Estimating neutron-capture rate uncertainties for iron isotopes using shell-model-based nuclear level densities in TALYS

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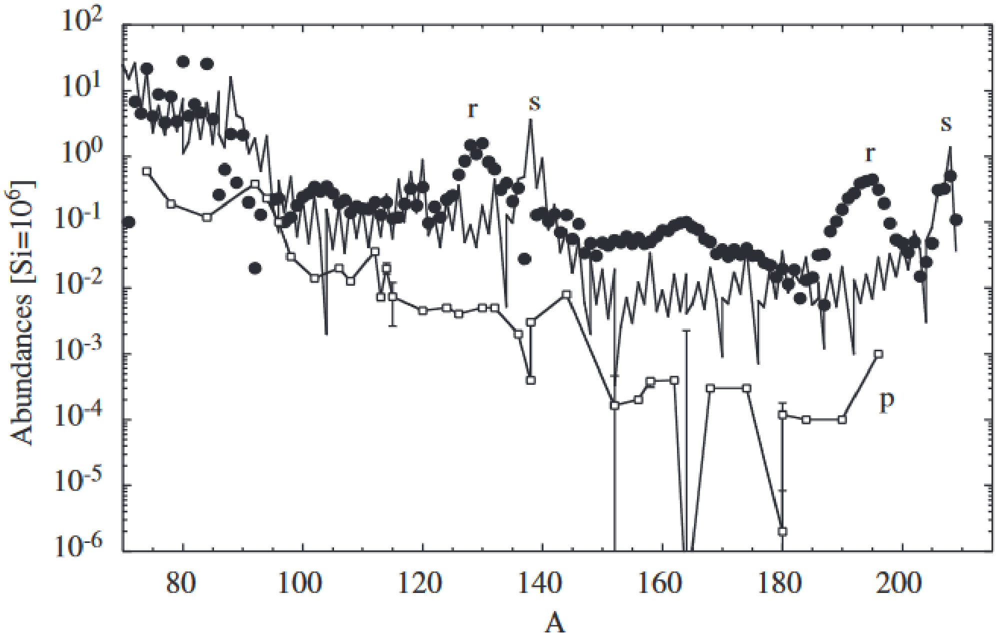
Grand Valley State University

Solar abundance distributions for heavy-element isotopes

Nuclear reaction data are required for many applications in both basic and applied science, including understanding elemental abundancies, operation of nuclear reactors.

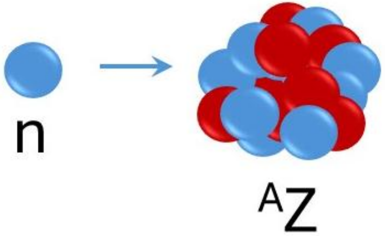


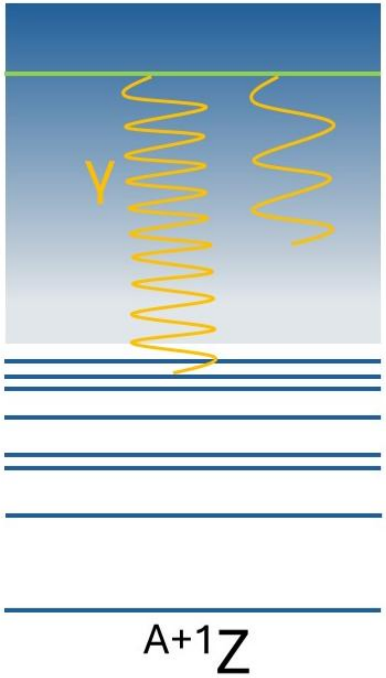
The exploration of the elemental abundances requires knowledge of the nuclear properties of thousands of neutron rich nu-clides. Simulations of elemental abundance distributions are obtained through nucleo-synthesis reaction network codes, with reaction cross-sections and rates being key inputs.

Neutron radiative capture reactions – Compound nucleus

To study the formation of neutron-rich nuclei, neutron radiative capture (n,γ) reaction rates play a crucial role. We treat these reactions within the compound nucleus framework.

- An incident neutron is absorbed by a target nucleus A, forming an excited compound nucleus A+1.
- According to Bohr's independence hypothesis, the compound nucleus "forgets" how it was formed and the decay probability depends only on the total energy given to the system.
- The compound nucleus then de-excites through various decay channels, including γ-ray emission.





Neutron radiative capture in compound nucleus framework

- The neutron radiative capture cross section is proportional to the probability of forming a compound nucleus and subsequently decaying by γ-ray emission.
- $\langle\sigma(n,\gamma)\rangle \sim \frac{T_n T_\gamma}{\sum T_c}$

T_n neutron transmission coefficient for formation of compound nucleus

T_γ total γ-ray transmission coefficient

T_c transmission coefficients of all possible outgoing channels

- When neutron scattering dominates $\langle\sigma(n,\gamma)\rangle \approx \frac{T_n T_\gamma}{\sum T_c} \approx T_\gamma \equiv \sum_{Xl} \sum_{I'\Pi'} \int T_{Xl}(E_\gamma)\rho(E_f, I', \Pi')\, dE_\gamma$

T_γ is obtained by summing over all possible γ transitions to all accessible final states

The level density $\rho(E_f, I', \Pi')$ determines how many final states are available for γ-decay

The γ-ray transmission coefficients $T_{Xl}(E_\gamma)$ determine the probability of each γ-ray transition

Level densities and γ-ray transmission coefficients introduce the largest uncertainty in the T_γ

Astrophysical reaction rates

$$N_A\langle\sigma v\rangle = N_A\left(\frac{8}{\pi\mu(k_BT)^3}\right)^{1/2}\int_0^\infty \sigma(E)\,Eexp\left(-\frac{E}{k_BT}\right)dE$$

In stellar environments, reactions occur over a distribution of neutron energies. The reaction rate is obtained by averaging the neutron capture cross section over the Maxwell-Boltzmann energy distribution.

Nuclear level density (NLD)

Definition: number of levels per energy interval

AUGUST 15, 1936 PHYSICAL REVIEW VOLUME 50

An Attempt to Calculate the Number of Energy Levels of a Heavy Nucleus

H. A. BETHE, *Cornell University*

(Received June 5, 1936)

state of energy U_0. We are interested in the energy levels of the nucleus which lie by a certain amount Q higher than the ground state, and we ask for the density of energy levels in this region, i.e., for the number of levels between Q and $Q+dQ$ which we may call $\rho(Q)dQ$. $1/\rho(Q)$ will then be the average spacing between neighboring levels.

We shall be particularly interested in such values of Q which are just sufficient to dissociate the given nucleus A into a neutron and a residual nucleus of atomic weight $A-1$. These energy levels will be important for the capture of slow neutrons by the nucleus $A-1$. In general, the

Nuclear level density (NLD)

Experimental NLDs

- Counting low-energy discrete levels
- Level density from average neutron resonance spacing (average energy spacing between adjacent neutron resonances), D_0 (l=0) and D_1 (l=1), at the neutron separation energy, S_n, primarily for stable nuclei.
- Oslo method and β-Oslo technique (simultaneously determines the functional form of the NLD and γ-ray strength function, stable/exotic species)
- Particle evaporation spectra in compound nuclear reactions

A. Schiller *et al*, N. Inst. Meth. Phys. Res., Sect. A 447, 498 (2000).

A. C. Larsen et al, Nuclei in the Cosmos XV. Springer Proc. in Phys., vol 219. Springer.

H. Vonach,, BNL Report No. BNL-NCS-51694, p. 247.

NLD - Phenomenological models

- Back-shifted Fermi gas model

$$\rho(E_x, J, \pi) = \frac{1}{2}\frac{2J+1}{2\sigma^2}\exp\left[-\frac{(J+1/2)^2}{\sigma^2}\right]\frac{1}{\sqrt{2\pi}\sigma}\frac{\sqrt{\pi}}{12}\frac{exp\left[2\sqrt{aU}\right]}{a^{1/4}U^{5/4}}$$

- Constant temperature model

$$\rho(E_x, J, \pi) = \underbrace{\frac{1}{2}\frac{2J+1}{2\sigma^2}\exp\left[-\frac{(J+1/2)^2}{\sigma^2}\right]}_{\text{spin distribution}}\frac{1}{T}exp\left[\frac{E_x - E_0}{T}\right]$$

Analytical formulas with parameters (a, U, E_0, T) determined from the available experimental data or from empirical expressions; less accurate far from stability

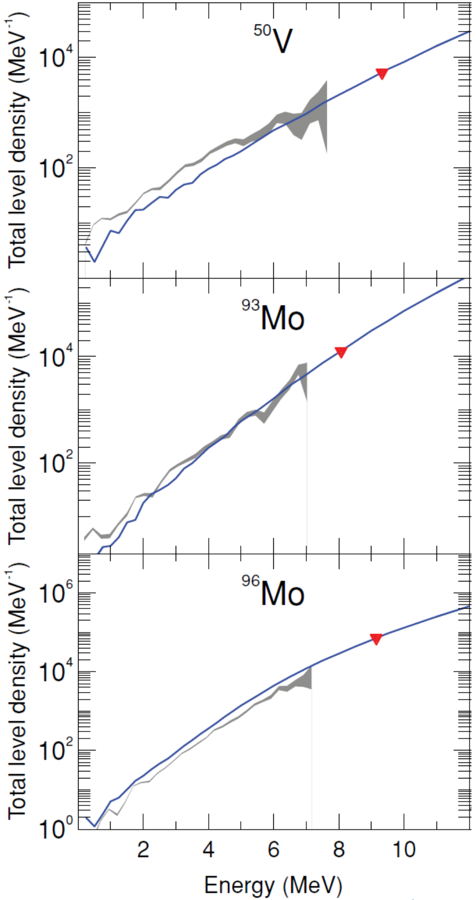
H. A. Bethe, PR 50 332 (1936)
A. Gilbert et al., CJP 43 1248 (1965)
T. Ericson, Adv Phys 9 425 (1960)

NLD - Microscopic models

- Skyrme and Gogny energy density functionals within the Hartree-Fock-Bogoliubov framework

✓ spin- and parity-dependent NLDs

✓ global level density predictions available for thousands of nuclides at high excitation energies and spins

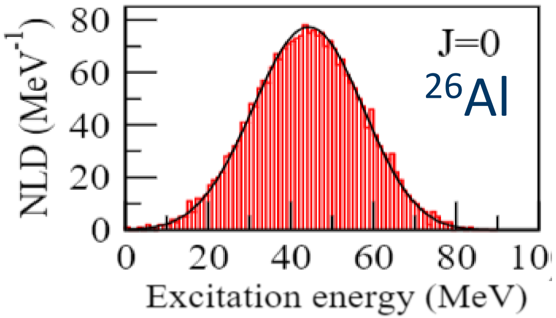


S. Goriely et al., ADNDT 77 311 (2001)   S. Hilaire et al., PRC 86 064317 (2012)   S. Goriely et al., PRC 78 064307 (2008)

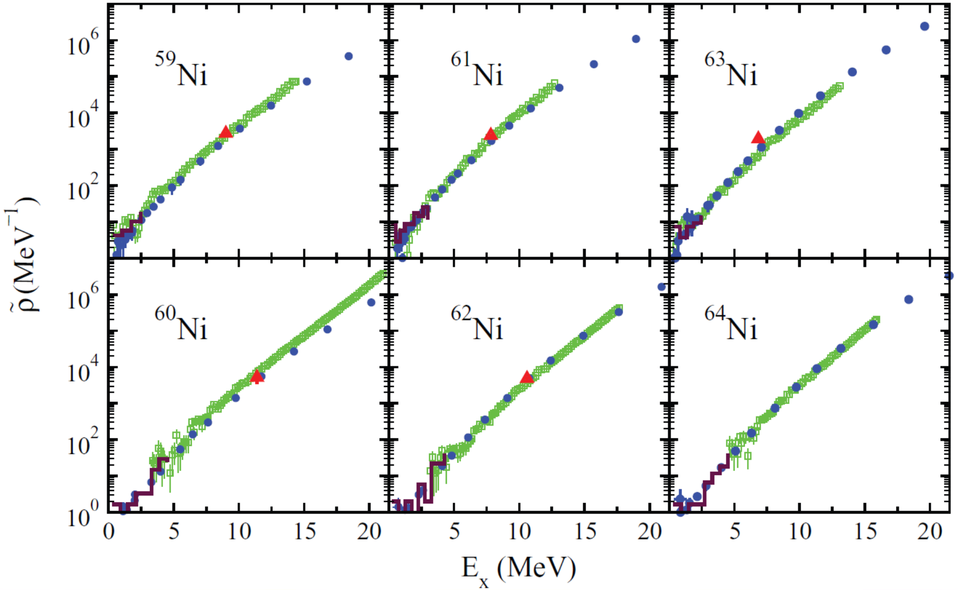
NLD – Shell model approaches

(spin- and parity-dependent NLDs)

– Configuration interaction shell model calculations using conventional diagonalization;
× *sd*-nuclei



– Shell Model Monte Carlo; mid-mass and heavy nuclei



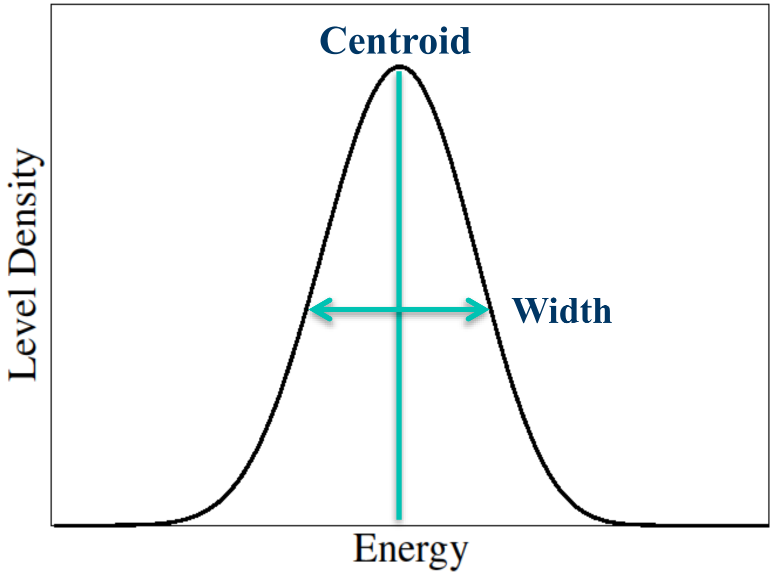
Y. Alhassid et al., PRL 99 162504 (2007)
M. Bonett-Matiz et al. PRC 88 011302 (R) (2013)

NLD – Shell model approaches: Moments Method

The code enumerates all proton/neutron partitions within a given model space:

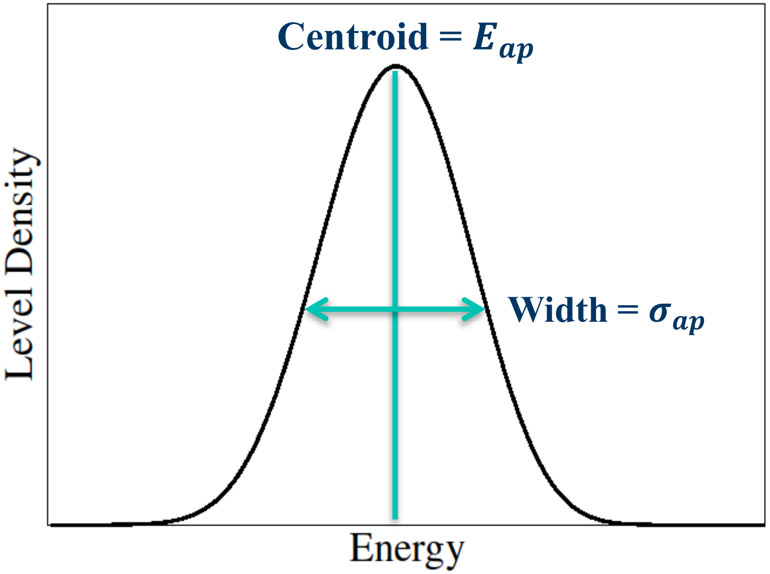
p	$d_{5/2}$	$s_{1/2}$	$d_{3/2}$
1	6	0	0
2	5	1	0
3	5	0	1
4	4	2	0
...	...	...	...
15	0	2	4

Each proton partition is combined with a neutron partitions to generate all possible states with fixed J and π arising from each p/n configuration.



CI shell model calculations show that states with fixed J and π from a given p/n configuration exhibit approximately Gaussian energy distributions.

NLD – Shell model approaches: Moments method



$$E_{ap} = \frac{1}{D_{ap}} Tr^{ap} H$$

$$\sigma_{ap}^2 = \frac{1}{D_{ap}} Tr^{ap} H^2 - E_{ap}^2$$

D_{ap}: dimension of partition

$$G_{ap} = G\left(E - E_{ap} + E_{g.s.};\ \sigma_{ap}\right)$$

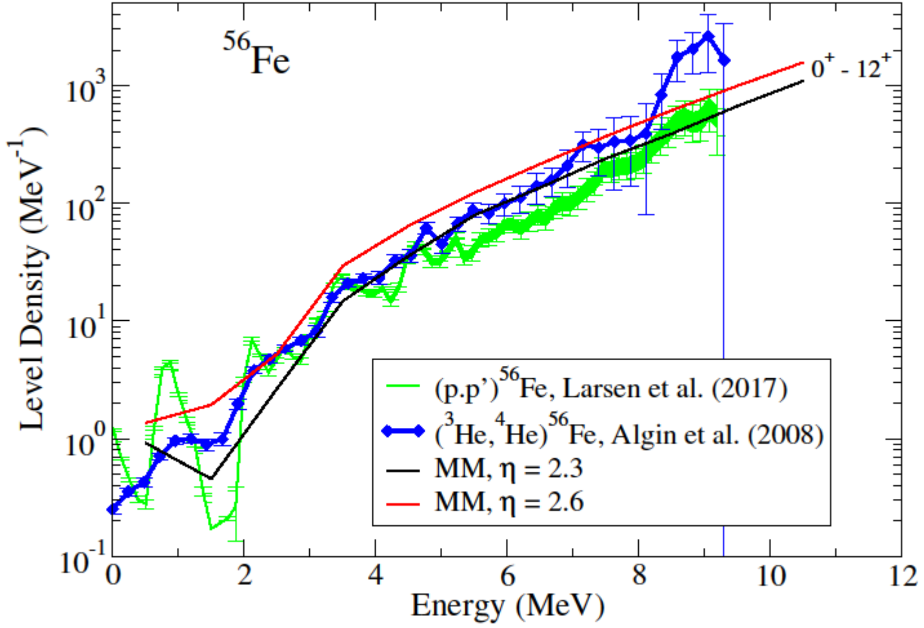
$$G(x;\sigma) = C \begin{cases} e^{-x^2/2\sigma^2}, |x| \leq \eta\sigma \\ 0, |x| > \eta\sigma \end{cases}$$

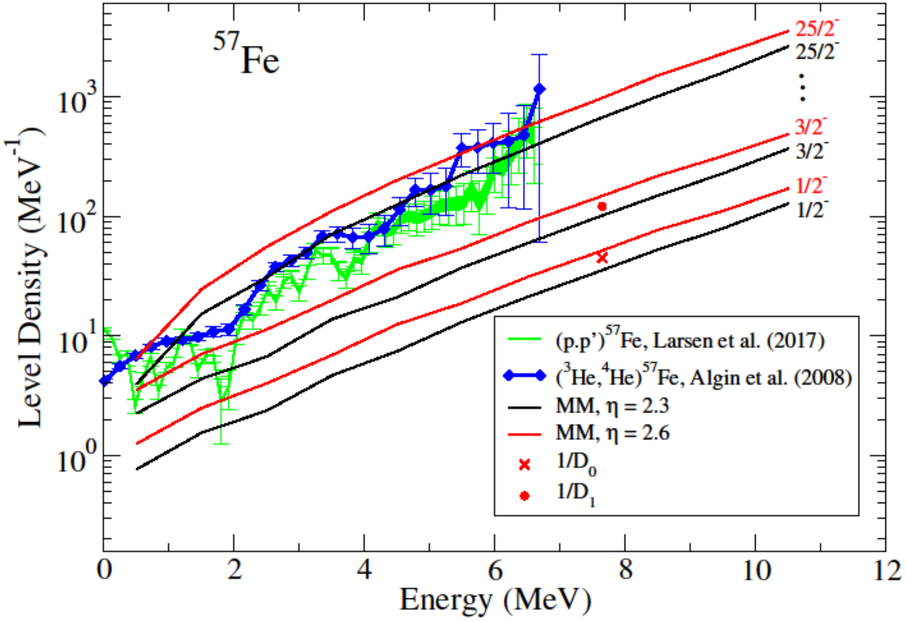
$E_{g.s.}$: ground state energy
η: cut-off (2.3 – 2.8)

$$\rho(\mathrm{E}, a) = \sum_p D_{ap}\, G_{ap}$$

The moments method code computes the first two moments of the Hamiltonian:
First moment → Centroid
Second moment → Width

Moments Method – comparison to experiment





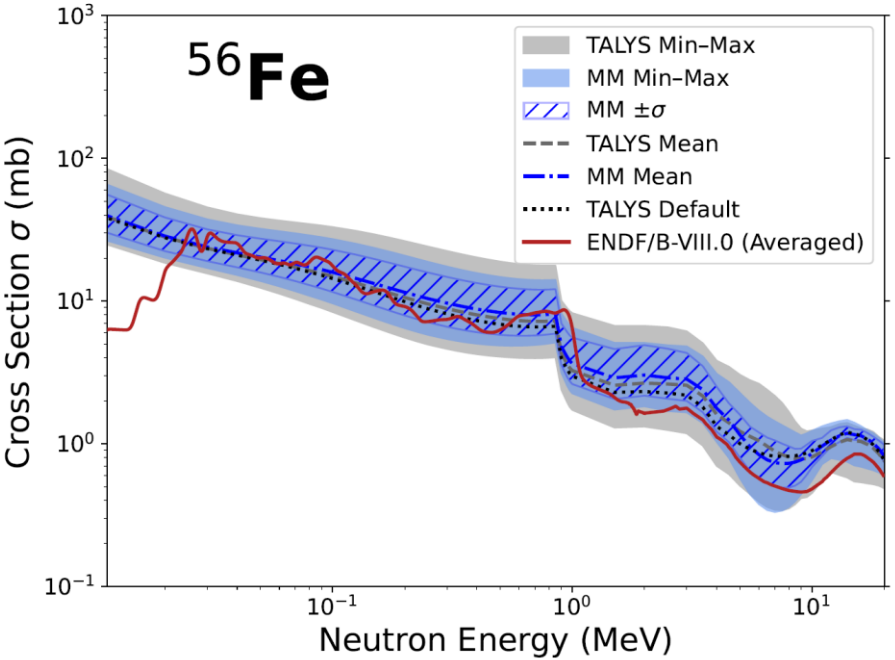
η: cut-off (2.3 – 2.6) is the uncertainty in calculations

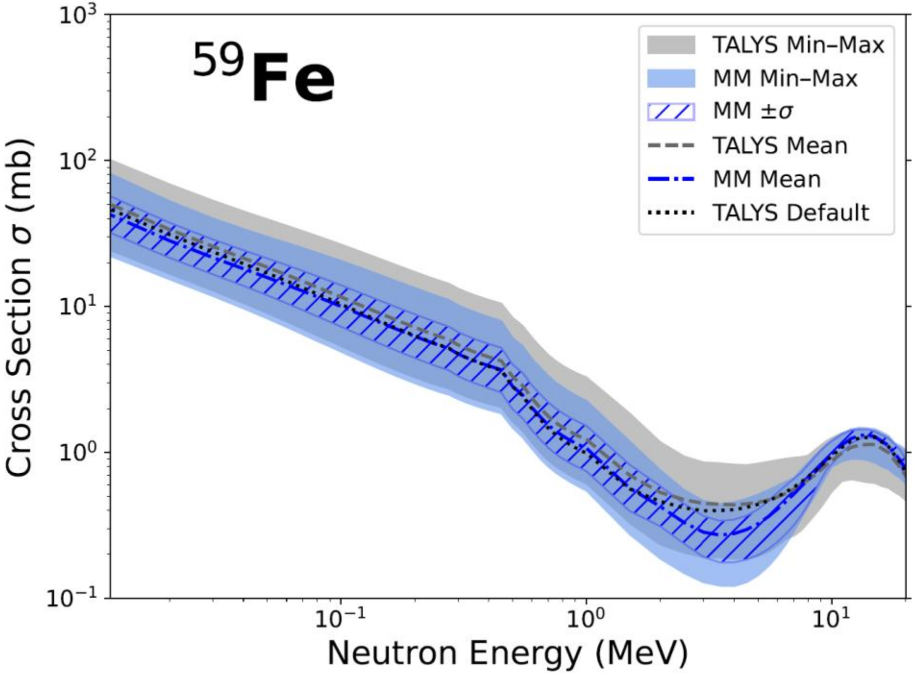
From NLDs to neutron capture cross-sections and reaction rates

The Moments Method (MM) provides spin- and parity- dependent NLDs. The next question is how these NLDs affect observables. To answer this, we import the MM NLDs into TALYS, a nuclear reaction code, and calculate neutron capture cross-sections and reaction rates.

TALYS already includes a variety of NLD and γSF models. To estimate the uncertainty band associated with these inputs, we generated an uncertainty band using 50 TALYS model combinations (5 NLD models paired with 10 γSF models). We then compared this band to the uncertainty obtained from the two MM NLD calculations, corresponding to $\eta = 2.3$ and $\eta = 2.6$, each combined with the same set of 10 γSF models.

^{56,59}Fe(n,γ) cross sections





Acknowledgement: Plots generated by Lucas Chouinard (GVSU undergraduate student)

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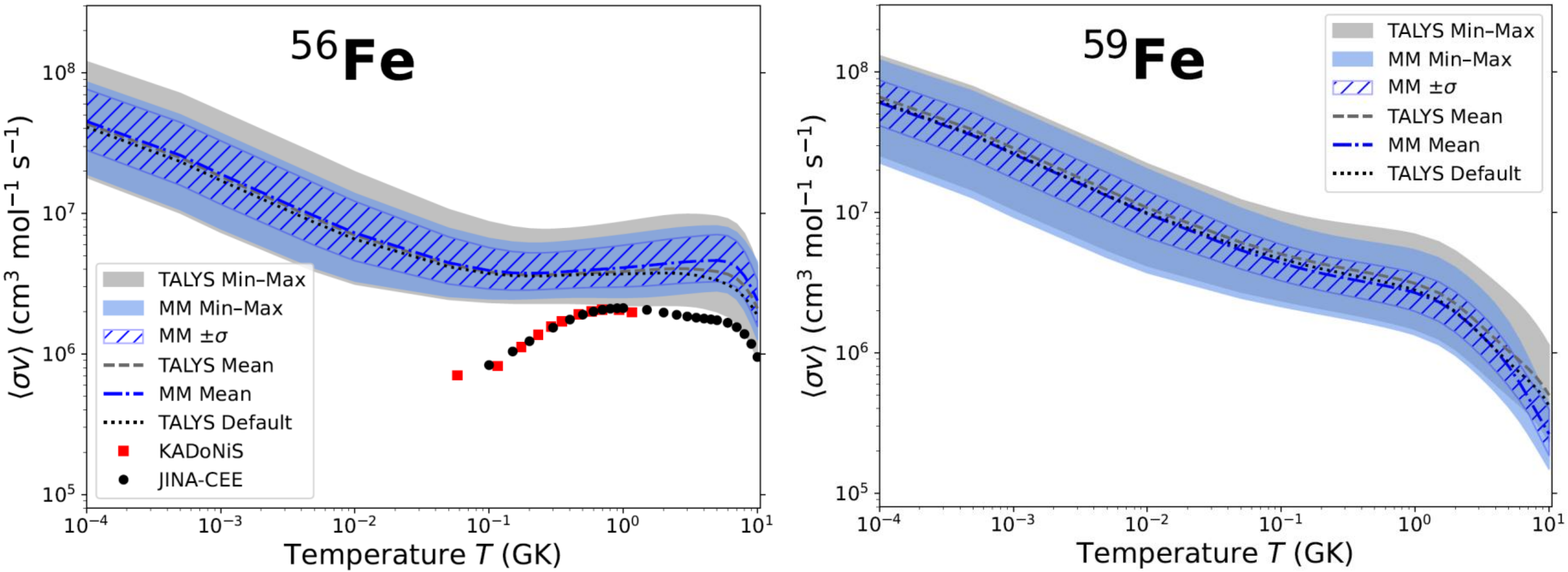
^{56,59}Fe(n,γ) reaction rates



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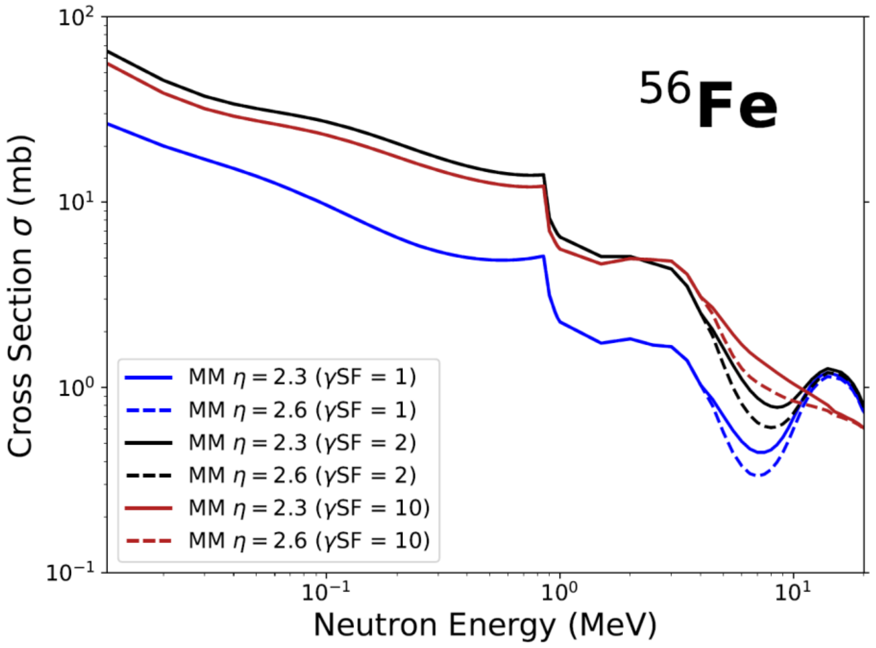
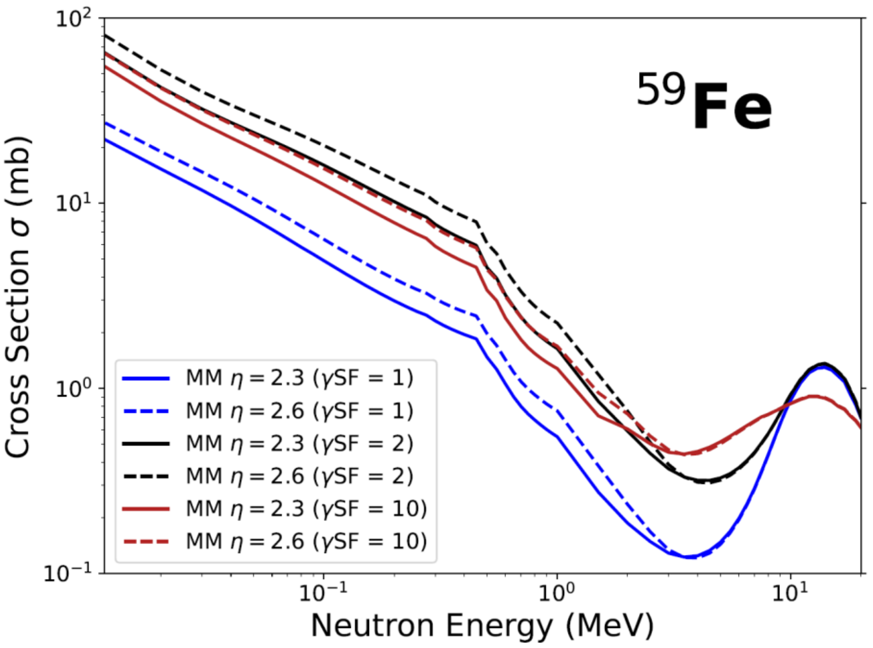
$^{56,59}Fe(n,\gamma)$ cross sections – MM vs strength dependence





γSF = 1, 2, 10

Different Lorentzian parameterizations of the E1 gamma-ray strength function.

Acknowledgement: Plots generated by Lucas Chouinard (GVSU undergraduate student)

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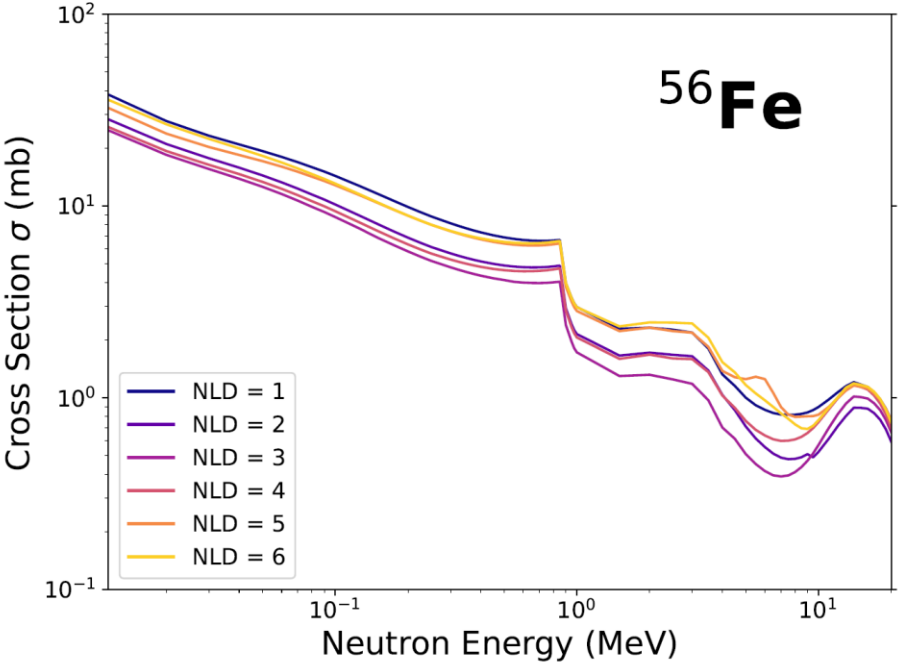
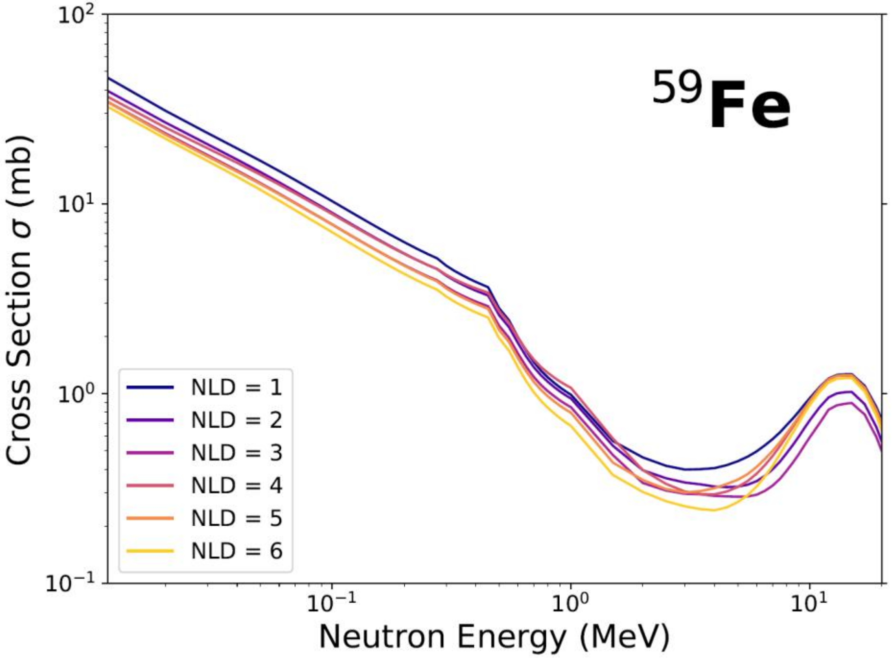
^{56,59}Fe(n,γ) cross sections – γSF fixed vs NLD dependence





NLD = 1 – 3: CT, BFG, GSM   NLD = 4 – 6: HFB microscopic

Different NLD models within TALYS

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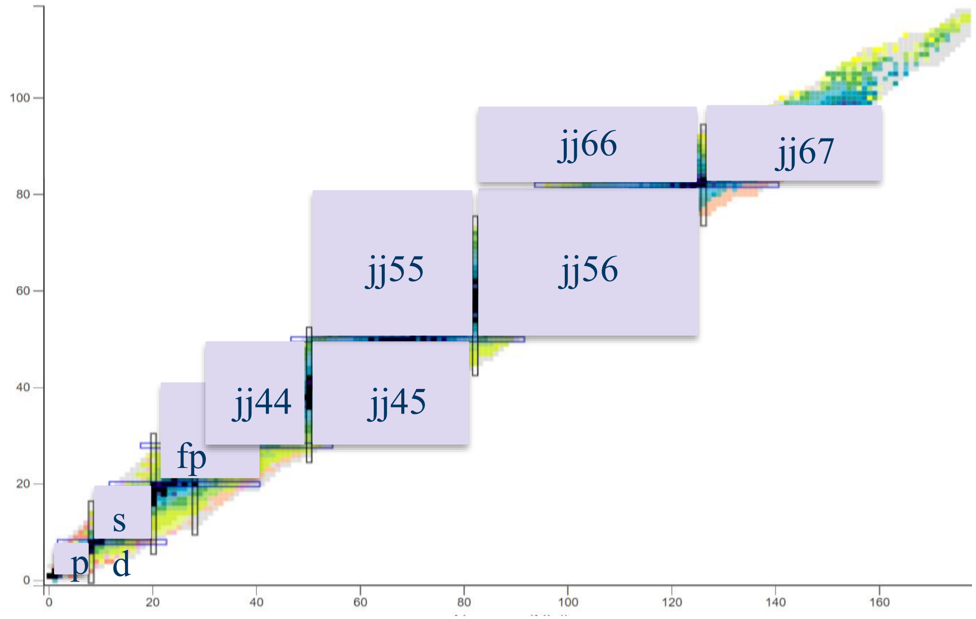
Future work - Challenges

* Develop a statistical uncertainty quantification framework for MM NLDs using Bayesian inference.
* Extend MM calculations to more exotic nuclei.
* The availability of reliable shell model interactions becomes increasingly limited far from stability, constraining predictions.
* For nuclei far from stability, protons and neutrons occupy different single-particle orbitals, whereas the Moments Method code was developed for model spaces in which protons and neutrons share the same single-particle orbitals.



Thank you

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