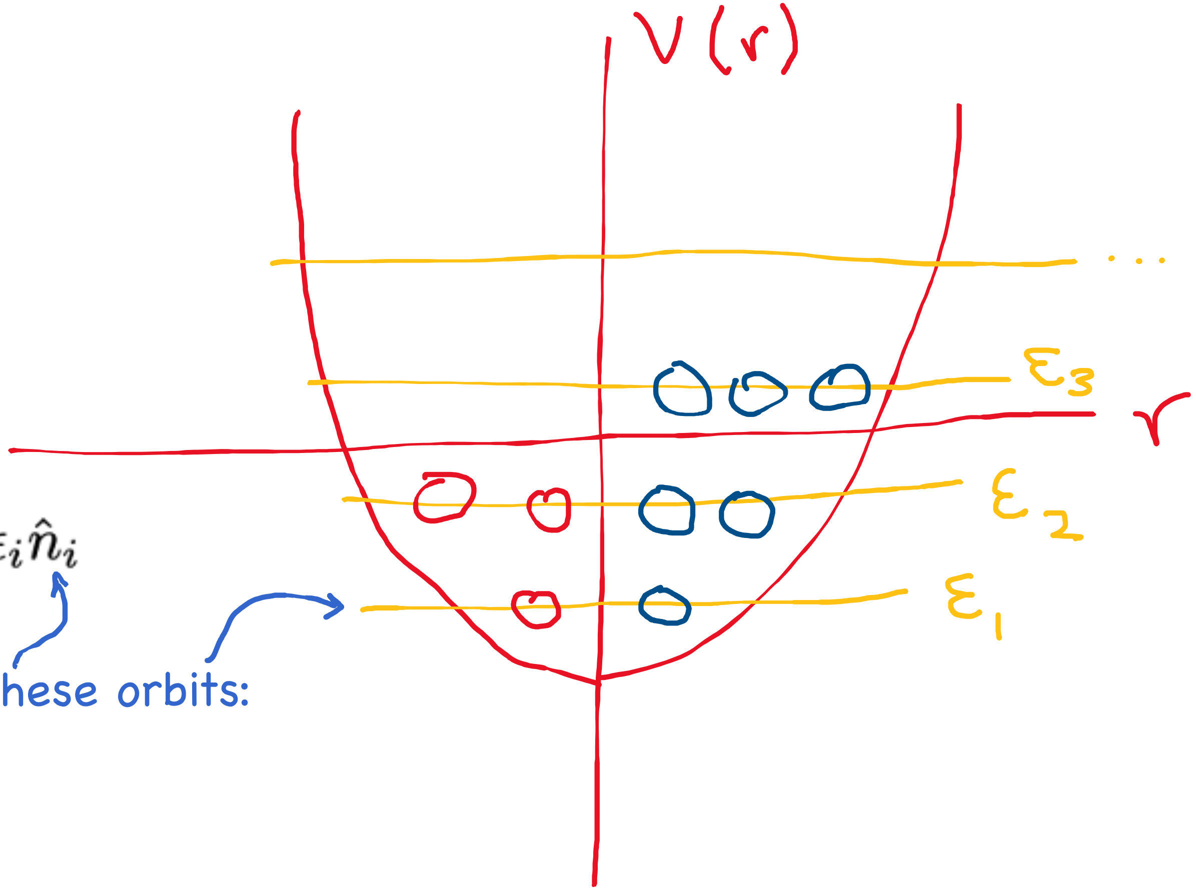
Claim: the **shell model** is the "closest-to-*ab-initio*" we can reasonably expect to meet these needs

Nuclear shell model as mean field theory



$$\hat{H}(\boldsymbol{c}) = \sum_i \epsilon_i \hat{n}_i$$

# of particles in these orbits:
Mean-field energy



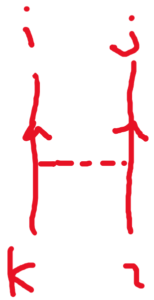
Single-particle energies should reproduce magic numbers, i.e. shell gaps.
(Requires modifications to HO potential, spin-orbit coupling, etc.)

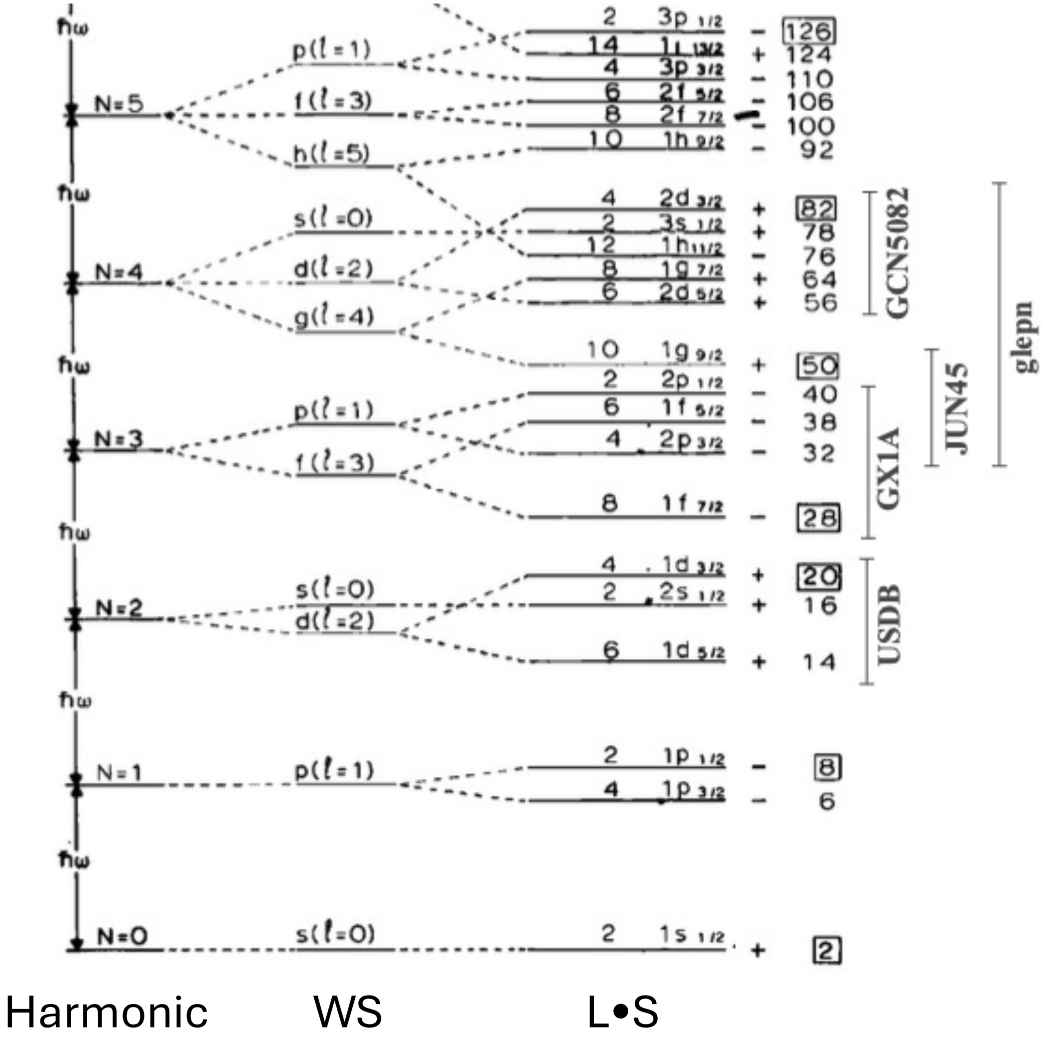
Nuclear shell model beyond mean field

$$\hat{H}(\boldsymbol{c}) = \sum_i \epsilon_i \hat{n}_i + \sum_{i\leq j,k\leq l;JT} V_{ijkl;JT}\hat{T}_{ijkl;JT}$$

Matrix elements:
Residual 2-body interaction

Get these from effective field theory

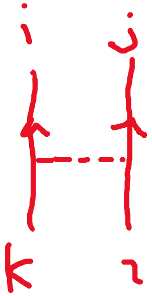




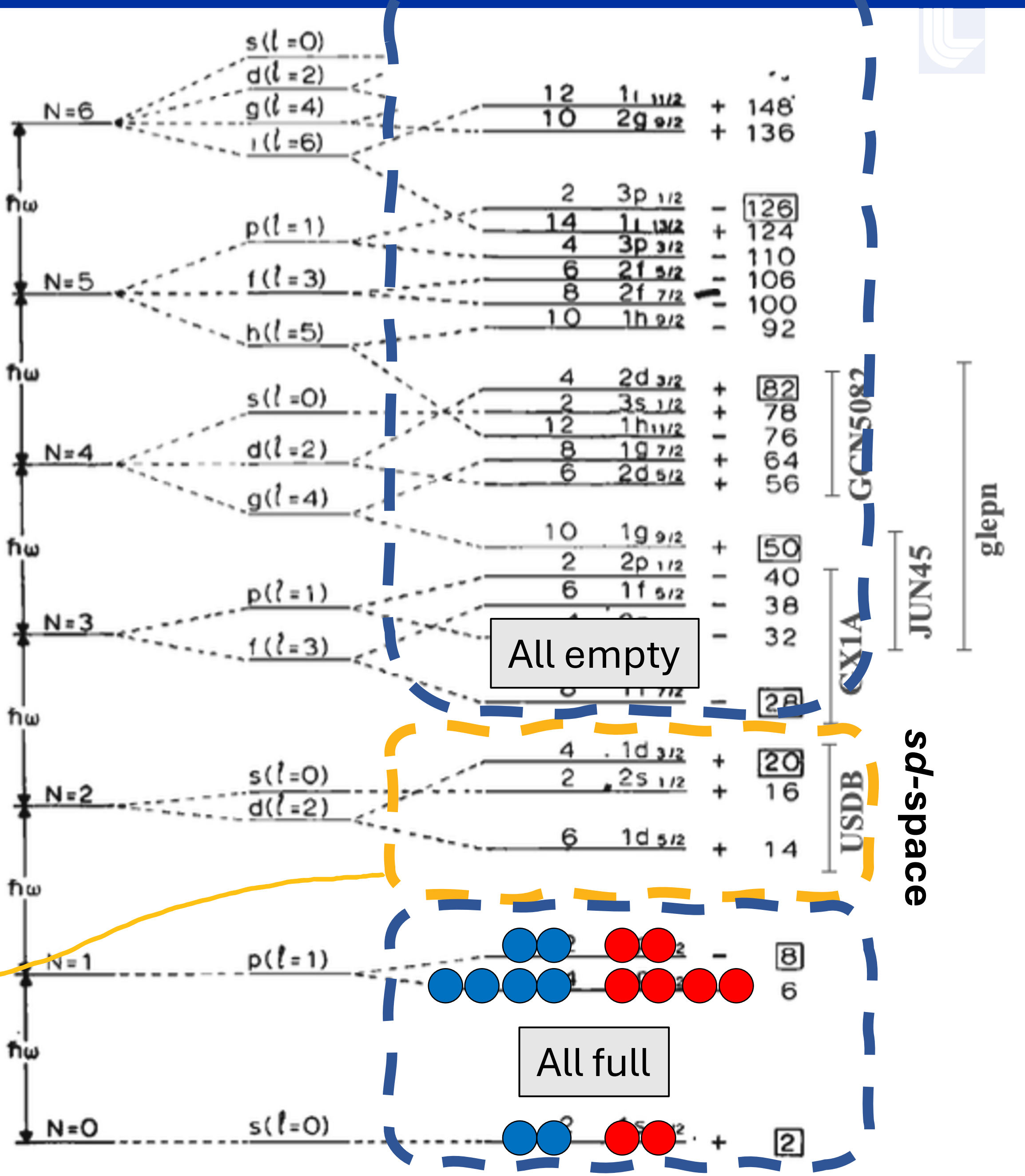
Phenomenological nuclear shell model (with core)

$$\hat{H}(\mathbf{c}) = \sum_i \epsilon_i \hat{n}_i + \sum_{i\le j,k\le l;JT} V_{ijkl;JT}\hat{T}_{ijkl;JT}$$

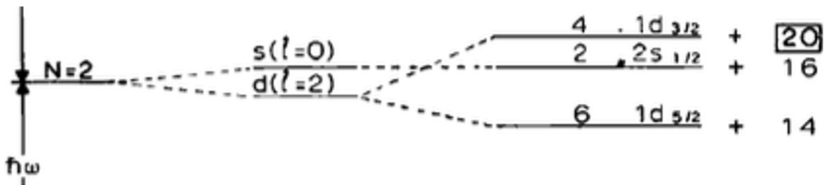
Renormalized "effective interaction"



$$\hat{H}(\mathbf{c}) = \sum_i \epsilon_i \hat{n}_i + \sum_{i\le j,k\le l;JT} V_{ijkl;JT}\hat{T}_{ijkl;JT}$$



Example: USDB interaction for the *sd*-shell



sd-space Hamiltonian:

- 3 single particle energies
- 63 residual TBMEs

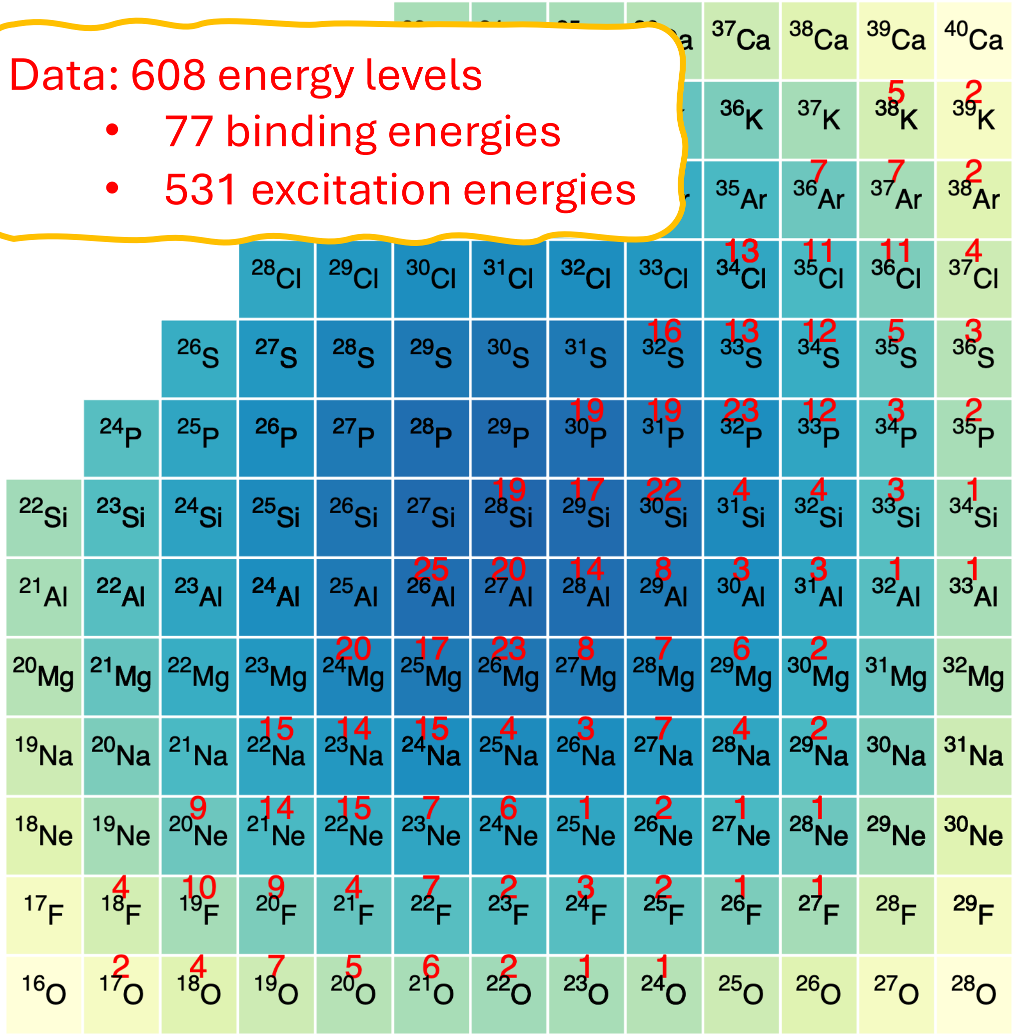
B. A. Brown *et al.*, PRC 74, 034315 (2006)

$H|\psi\rangle = E|\psi\rangle$

Adjust to fit

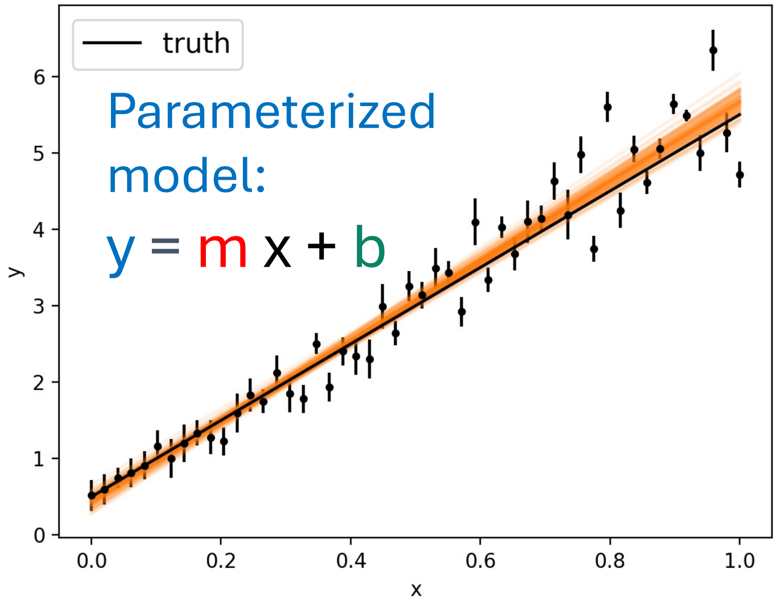
Data: 608 energy levels

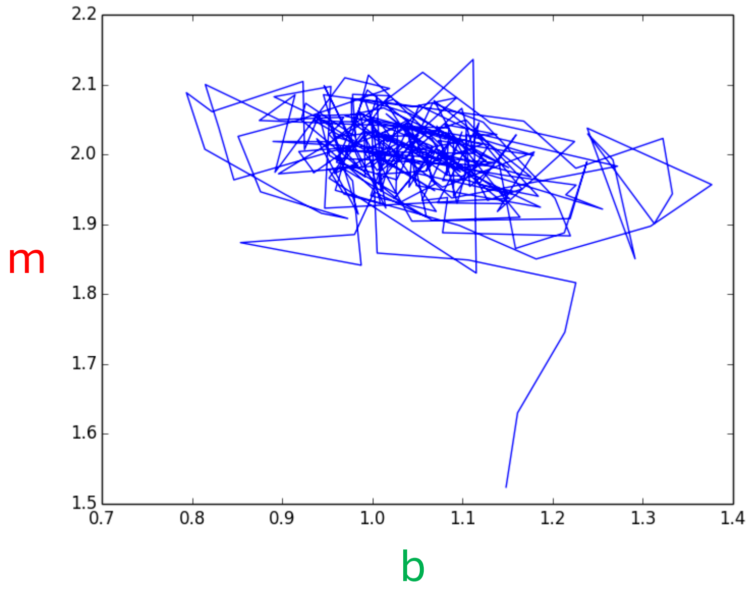
- 77 binding energies
- 531 excitation energies

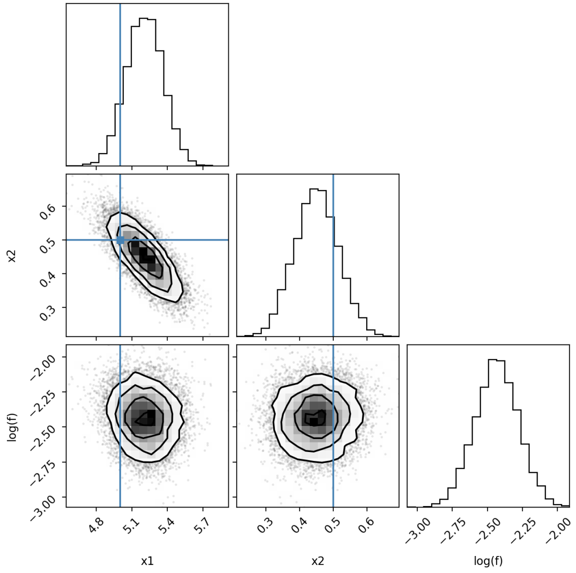


We gain significant accuracy, but we lose perturbation theory.
How do we assess uncertainty?

Markov Chain Monte Carlo (MCMC) for more robust statistics

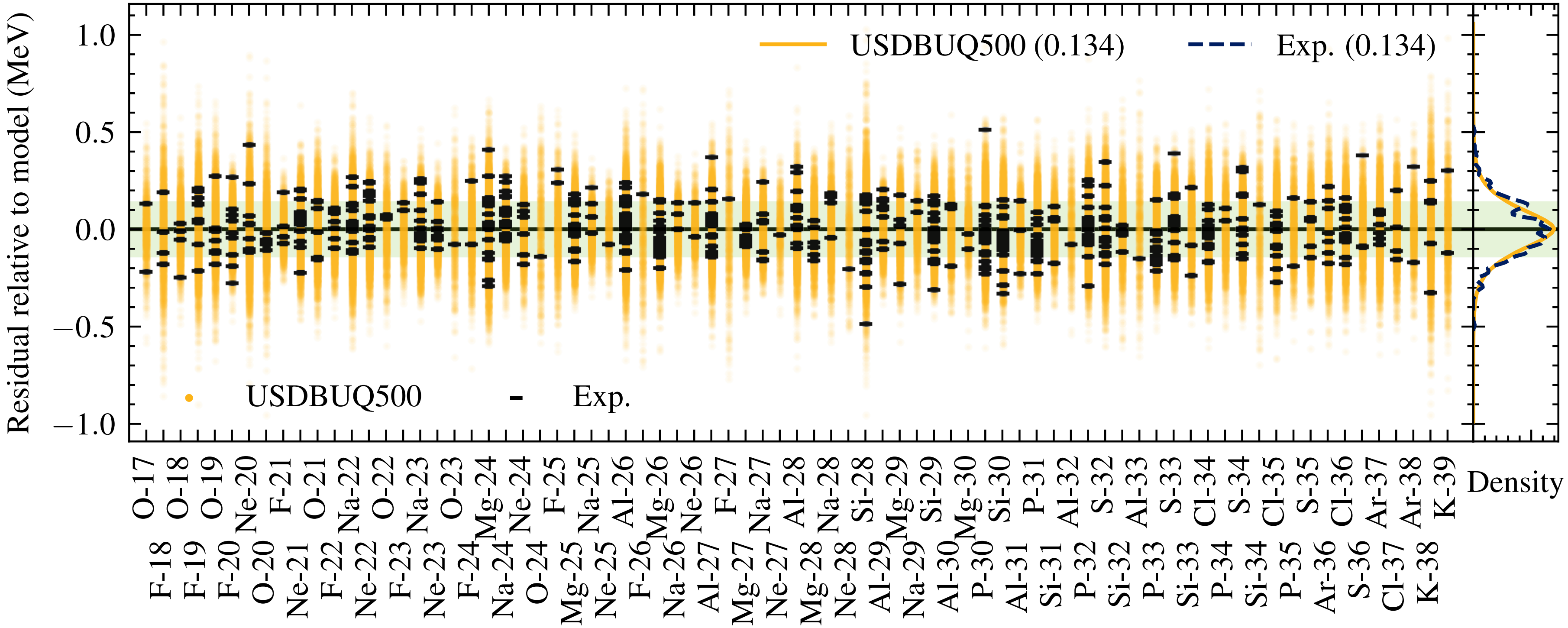






Result: *probability distribution* for the underlying parameters

USDBUQ-500: a new UQ shell model interaction



USDBUQ500 stats sheet

Standard error of a **random prediction**:

- 190 keV (USDB is 130 keV)

Standard error of an **averaged prediction:**

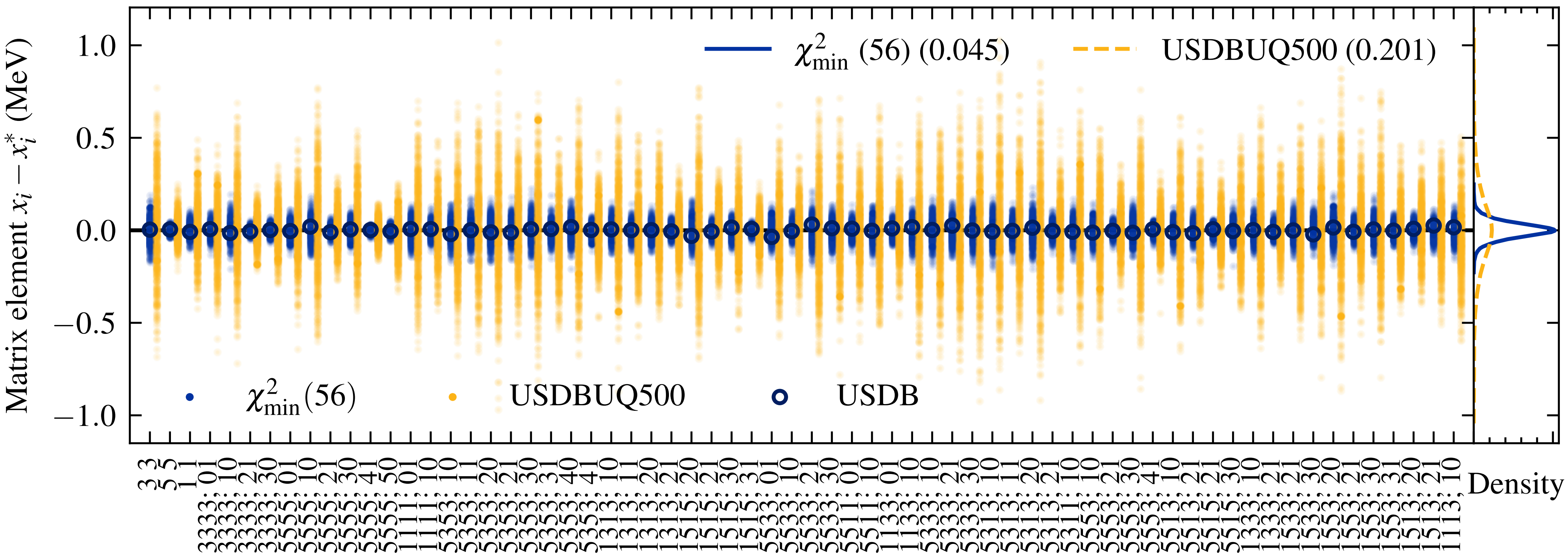
- 134 keV

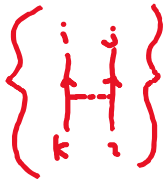
Average reported **error bar**:

- 134 keV

The result is a probability distribution for the Hamiltonian matrix elements

$$\hat{H}(\boldsymbol{c}) = \sum_i \epsilon_i \hat{n}_i + \sum_{i \le j, k \le l; JT} V_{ijkl;JT} \hat{T}_{ijkl;JT}$$





Physical Review C

ACCEPTED PAPER

Toward shell model interactions with credible uncertainties

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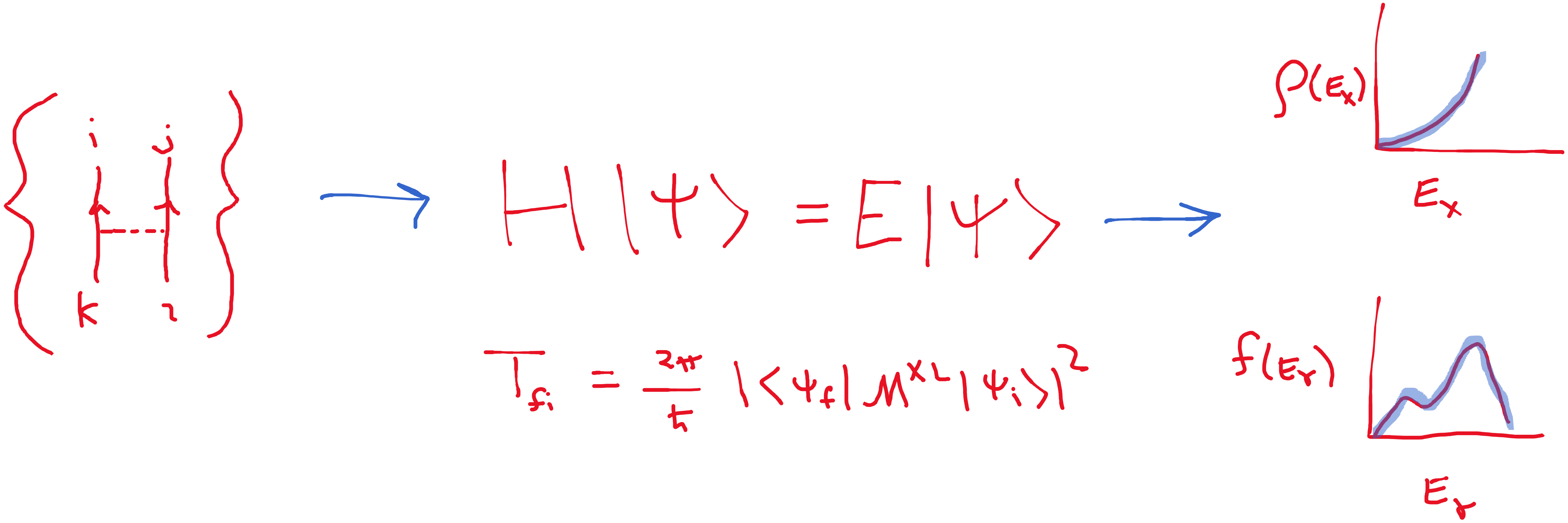
Abstract

[Background] The nuclear shell model is a powerful framework for predicting nuclear structure observables, but relies on interaction matrix elements fit to experimental data as its inputs. Extending the shell model's applicability, particularly toward dripline nuclei, requires efficient fitting methods and credible uncertainty quantification. Traditional approaches face computational challenges and may underestimate uncertainties. [Purpose] We develop and test a framework combining eigenvector continuation and Markov Chain Monte Carlo to efficiently fit shell model interaction matrix elements and quantify their uncertainties. [Methods] Eigenvector continuation is used to emulate shell model calculations, reducing computational costs. The emulator enables Markov chain Monte Carlo sampling to optimize interaction matrix elements and rigorously assess parametric uncertainties. The framework is benchmarked using the USDB interaction in the sd-shell. [Results] The emulator reproduces the USDB interaction with negligible error, validating its use in shell model fitting applications. However, we find that to obtain credible predictive intervals, the model defect of the shell model itself, rather than experimental or emulator error, must be taken into account in order to obtain credible uncertainties. [Conclusions] The proposed framework provides an efficient and rigorous approach for fitting shell model interactions and quantifying uncertainties. Further, the normality assumption used in the past appears sufficient to describe the distribution of interaction matrix elements. However, it is crucial to account for model correlations to avoid underestimating uncertainties.

We can turn UQ shell model into UQ LDs and GSFs

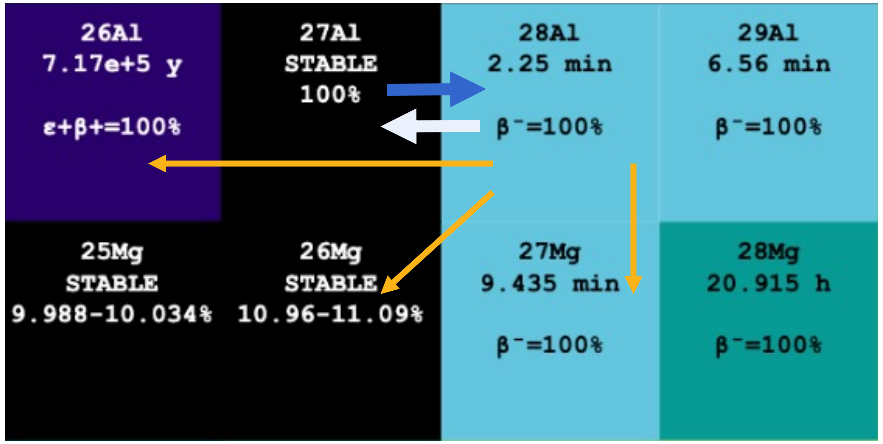


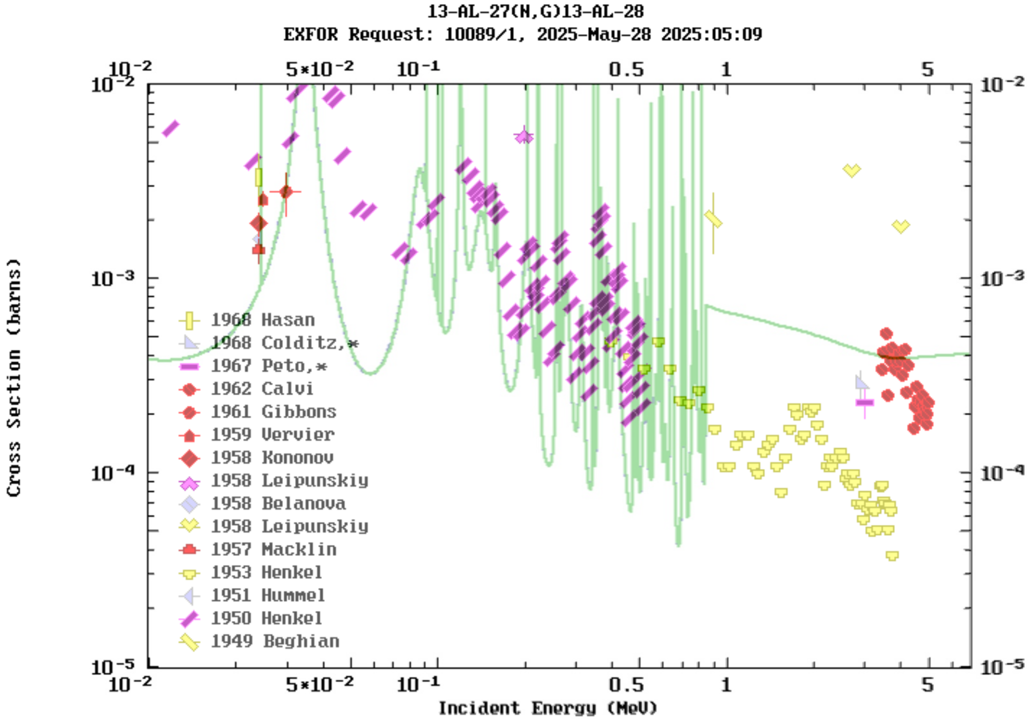
Advantages:
- Microscopic and high fidelity
- Self-consist LD and GSF (OMP?) across entire region
- Full covariance information

Disadvantages:
- Limited to low energies
- E1 GSF needs large model space
- Availability of interactions

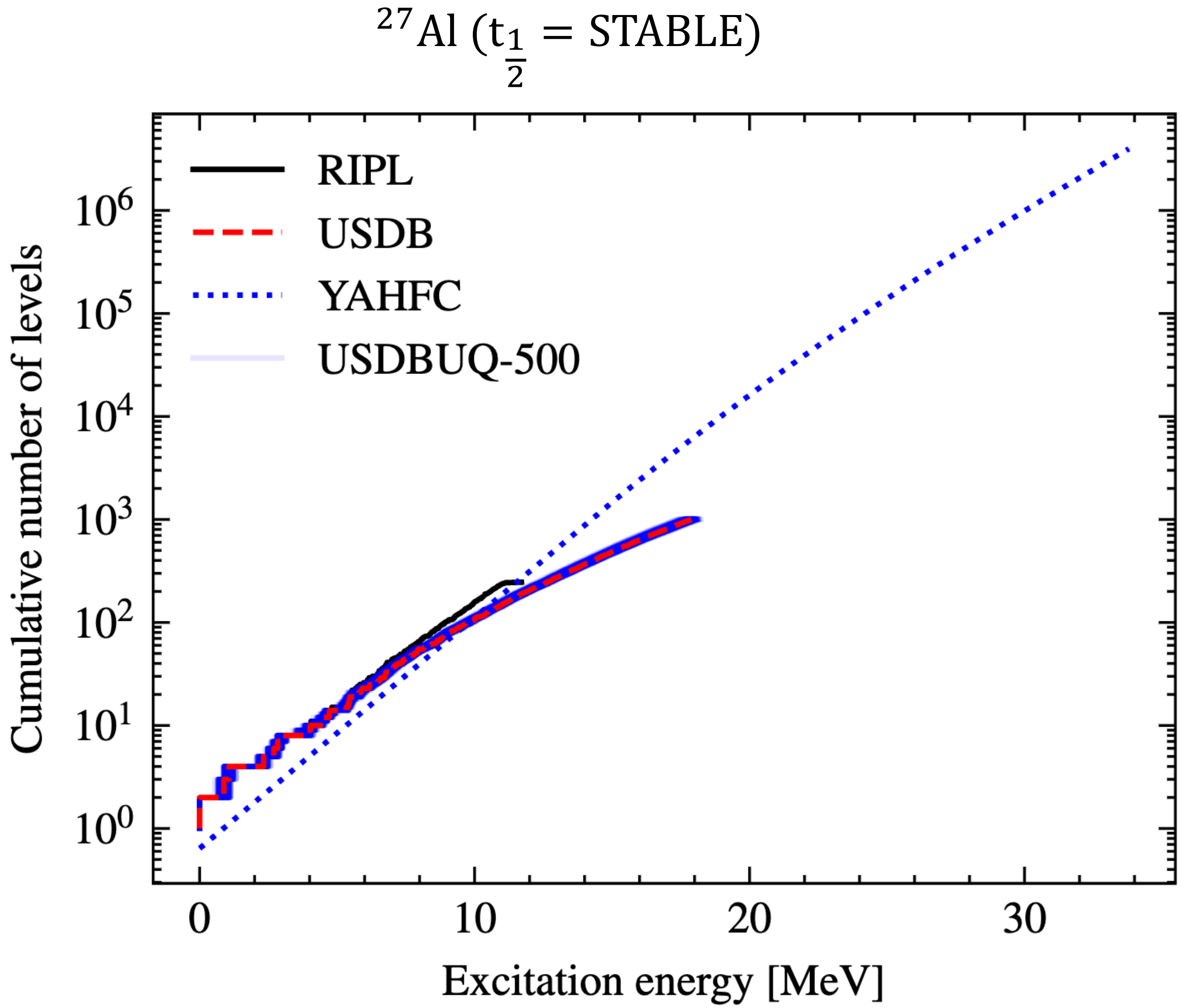
Example: neutron capture on ^{27}Al

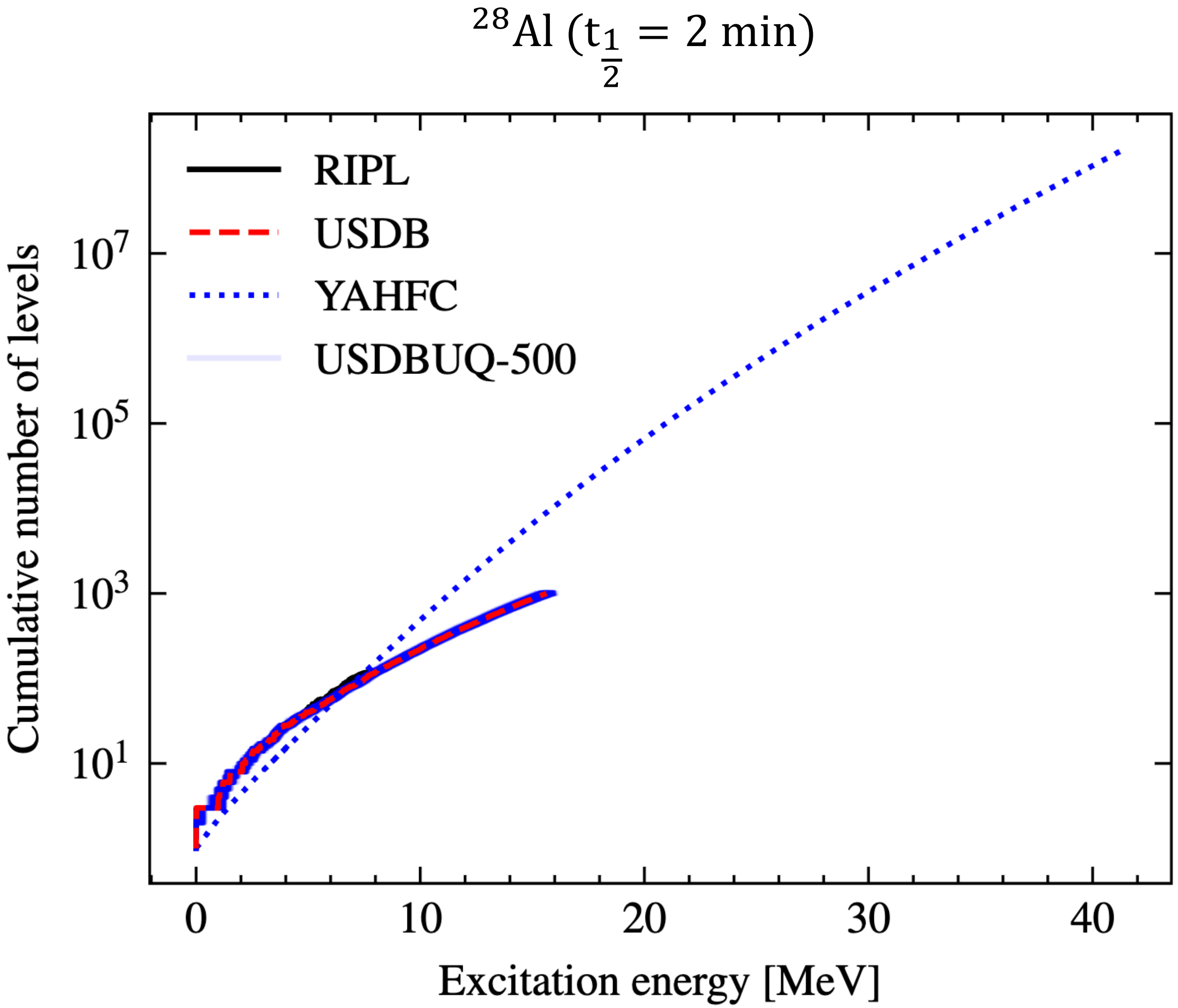
$^{27}\mathrm{Al}(n,\gamma)^{28}\mathrm{Al}$



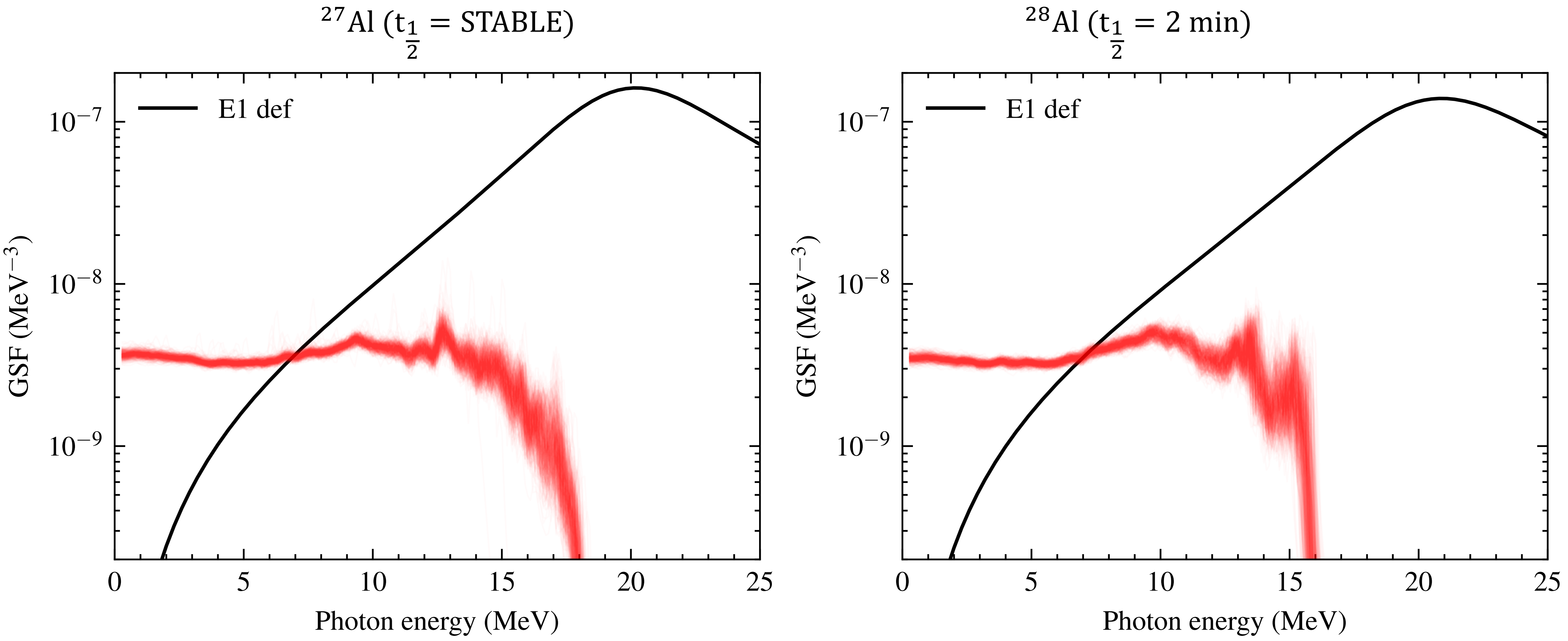


Level densities from shell model

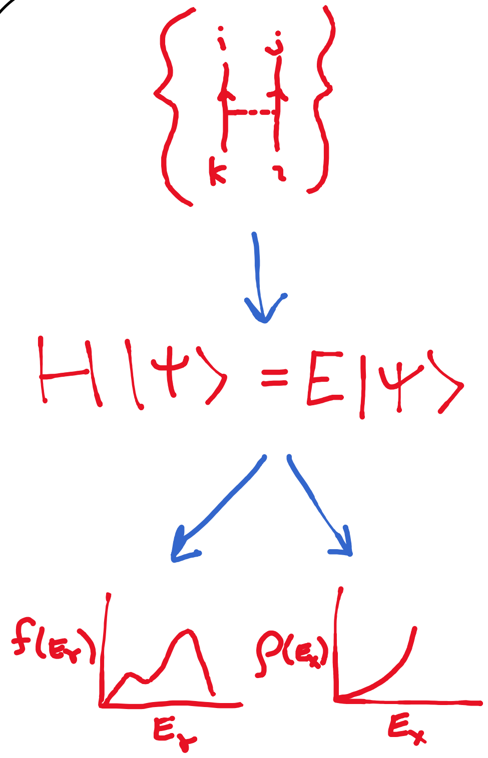




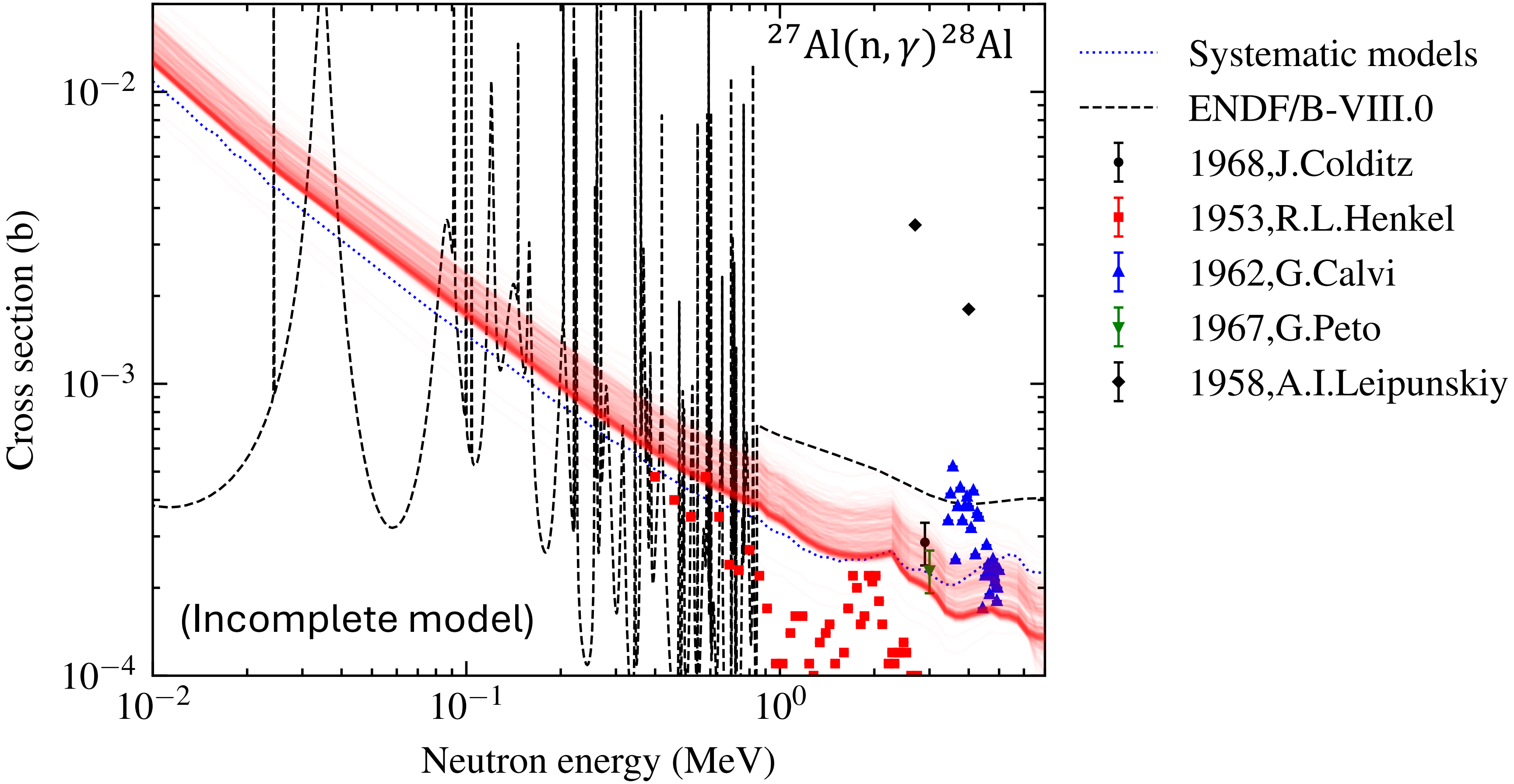
M1 gamma strength functions from shell model



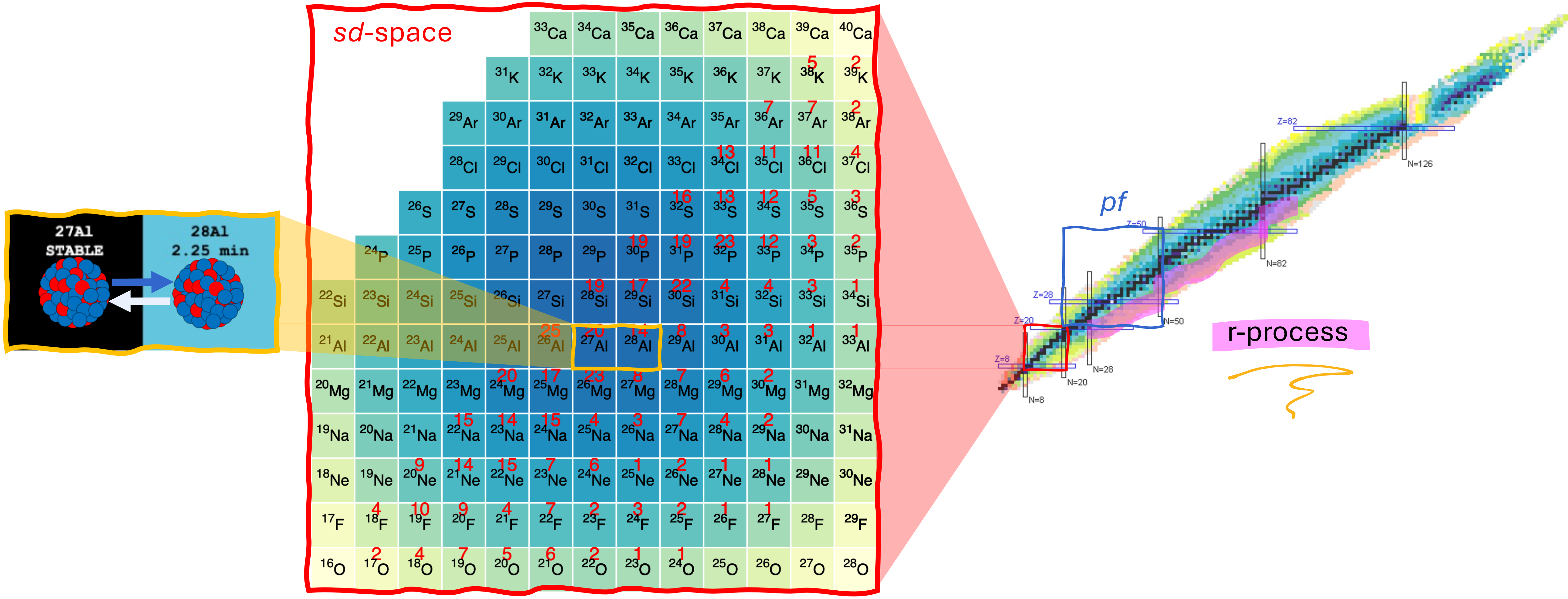
Neutron capture cross section computed with UQ level densities and M1 strength functions

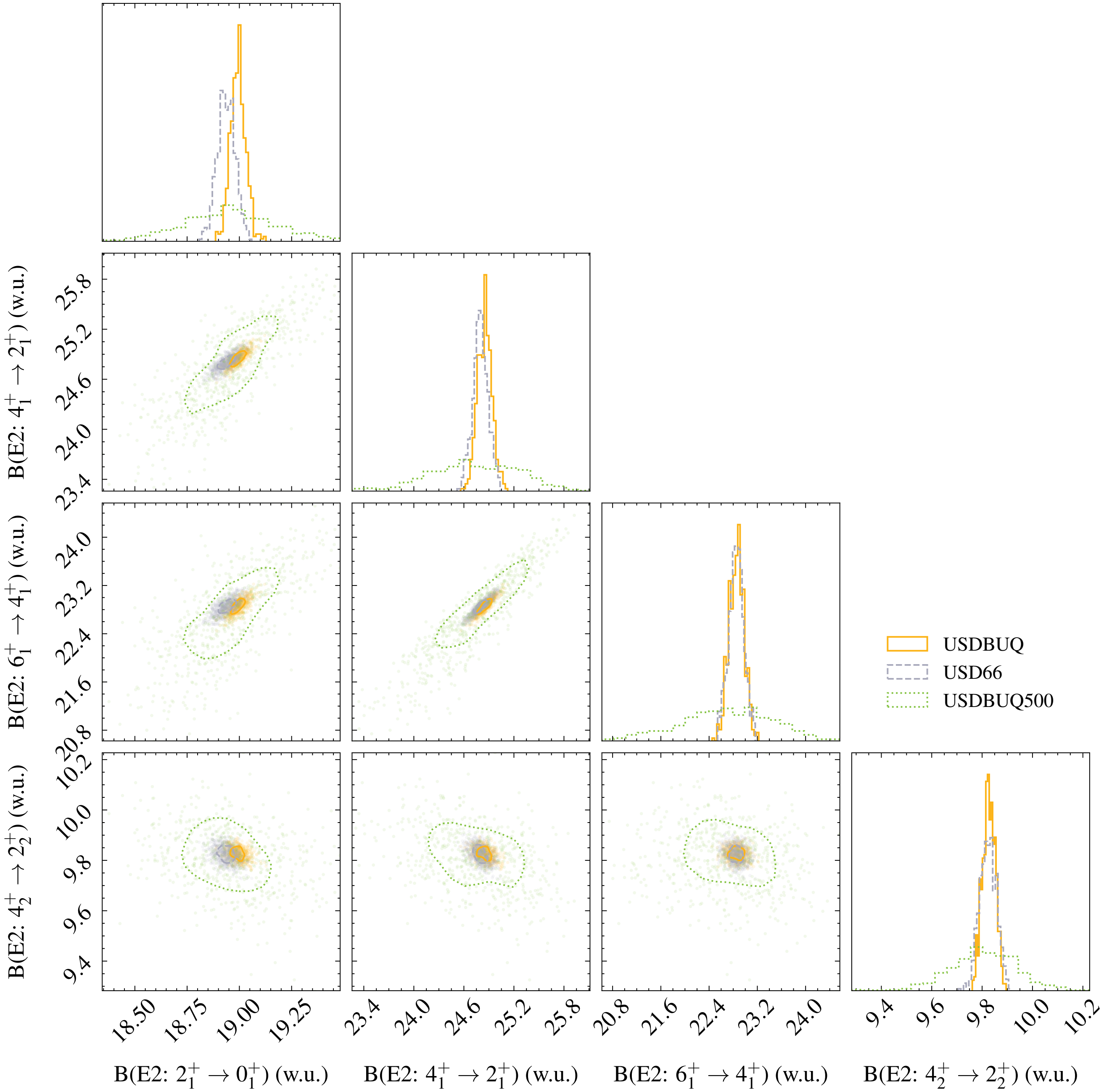


$N = 560$



Shell model for ***future*** astrophysics and nuclear technologies

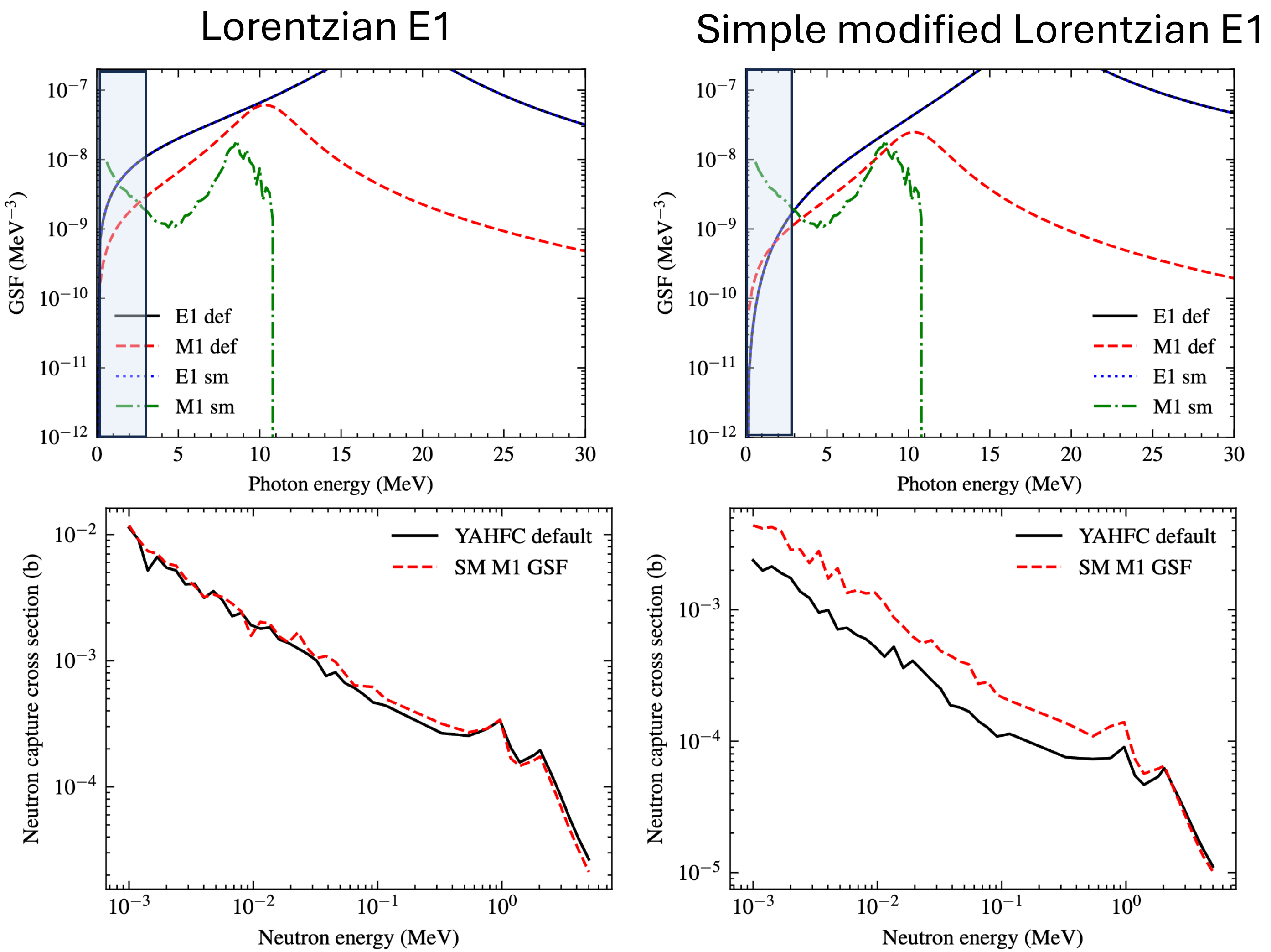



B(E2: $4_1^+ \to 2_1^+$) (w.u.)
B(E2: $6_1^+ \to 4_1^+$) (w.u.)
B(E2: $4_2^+ \to 2_2^+$) (w.u.)
B(E2: $2_1^+ \to 0_1^+$) (w.u.)
USDBUQ
USD66
USDBUQ500

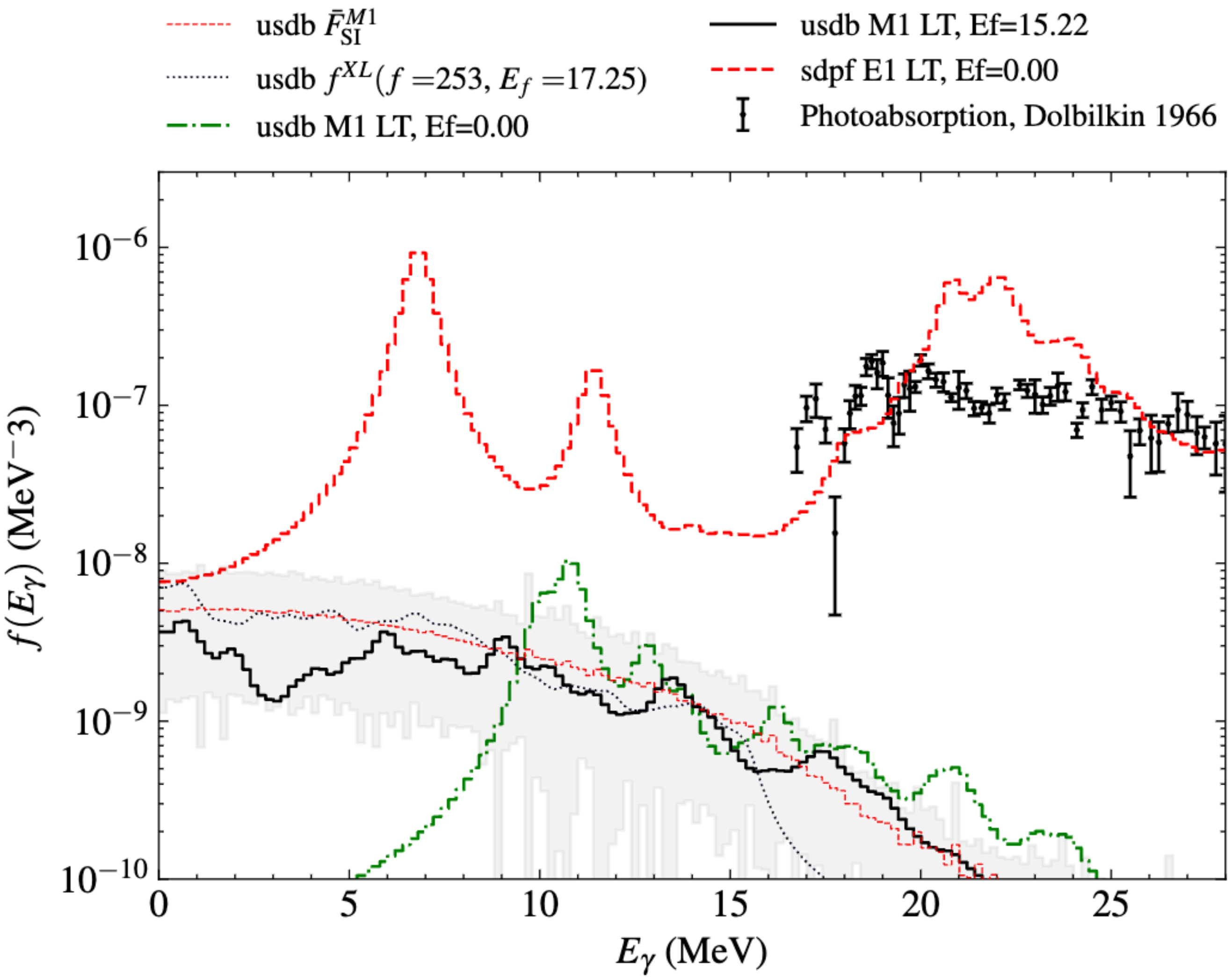
Impact on neutron capture cross sections

Ti58 (Ti59 cn and gsf)

Sn(Ti59)=3.034 MeV

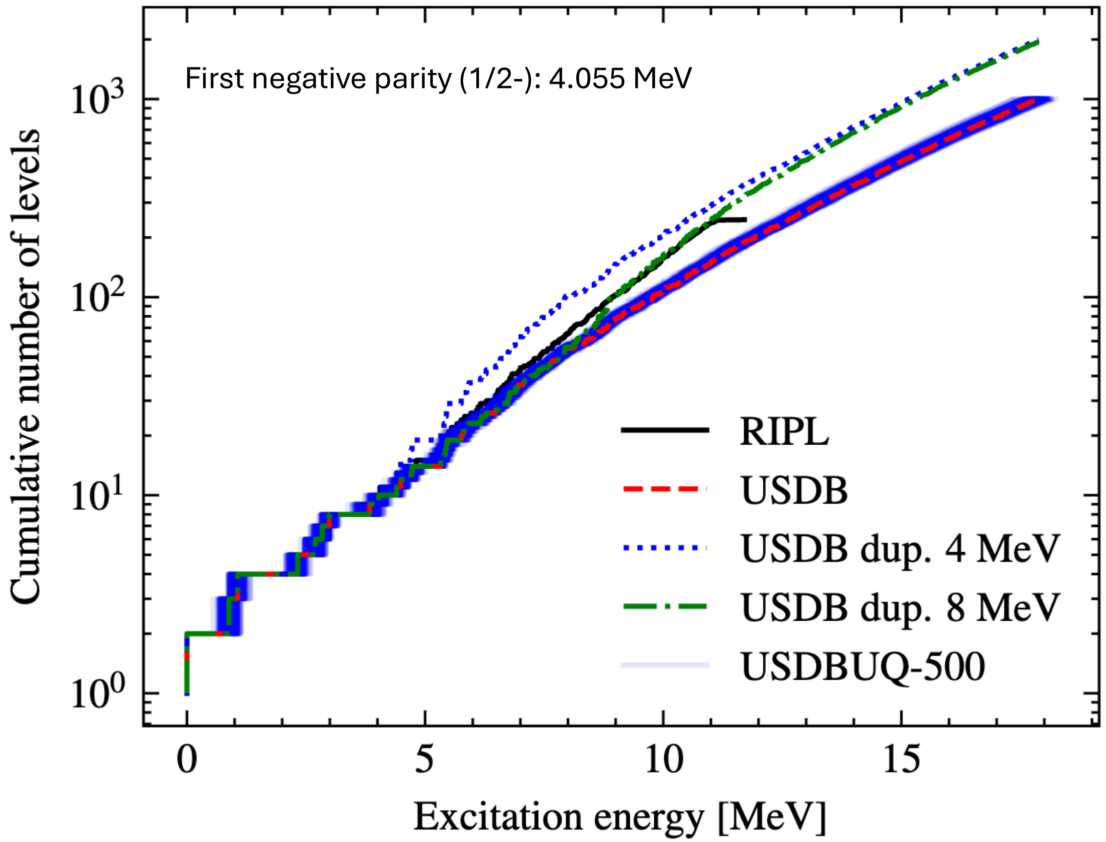


We can better understand the composition of GSFs



Valence space is eventually exhausted

Sn(Al-27)=13.058



Level density "mirage" can compensate