A Nuclear Data perspective for Nuclear Level Densities

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U.S. DEPARTMENT OF ENERGY

National Nuclear Data Center

1st RCM on Updating and Improving Nuclear Level Densities for Applications
IAEA, Vienna, Austria
March 24-28, 2025

Outline

- Nuclear Data
- Evaluations and modeling
- Experimental constraints
- Challenges in employing experimental NLD in evaluations
- Propositions to overcome these challenges

Before we begin…

… a brief advertisement

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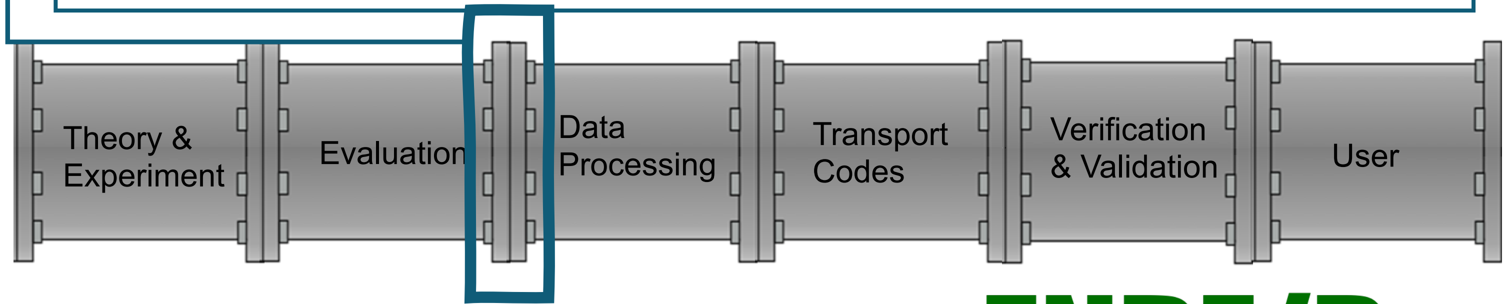
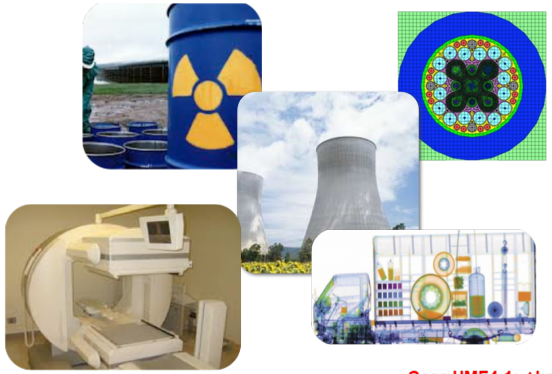
ENDF/B releases are a key interface in the improvement of the nuclear data that reaches the users' community!





The previous release (VIII.0) was great, but…

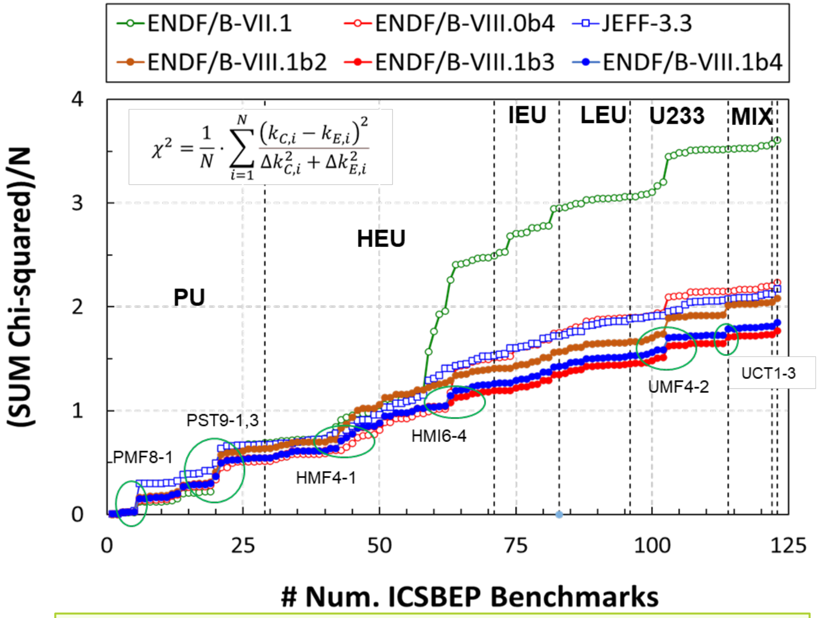
- Underpredicted depletion at high burnup
- Had deficiencies in leakage benchmarks
- Many other contributions since then

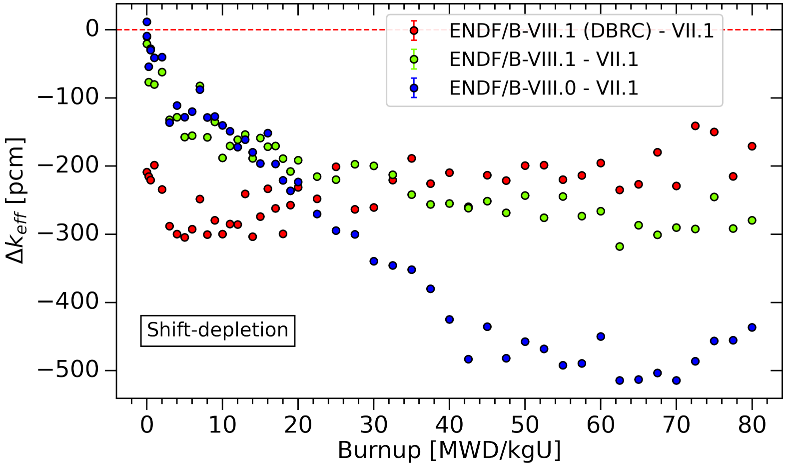
ENDF/B VIII.1

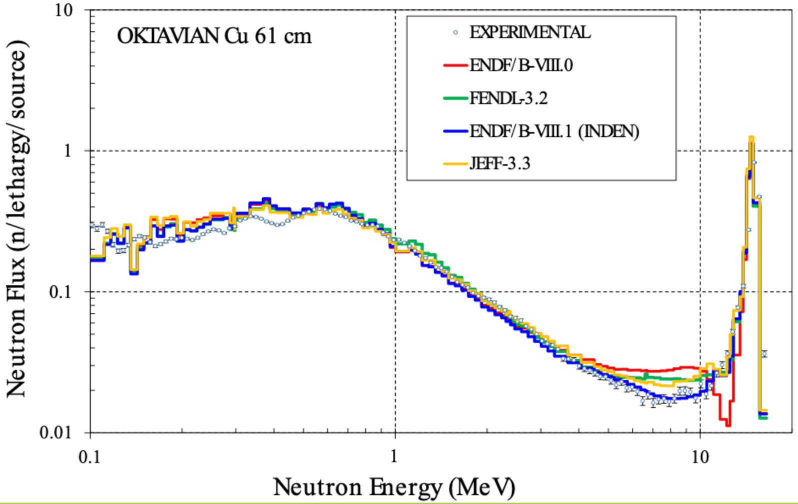
was released Aug 30, 2024!

Mosteller's Suite - 123

Case HMF4.1: Δkeff EXP=30 pcm







VIII.1 dramatically improves depletion performance,…

…performs much better in leakage and shielding experiments due to updates in Cu, Fe, Cr, Pb,…

…all while further improving the performance in criticality benchmarks, with updates to ^{239}Pu, ^{235,238}U, et al.!!

https://www.nndc.bnl.gov/endf-releases/

End of the ENDF/B-VIII.1 advertisement

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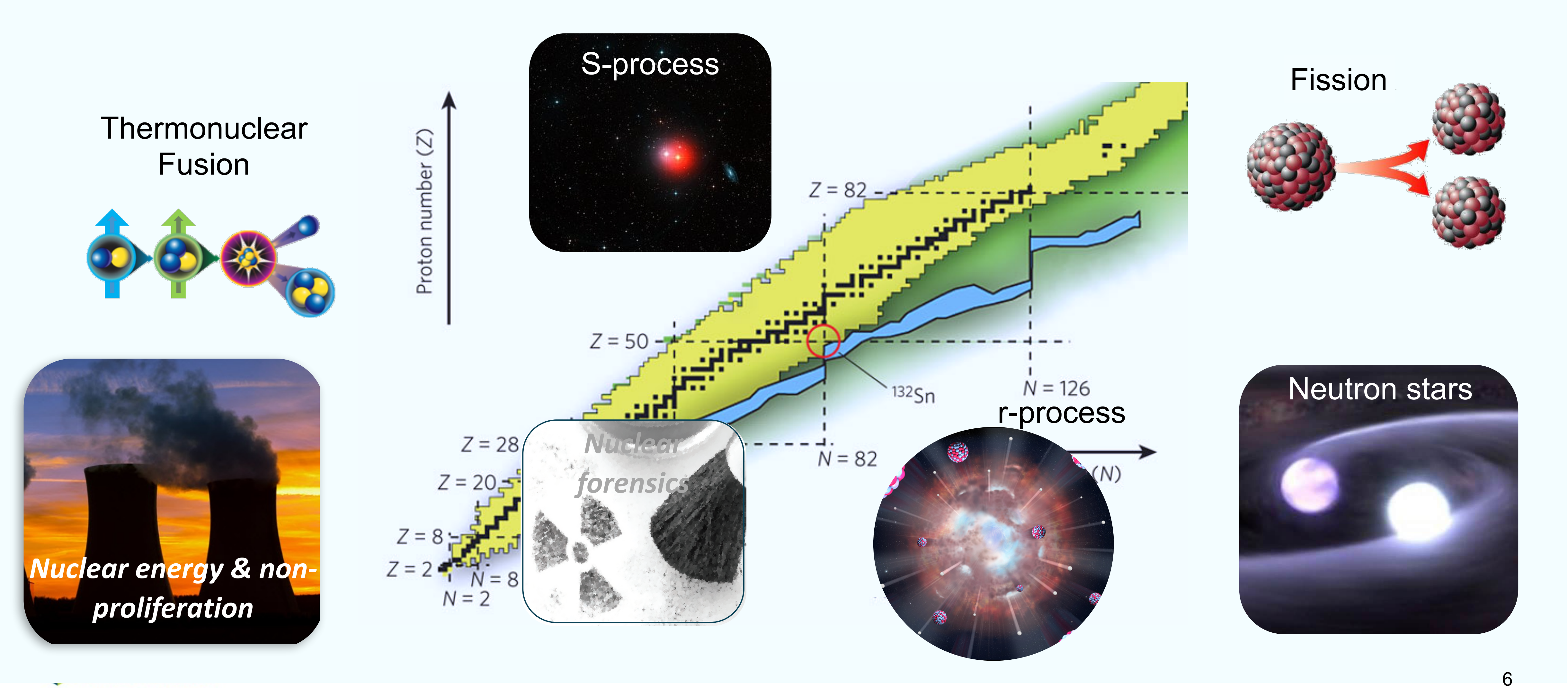
Nuclear Data is the interface between nuclear physics and science and technical application that depend nuclear physics



Updating and Improving Nuclear Level Densities for ***Applications***

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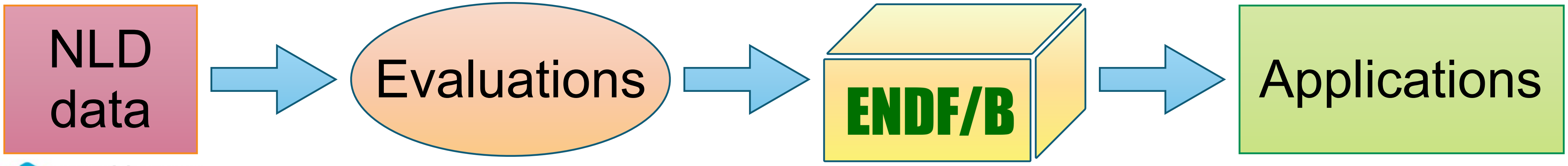

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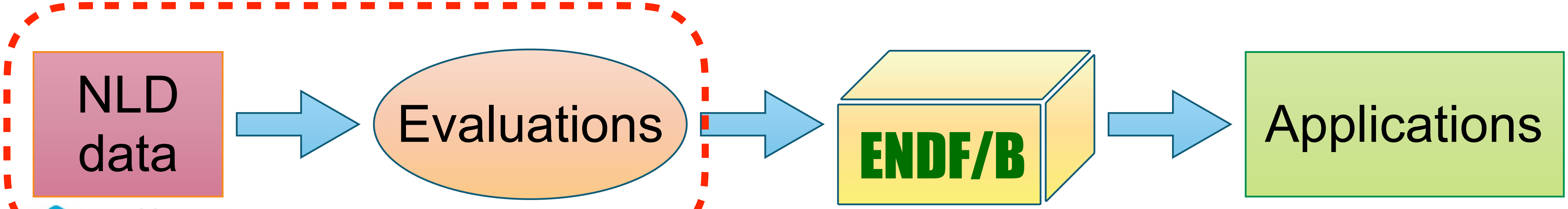
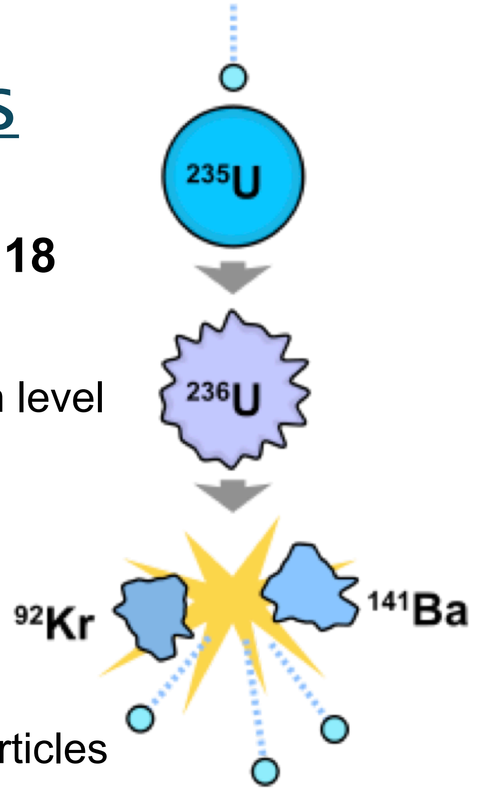
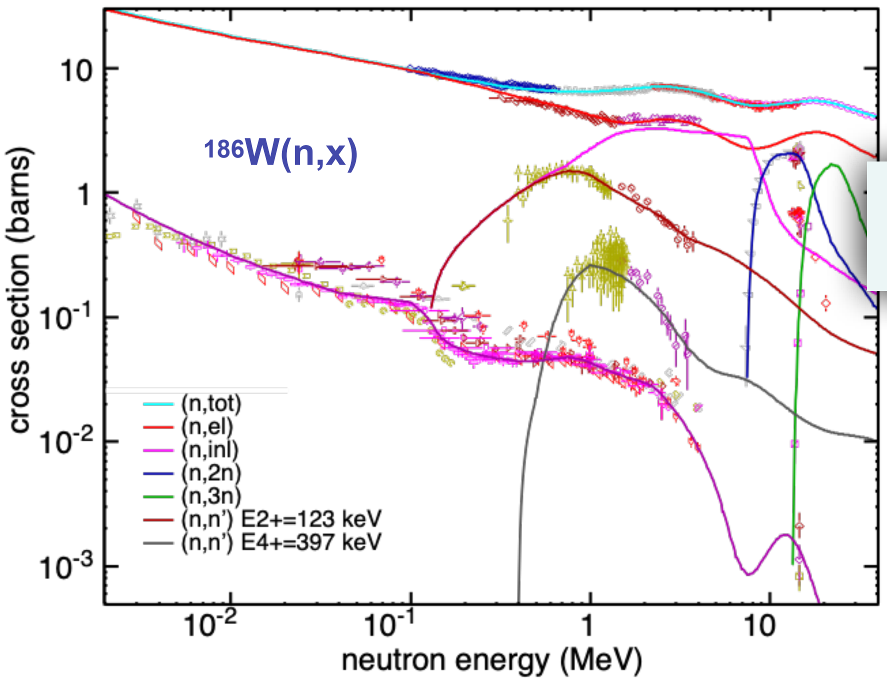


Evaluated Nuclear Data File: Nuclear reactions

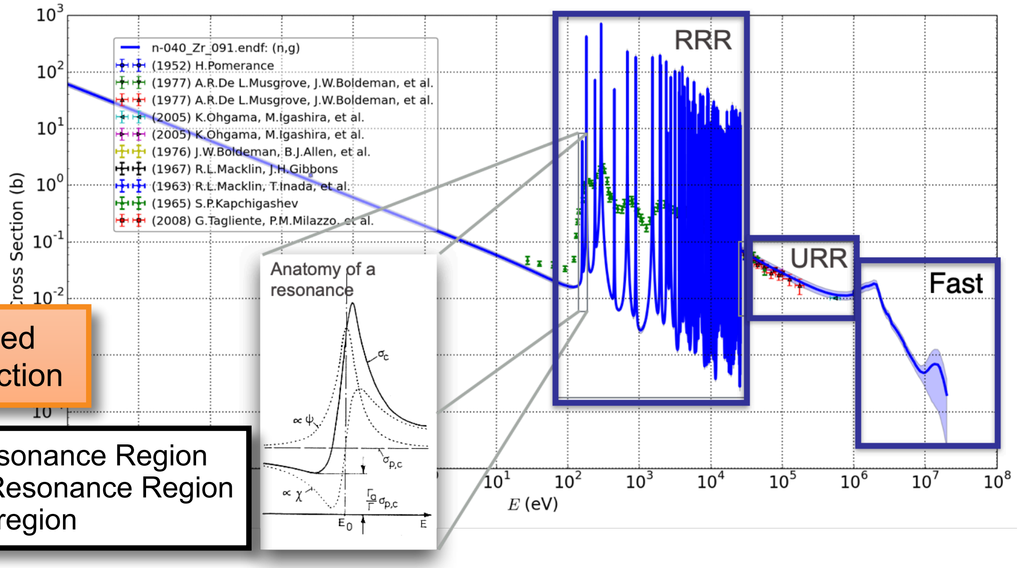


A **reaction evaluation** is the description of **everything** that can happen from the nuclear reaction between a **projectile** and a **target**

- **Typical neutron incident on non-actinide has ~ 18 relevant reactions**
  - ~ 5 threshold reactions: (n,2n), (n,3n), (n,p), etc.
  - ~ 10 discrete level excitation reactions: (n,n’) for each level in residual nucleus
  - 3 non-threshold reactions: (n,tot), (n,el), (n,γ)
- **Actinides add fission, (n,f)**
- **For transport studies, need:**
  - Cross sections
  - Multiplicities of all emitted particles
  - Outgoing energy-angle distributions for all emitted particles



Experimental data never enough: need theory to fill in gaps



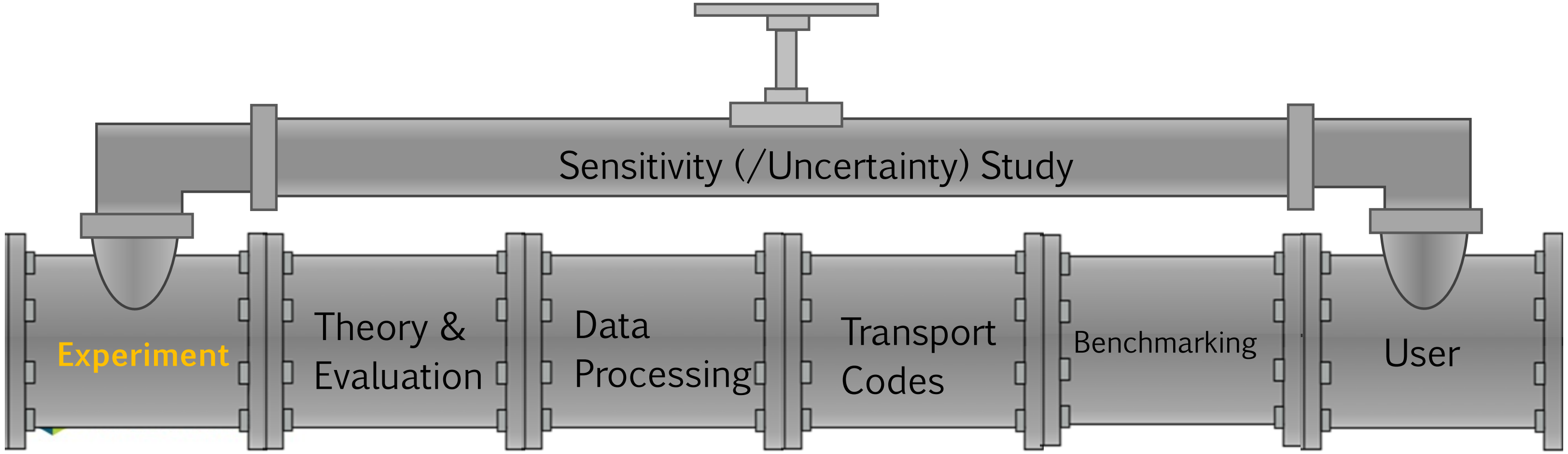
Typical evaluated capture cross section

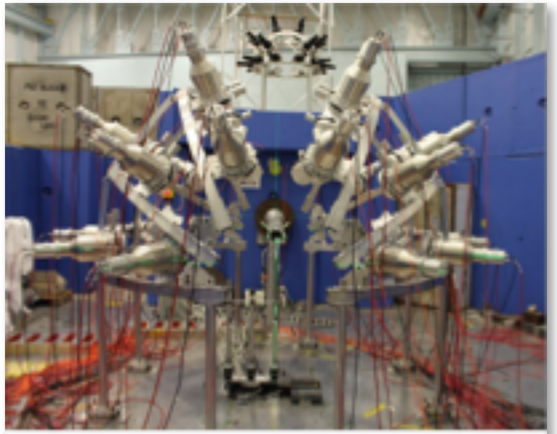
RRR: Resolved Resonance Region
URR: Unresolved Resonance Region
Fast: Fast-neutron region

Why do we need experiment?

- We do not fully understand the physics
- We can not theoretically calculate Nuclear Data with sufficient accuracy required by applications
  - Experiments constrain the uncertainty of evaluated data
  - Test the accuracy of evaluated files and codes physics

AMANDA Li-Glass detector array at RPI



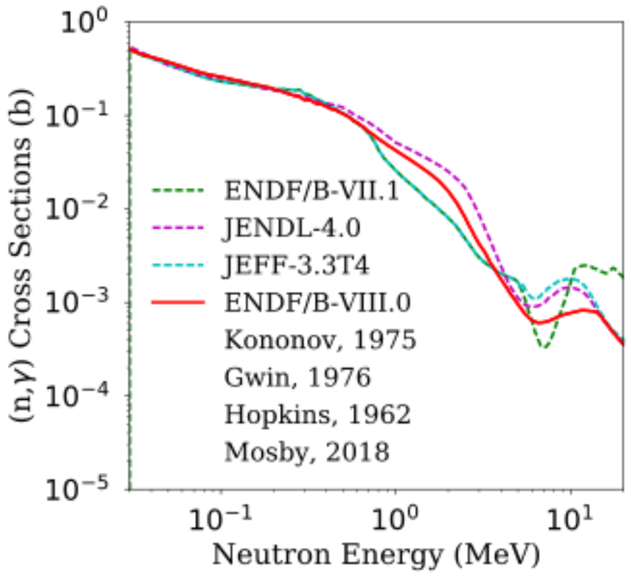


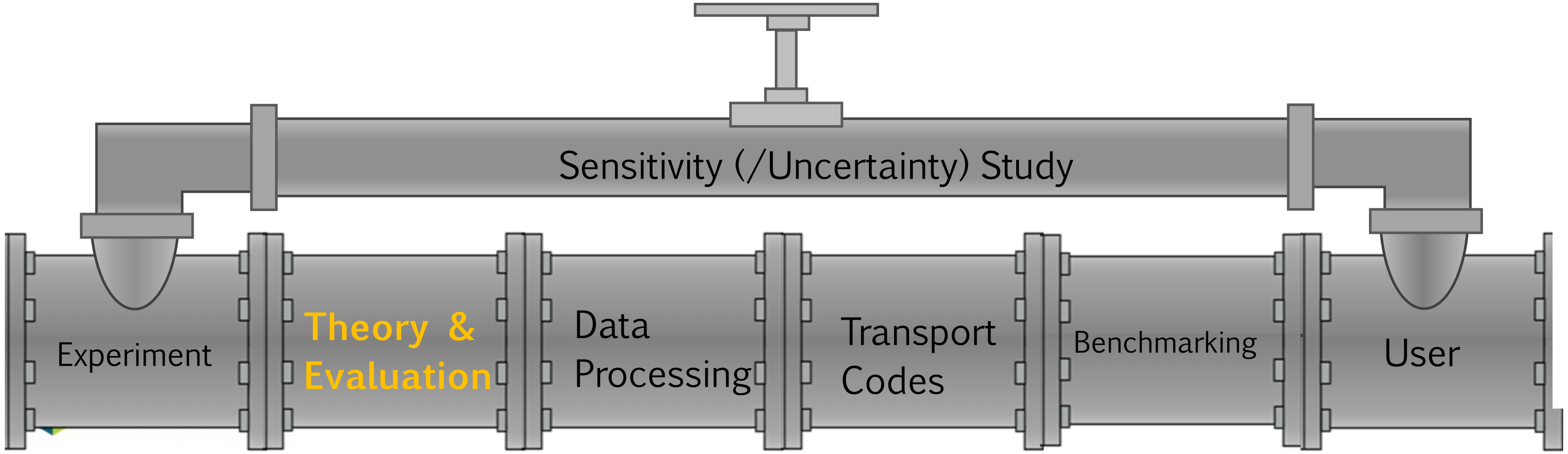
Chi-Nu EJ-309 Detector array at LANL

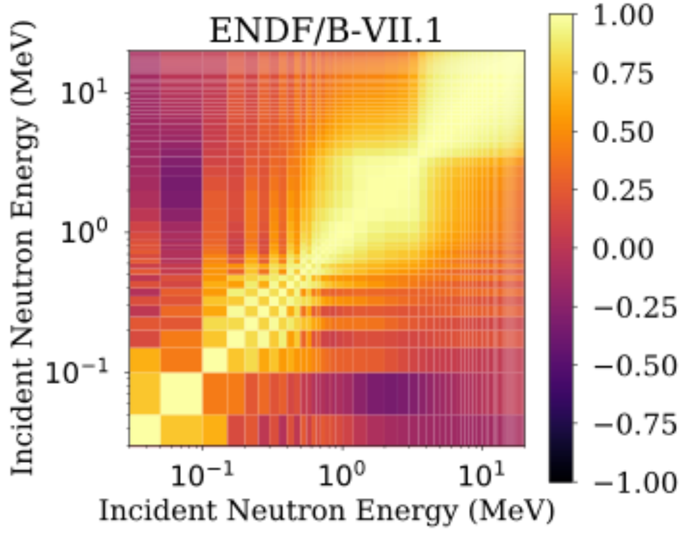
Slide based on Y. Danon's WANDA 2020 Pipeline Talk

Theory + Experiment + Statistics = Evaluation

- Experiments rarely cover all that users want
- Nuclear Theory is needed!
  - Complete data files for users
  - Make predictions/extrapolate (beyond calibration)
  - Provide estimates of uncertainties & correlations
- Statistics provide the glue
  - "To the best of our knowledge..." (given time, location, resources)
  - Bayesian statistics / Uncertainty Quantification







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Evaluations: theory and experiments

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The (mis-)interpretation of what the **data** is *actually* telling us can also be a **challenge**.

Some examples from nuclear data evaluations

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- Unitarity among reaction channels

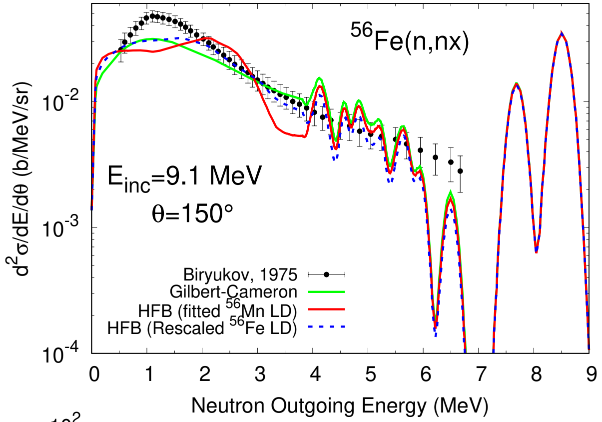
How about NLD data?

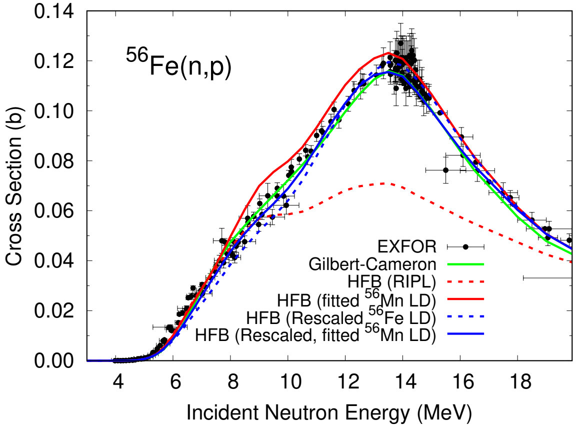
- Models are not perfect: Experimental NLD data are essential to constrain models
  - Phenomenological NLD models normally can get the job done, if we don't look too deep in the details
  - Parameter tuning can mask important physics and model deficiencies
  - Microscopic models: less flexible, but more realistic in the details

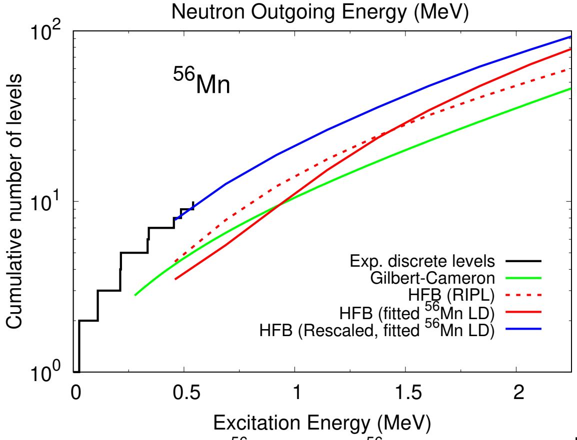
There are many benefits to data-constrained NLD

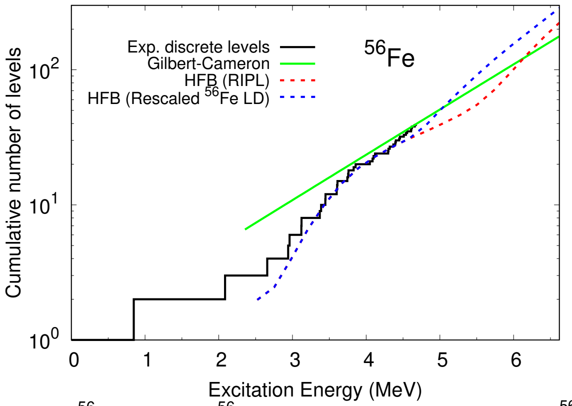
- Reduce unknowns
- Lower evaluated cross section uncertainties
- Help identify improvement needs for experiments and theory
- More consistent predictions, not only in general, but in the specifics:
  - correlation between NLD structure and neutron spectra
  - inelastic gamma cross sections and gamma spectra
  - extrapolation to unstable nuclei
  - etc.

Examples of impact of NLD details



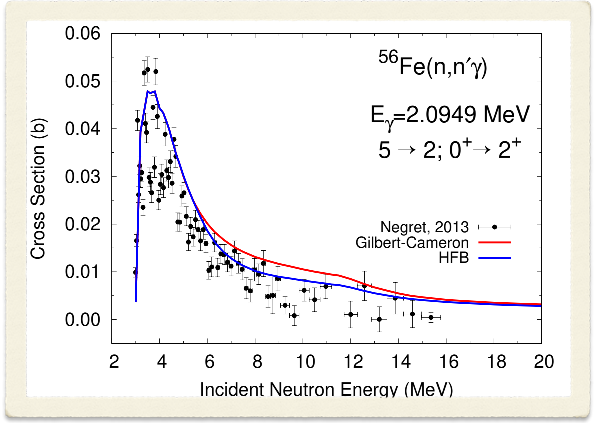


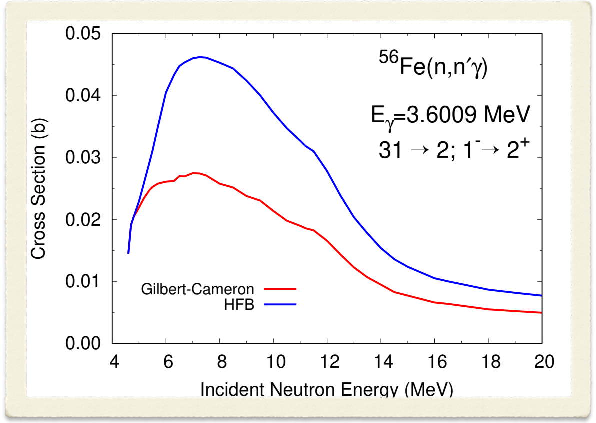


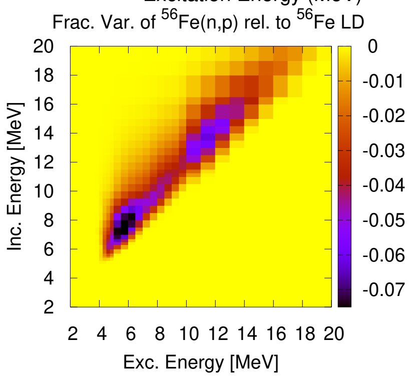


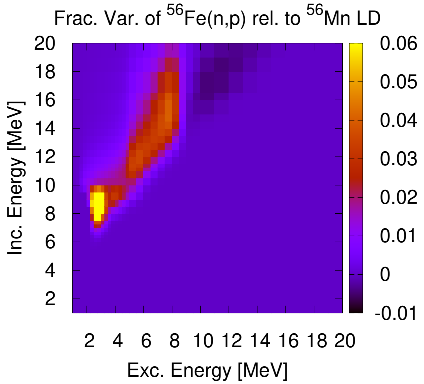
Correlations between NLD and cross sections for the many reaction channels!

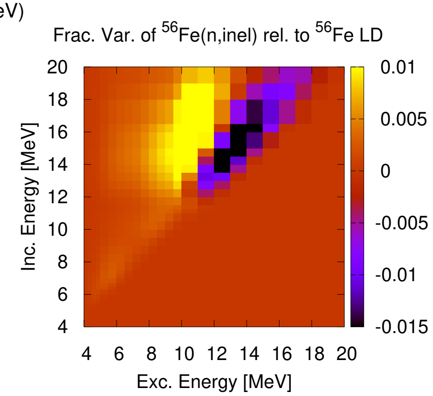
Can also impact inelastic gammas!

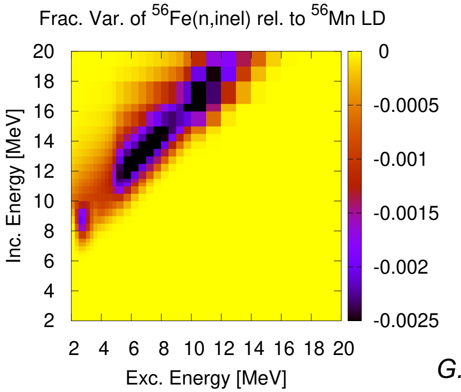












*G.P.A. Nobre et al., PRC**101** (2020) 034608*

NLD experimental methods

- There are many methods and approaches: Oslo method, shape method, etc.
- WARNING: I'm not an experimentalist, so I won't dare to go in the details about their commonalities, differences and subtleties
- I will use the Oslo method as an example
  - Successfully measured NLD and GSF data for broad variety of nuclei from primary gammas
  - Website with NLD data and associated publications*

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*"As only the functional form of the NLD and gSF can be deduced from the primary g spectra, the slope and absolute normalization must be determined from auxiliary data.**"*

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Normalization:

Low energy: discrete levels
Separation energy: resonance spacings

Things are often not so clear…

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^{56}Fe	5	5	20	20	54	55	109	117
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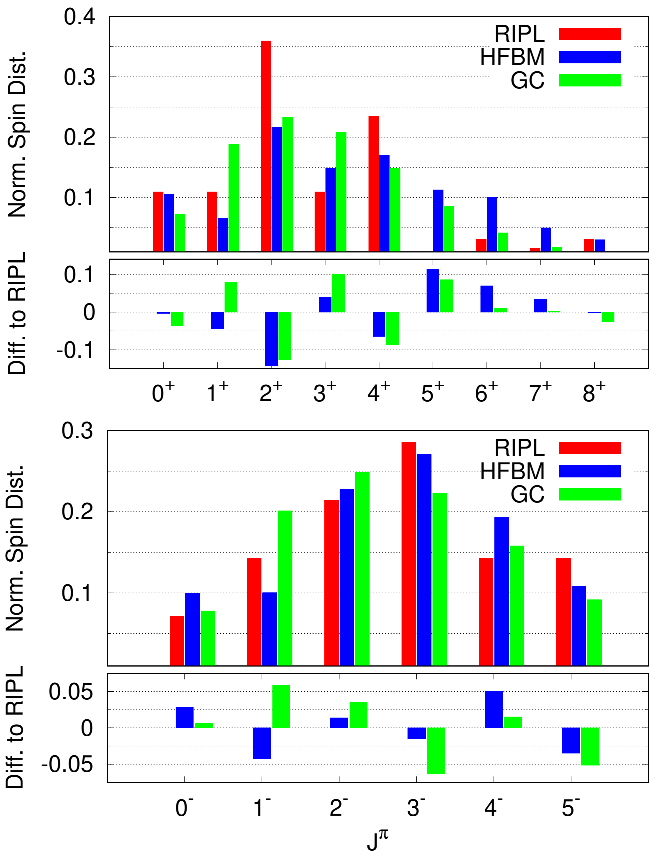
  - Also, spin/parity assignments may have changed
  - Poor match between measured levels and NLD models



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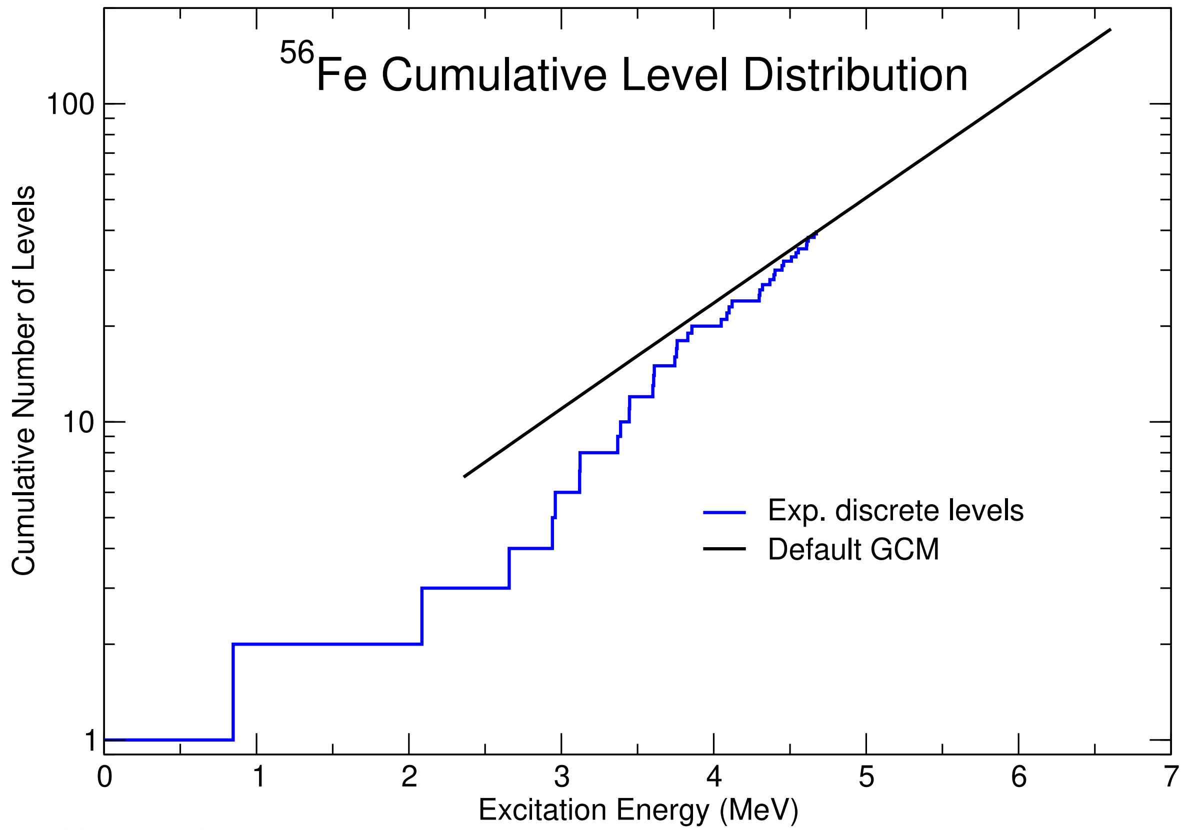
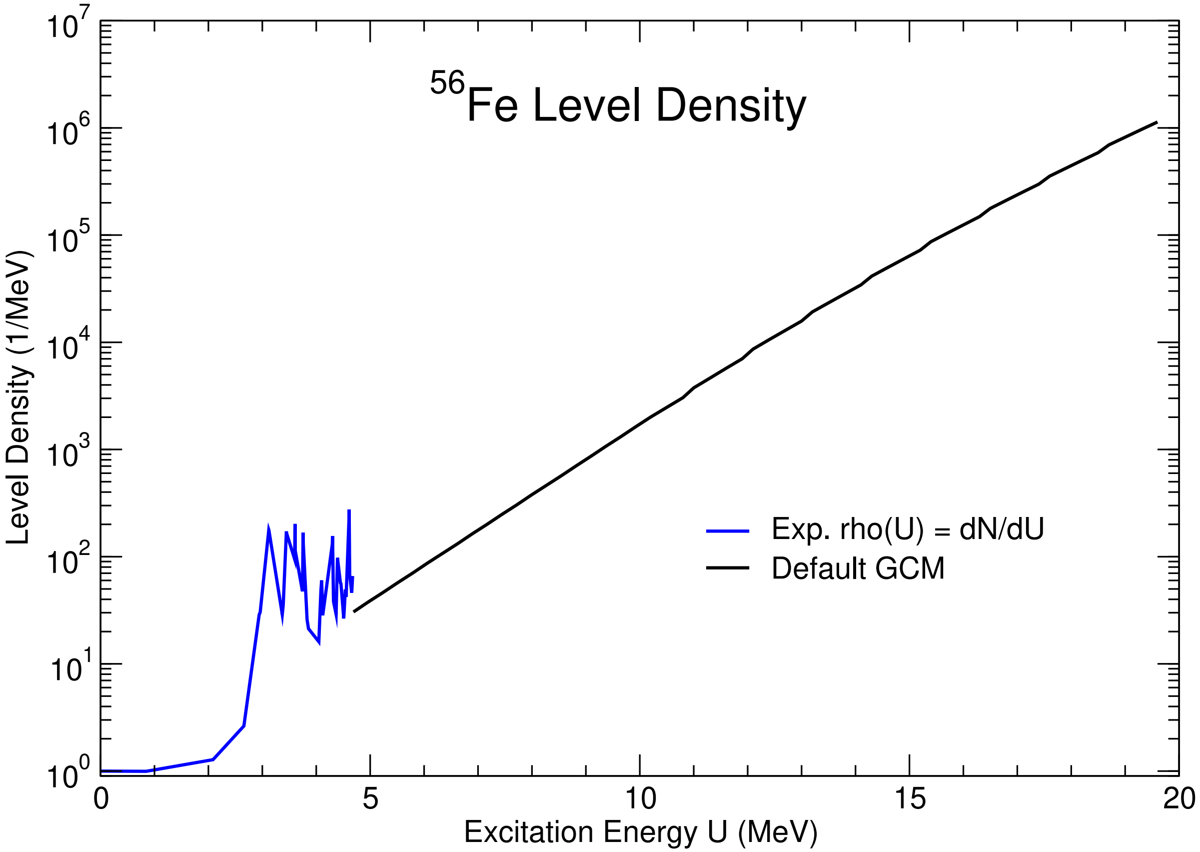
- However (2):
  - As excitation energy increases, we start to miss observed levels
  - Cut-off where ALL discrete levels are assumed to be known can be subjective





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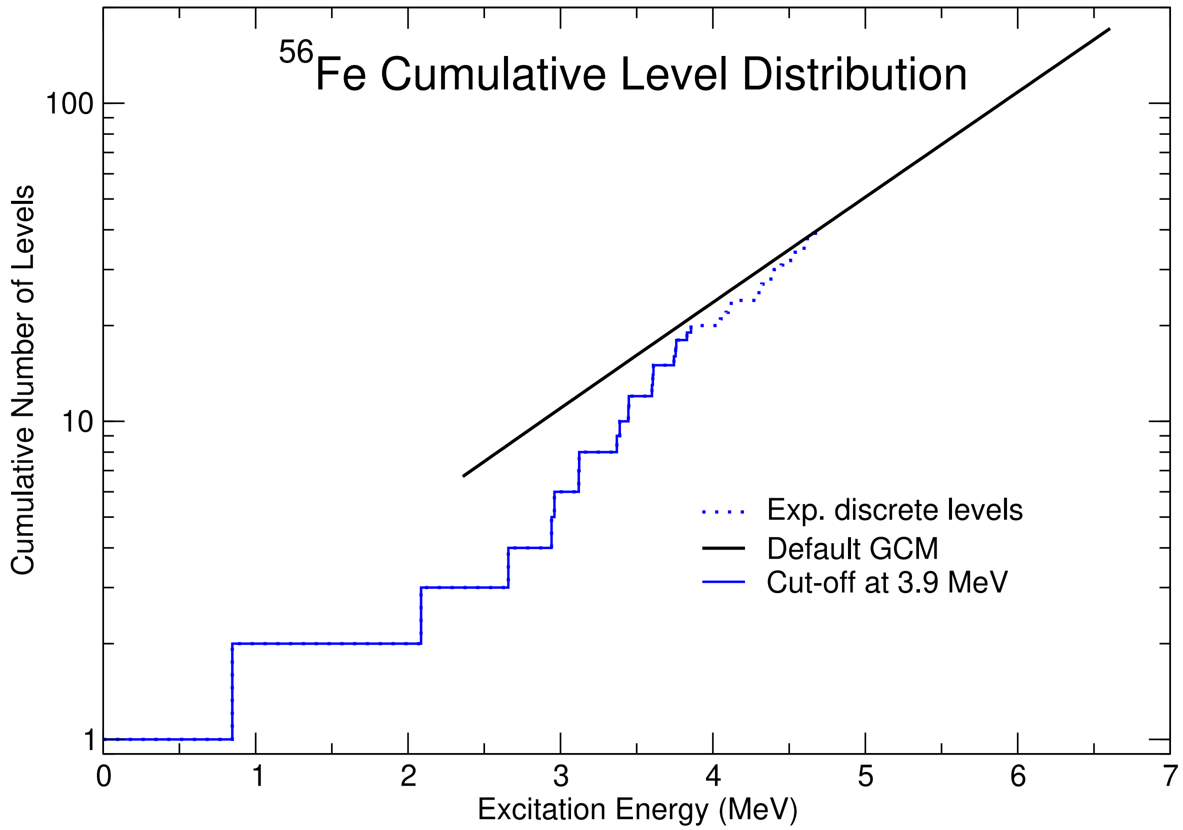

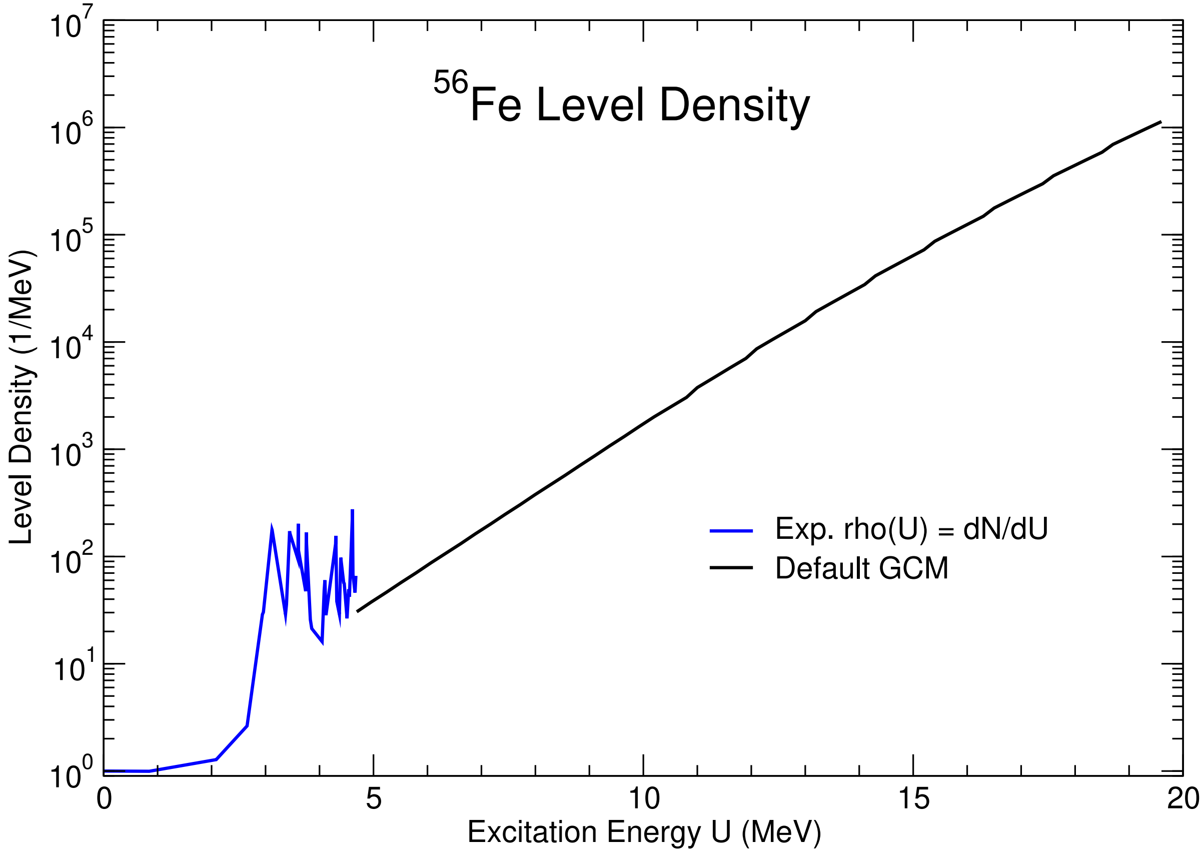

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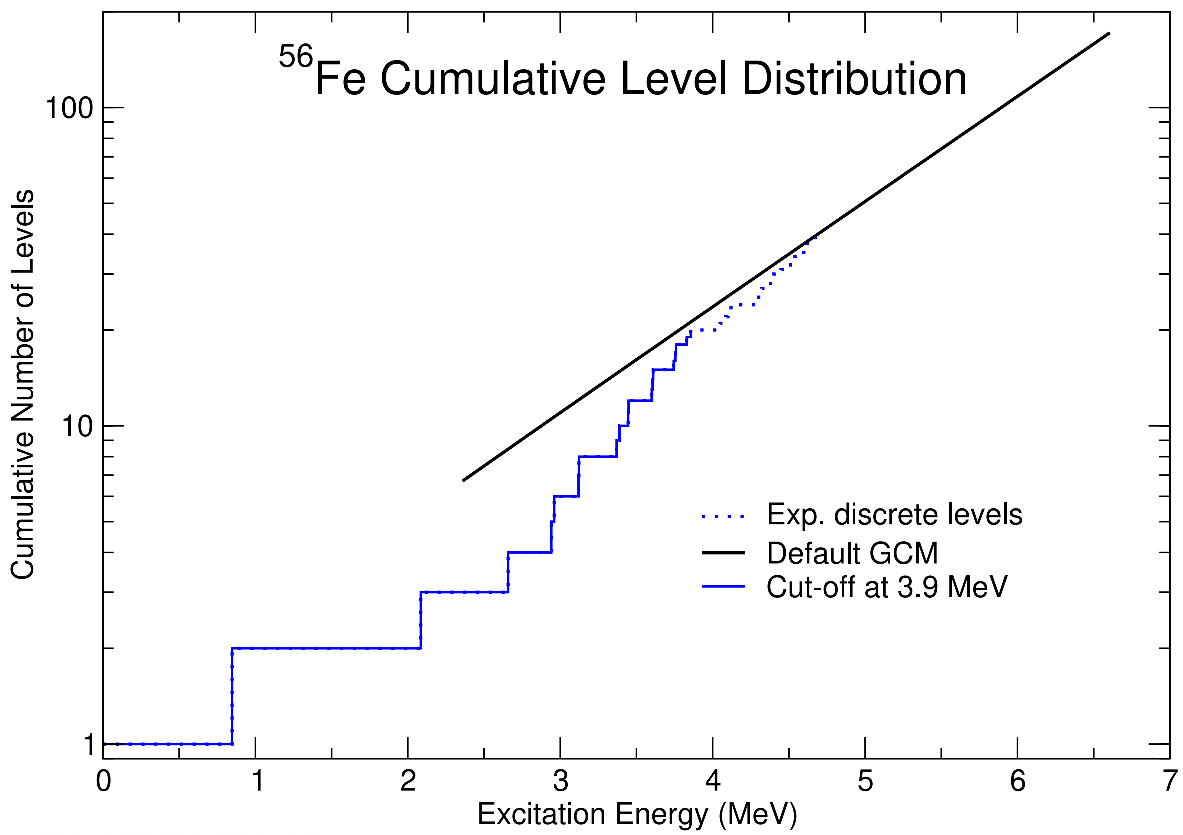

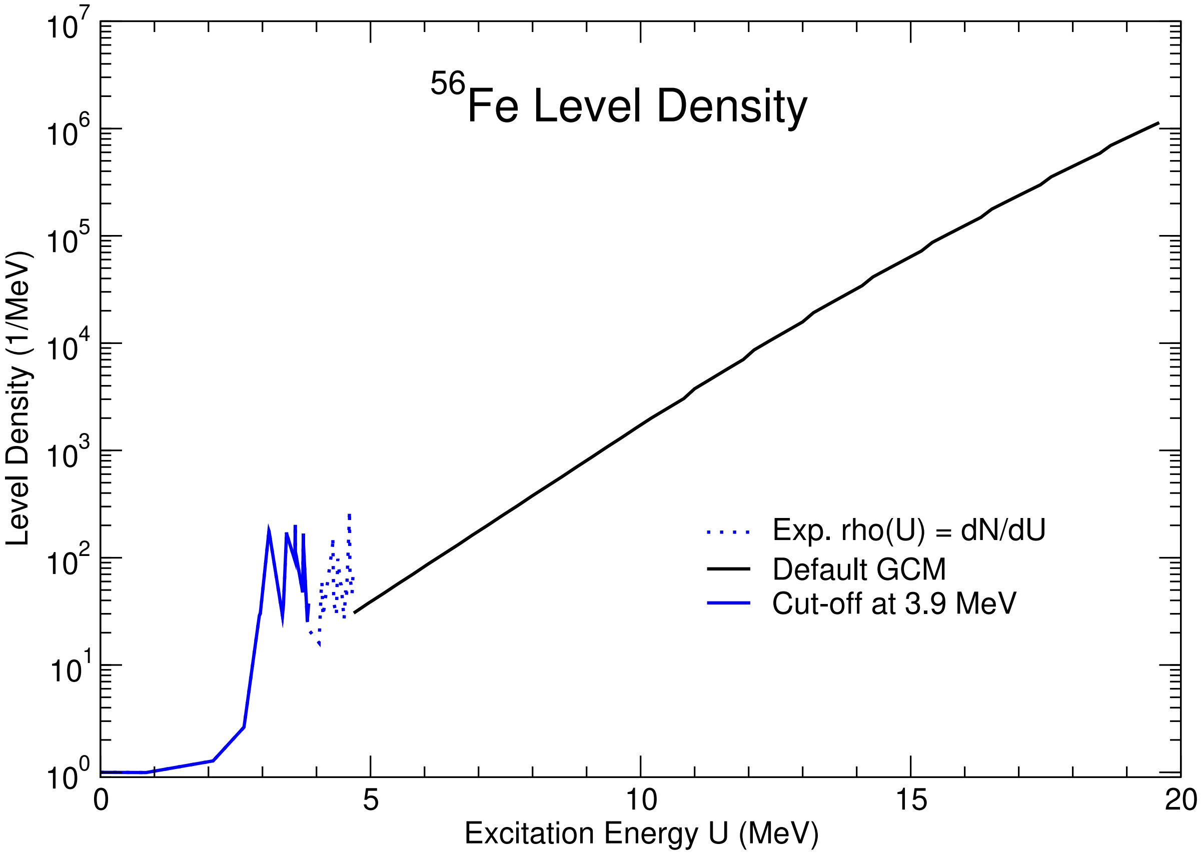

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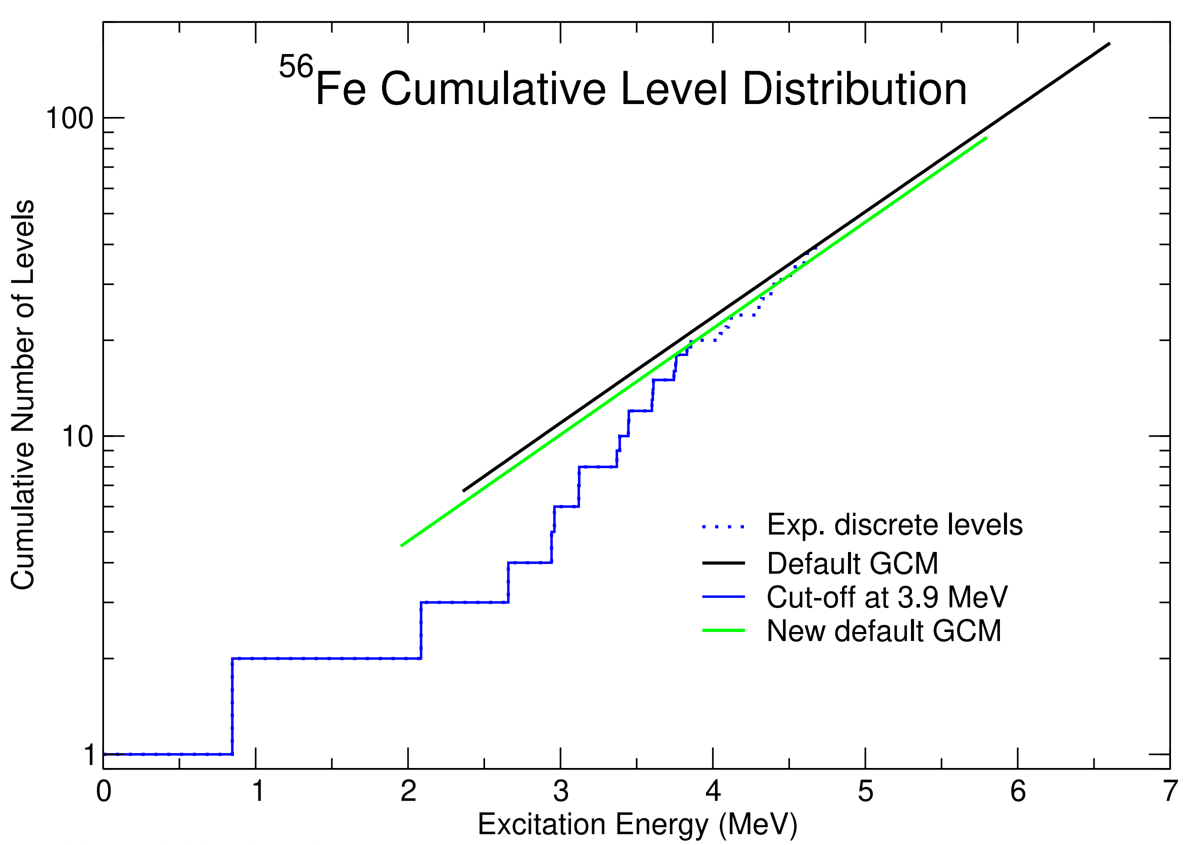

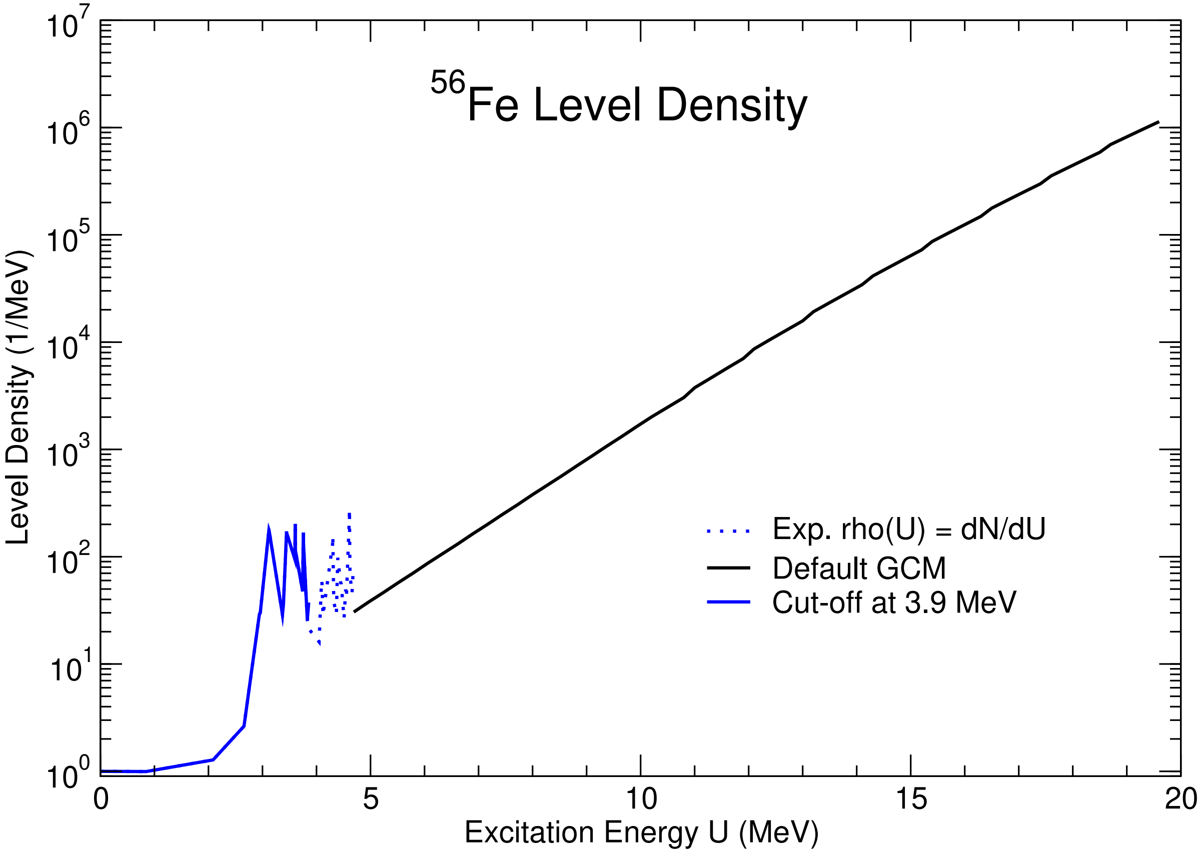

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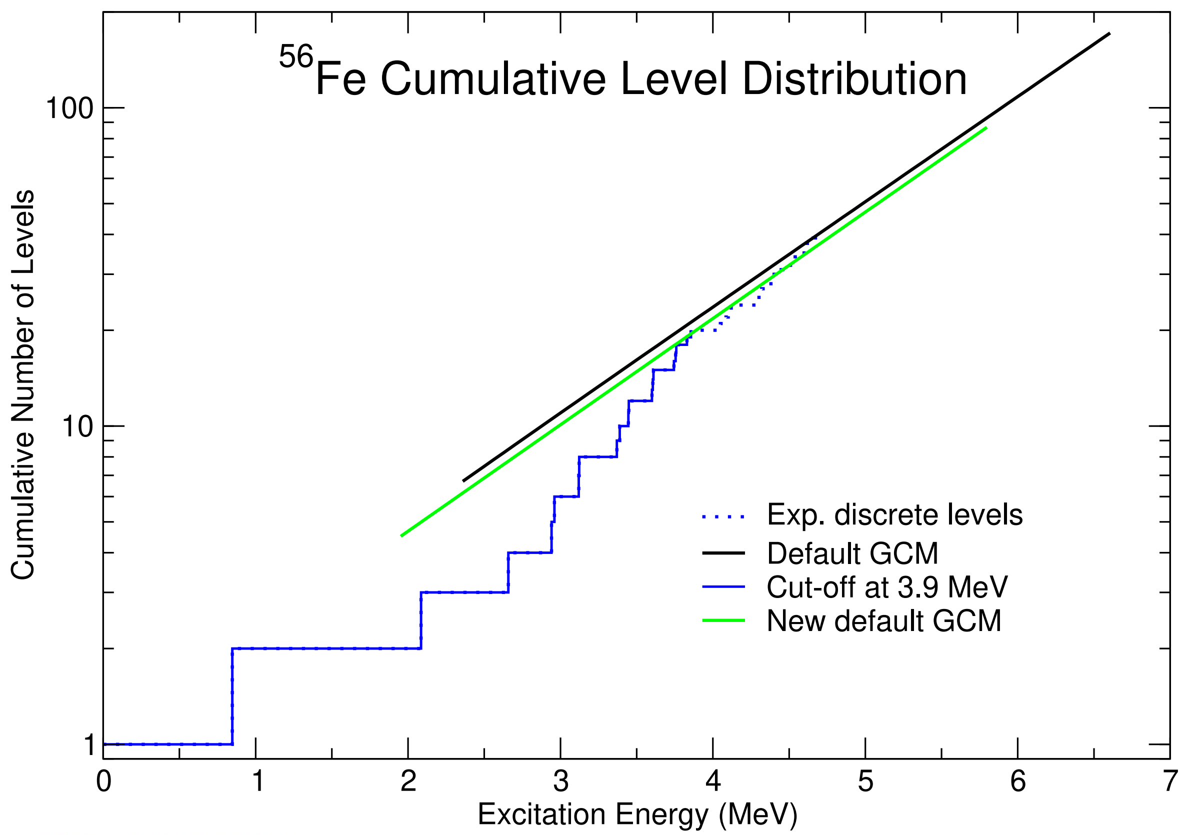

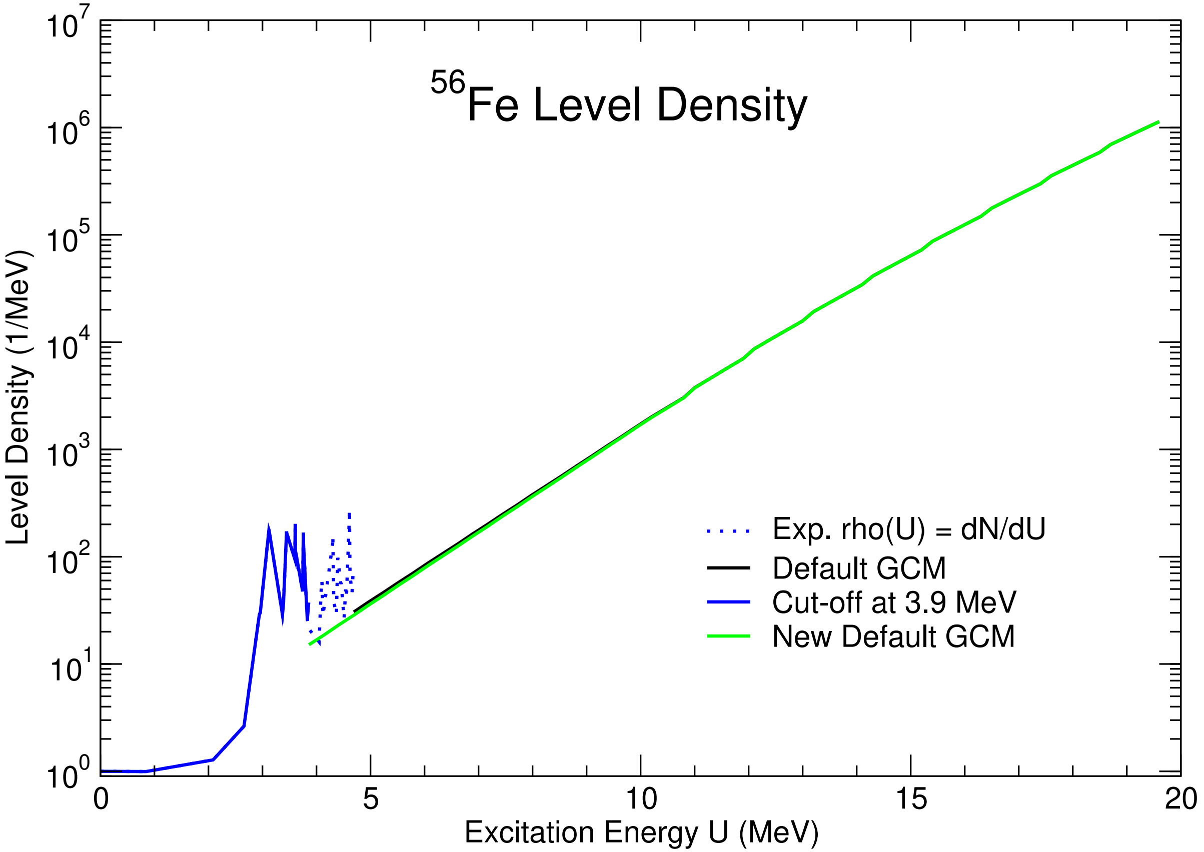

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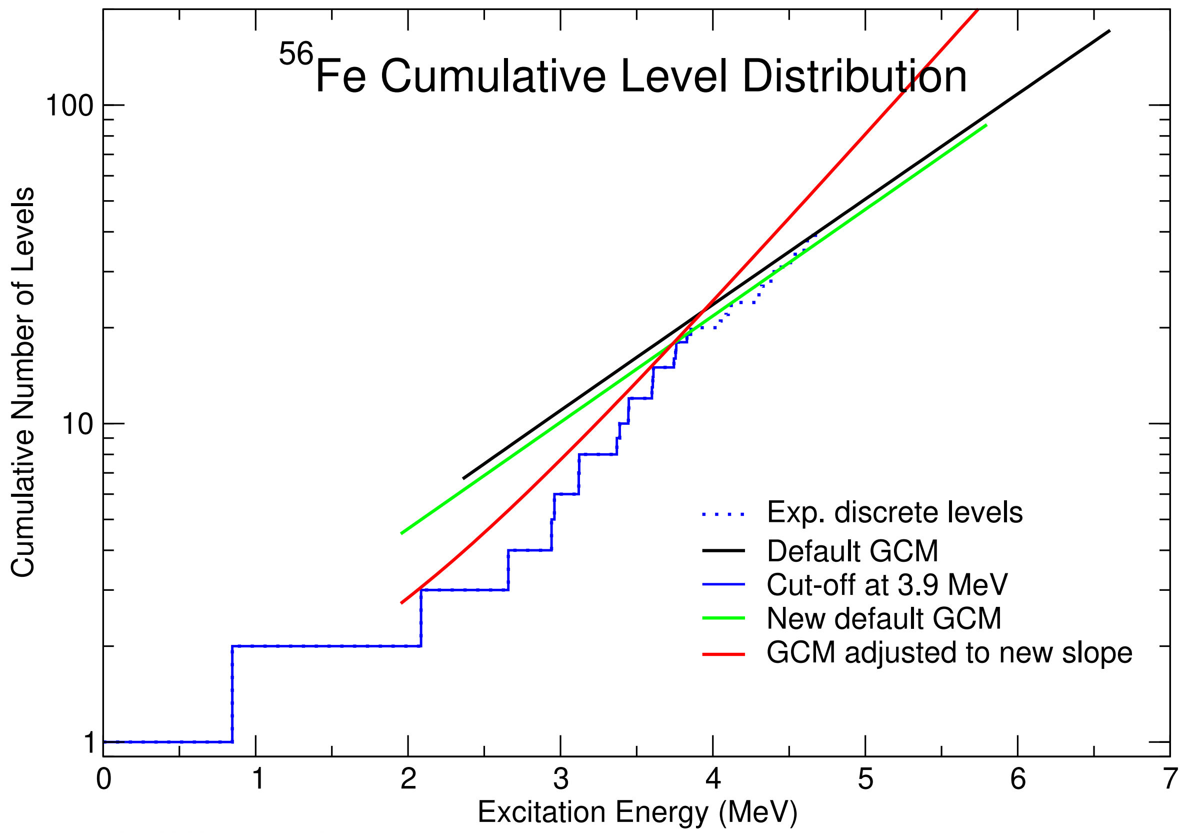

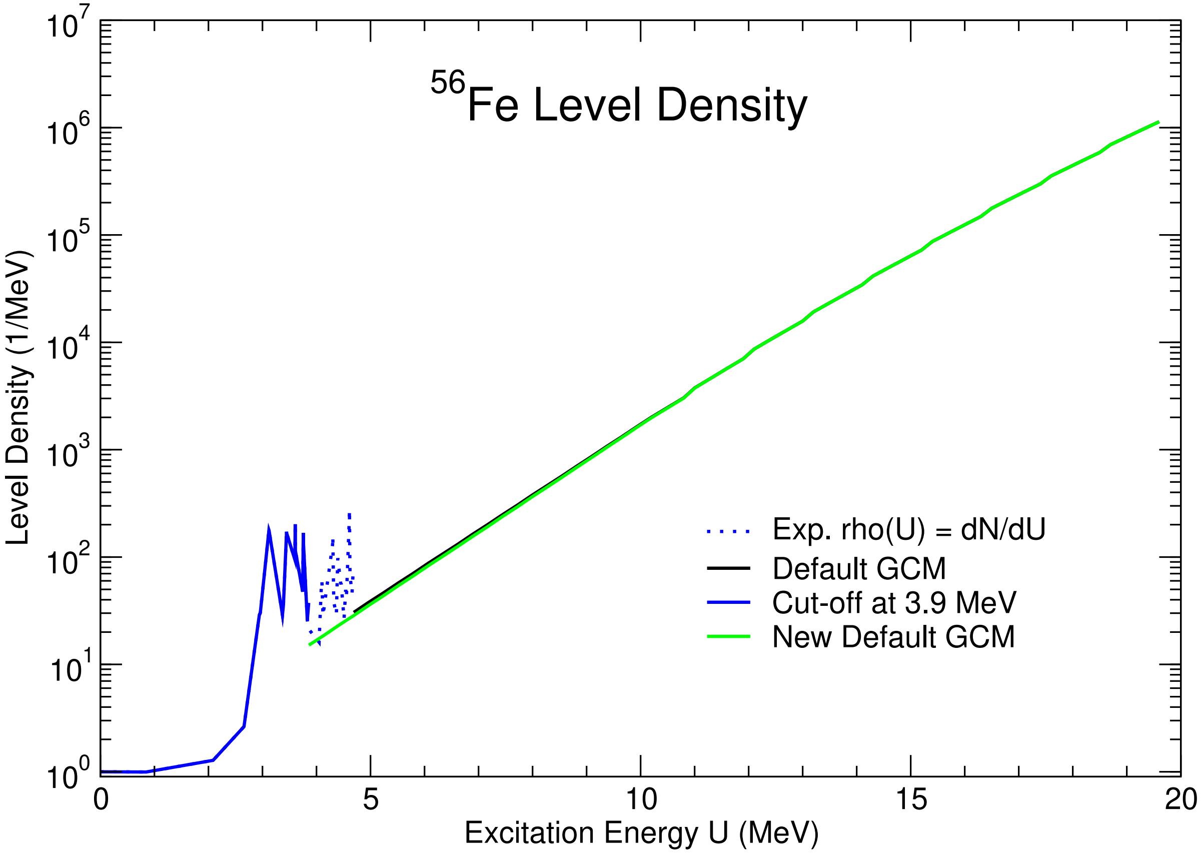

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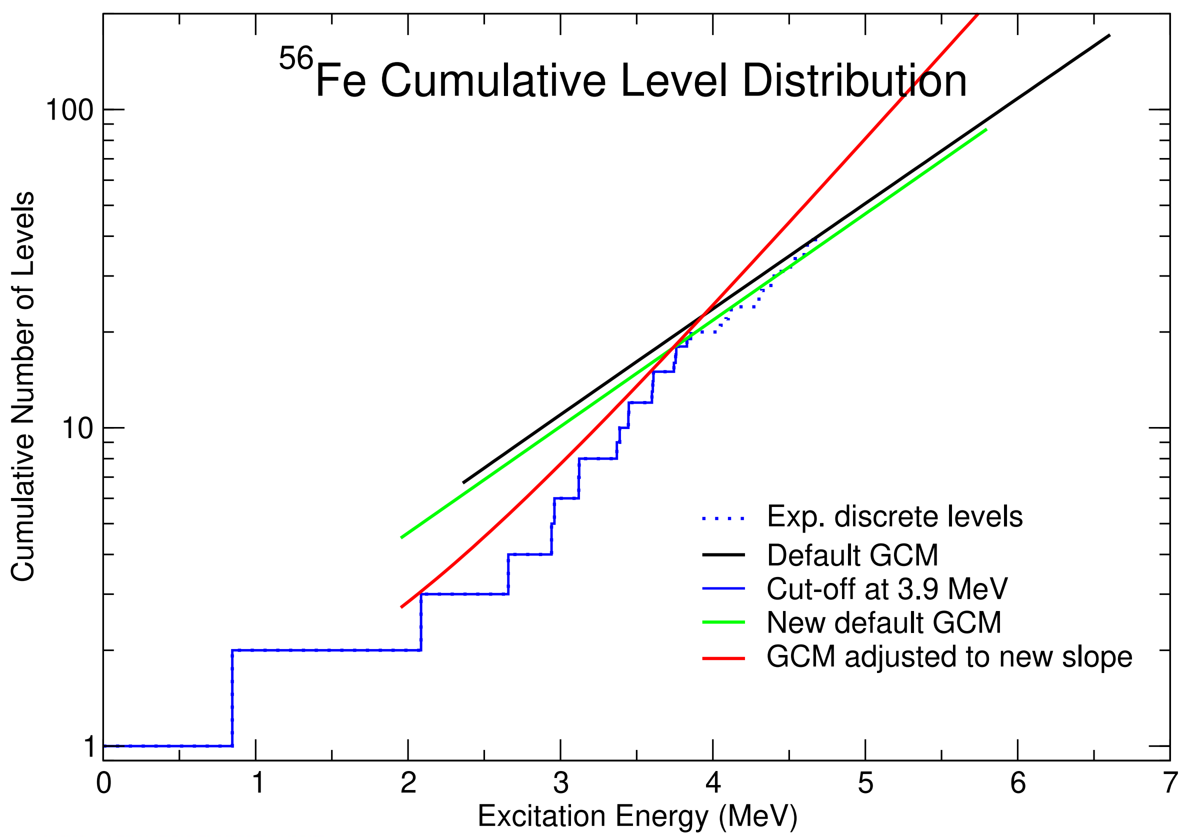

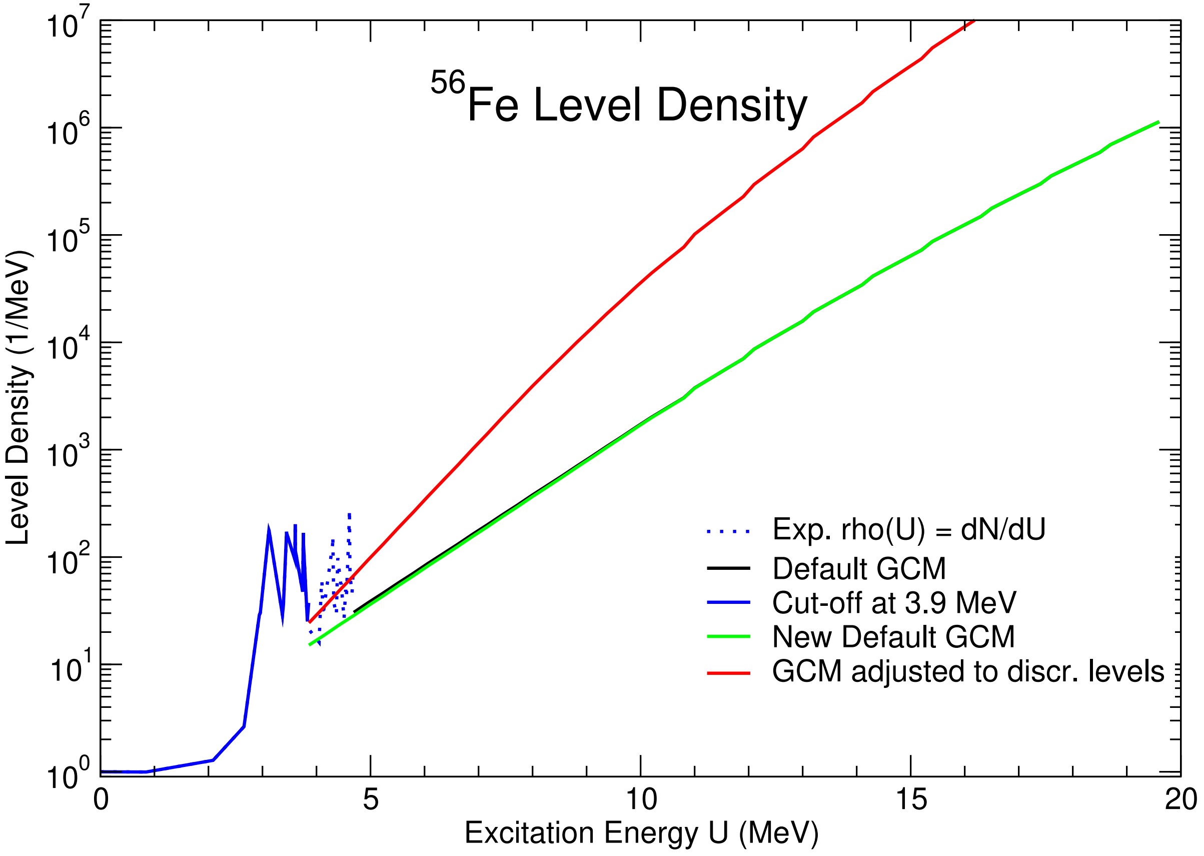

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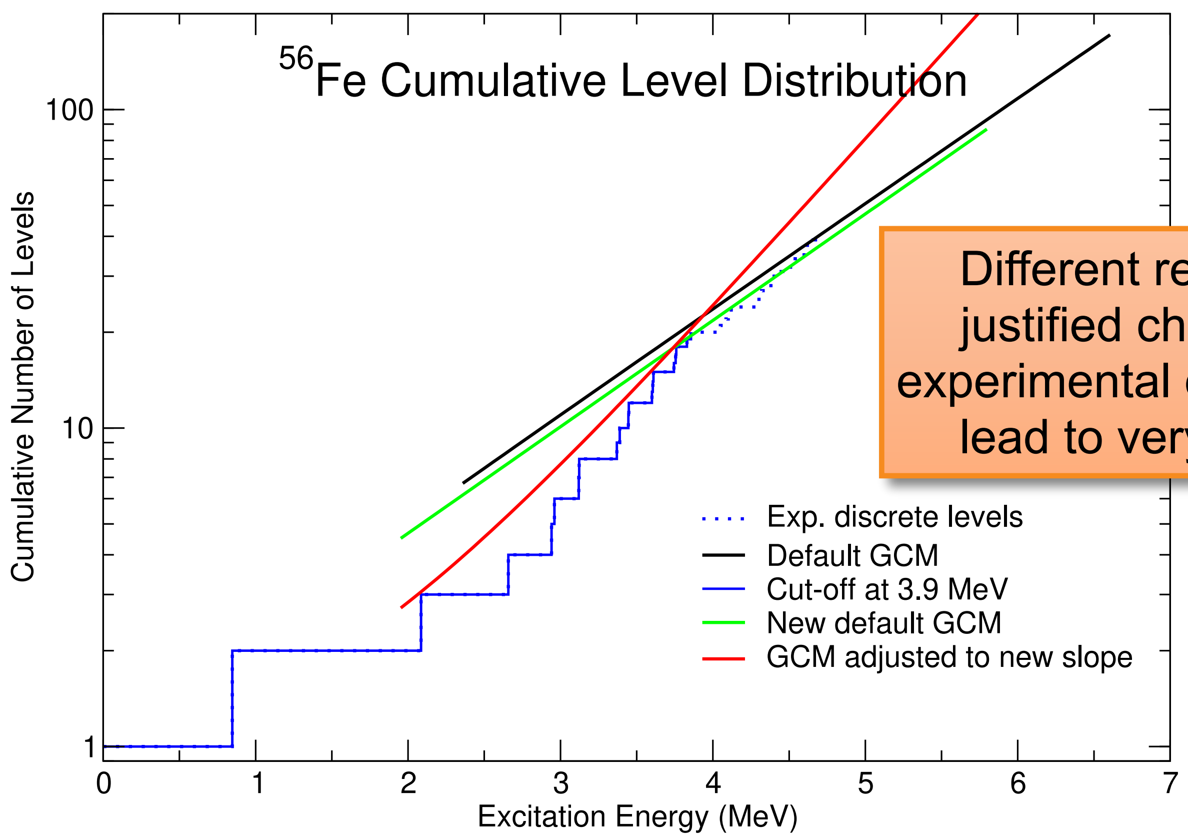
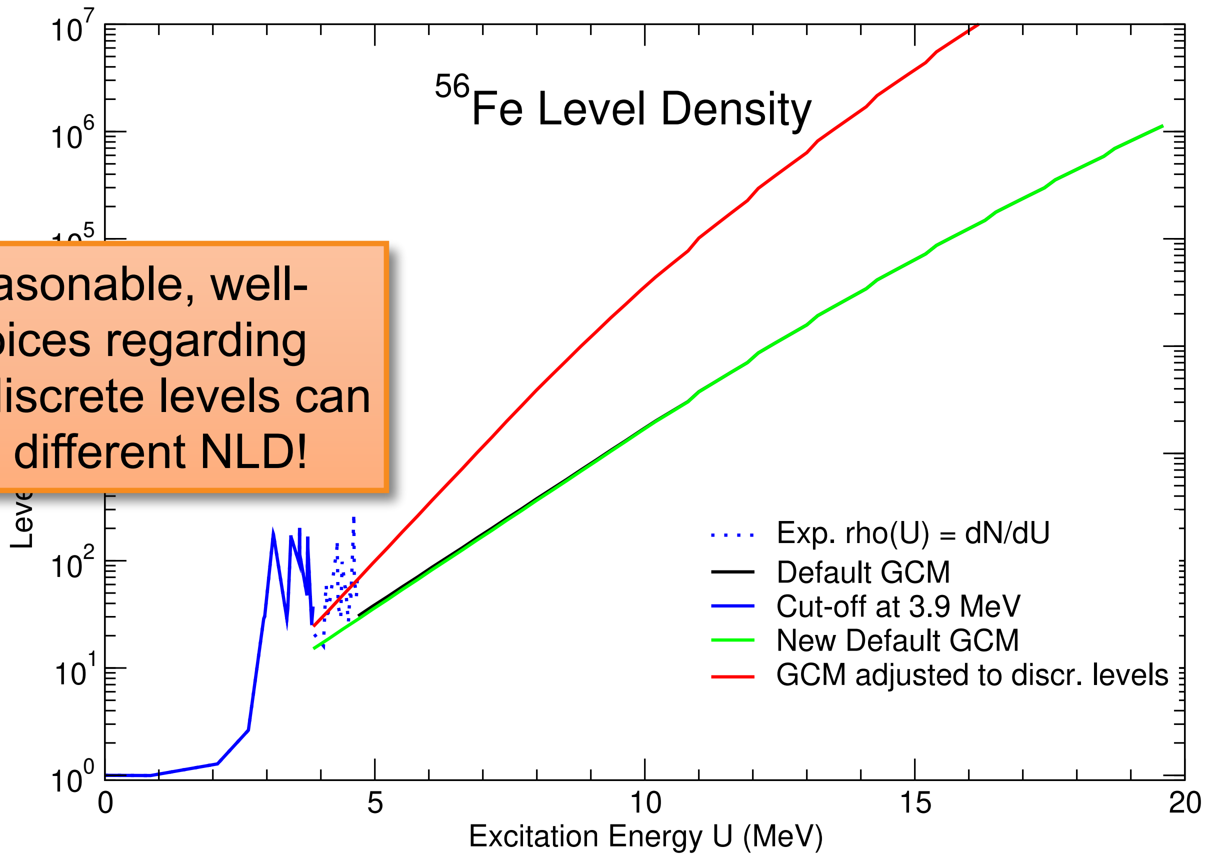




Different reasonable, well-justified choices regarding experimental discrete levels can lead to very different NLD!

High-energy constraints: resonance spacings

- We can use average spacings of s/p/d…-wave resonances (D_0, D_1, D_2,…) to constrain NLD for certain spins and parities at the neutron separation energy

$\widetilde{S}_n = S_n + \Delta E/2$, where ΔE is the energy interval for which the resonances are determined (which is much smaller than S_n, so $\widetilde{S}_n \approx S_n$), this relation can be generalized in the following expression:

$$D_L^{-1} = \sum_{J=J_{\min}}^{J_{\max}} \rho(\widetilde{S}_n, J, (-1)^L \pi_0), \qquad (5)$$

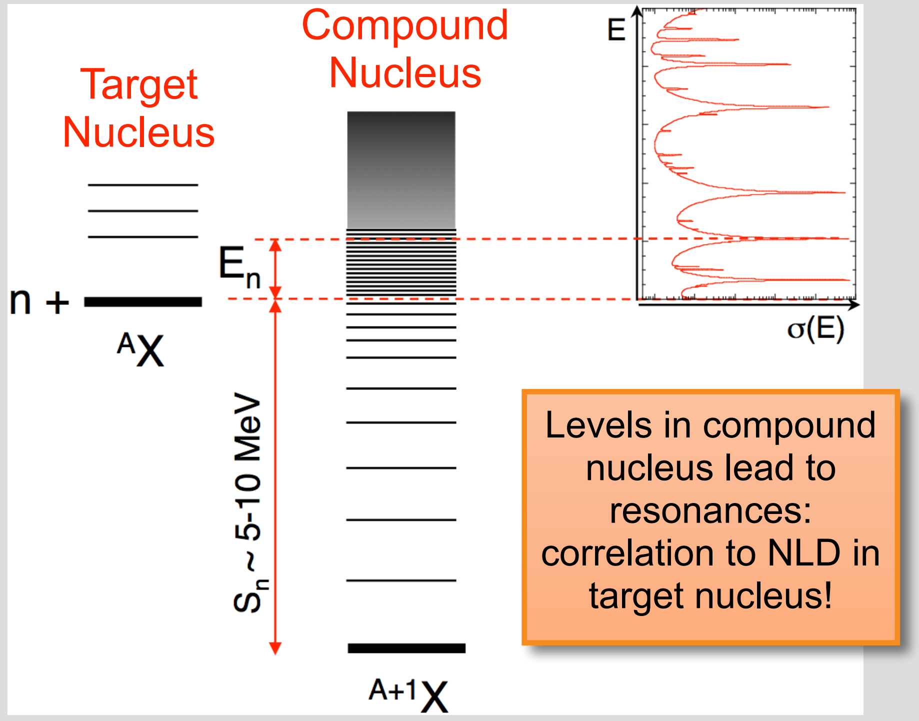
where I_0 and π_0 are, respectively, the spin and parity of the target nucleus, D_L is the average spacing of resonances of angular momentum L, and

$$J_{\min} = \max\left(0, |I_0 - L| - \tfrac{1}{2}\right) \qquad (6)$$

and

$$J_{\max} = I_0 + L + \tfrac{1}{2}. \qquad (7)$$

*G.P.A. Nobre et al., PRC**101** (2020) 034608*



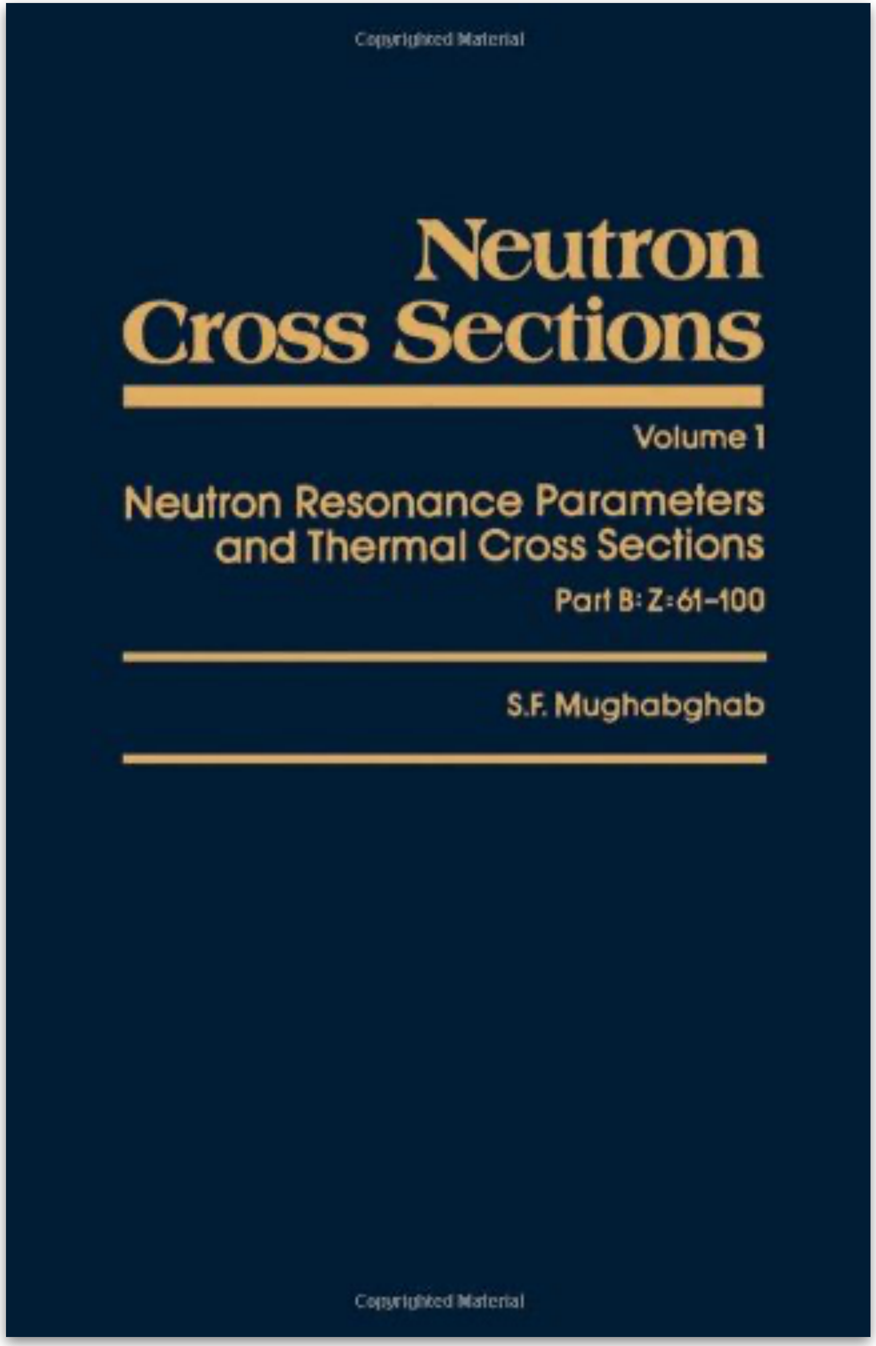
- That's not always available (e.g., **^{56}Fe**), and then more model assumptions have to be introduced
- *<u>When we have them</u>*, D_0 and D_1 are not as well-defined as one would expect.
    - Atlas is a fantastic resource, but it is far from perfect
    - Resonance sequences are filled with spin mis-assignments, to varying degrees.

The *Atlas* is foundational for much of nuclear science

- Comprehensive compilation of neutron resonances parameters and resonance properties
- Invaluable reference for resonance physics and phenomenology
- Regarded as “Standard values” for much of basic and applied physics

3 essential readings for neutron science:
***Atlas*, JEFF-18, Lane & Thomas**

Brookhaven National Laboratory



Behind the scenes, the *Atlas* production hasn't changed much since the 1970's

- ***Atlas*** **electronic files use original BNL-325 format, adjusted by Said**
  - 80 column format
  - "undocumented"

- ***Atlas*** **publication formatting tools are undocumented and unmaintained**
  - Tools build postscript directly from files (Did not build latex files)
  - Legacy fortran code psdsply.for
  - Written by BNL retiree Bob Kinsey?

- ***Atlas*** **files updated "by hand"**
  - Updated using text editor
  - No version control
  - Statistical analysis done with combination of codes from EMPIRE (wriurr.f, ptanal.f) and SAS analysis package (https://www.sas.com)

- **Issues**
  - "Compilation not evaluation"
  - Provenance of data - common problem in many older compilations
  - Typos galore
  - MLBW vs. RM vs. actual R matrix
  - Comments hiding beyond 80th column or hand written scrawl in personal copy

We adopted a multipronged approach to understanding the *Atlas*

1. Document the Atlas electronic file format
2. Develop simple Atlas API
3. Typo fixing by students (need statistics)
4. Match Atlas bibliography to EXFOR/NSR
5. Mean spacings and capture widths
6. BRR - tried to get provenance of D, went down rabbit hole

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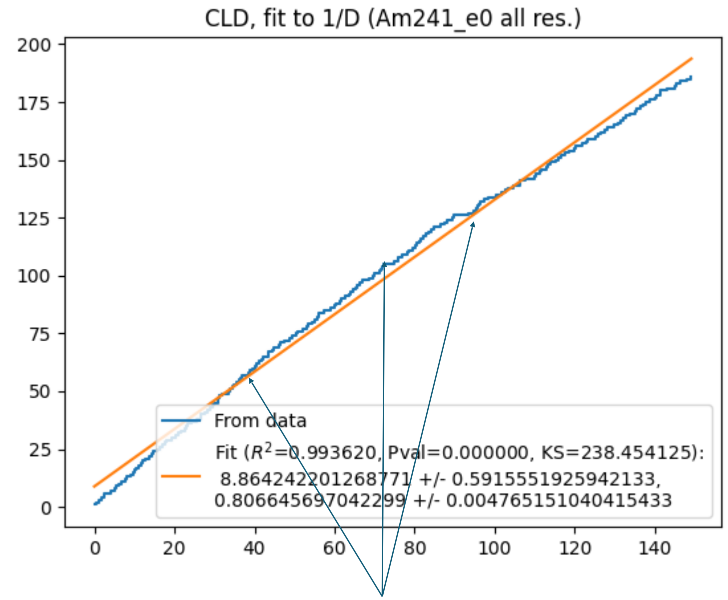
Extracting the mean resonance spacing is surprisingly difficult

- Big Problems:
  - Missing resonances
  - Spingroup missassignments*
  - Resonances from different nuclei altogether
- State of the art has not advanced much
  - Option #1: Build a cumulative level distribution (CLD), fit a line
  - Option #2: Just average the spacings
- But what spacings should you keep in your set? How will you deal with correlations? Can you “add in” (impute) missing resonances?



Obvious gaps could be imputed

*Foils usage of Δ_3 statistic and other RMT-inspired approaches

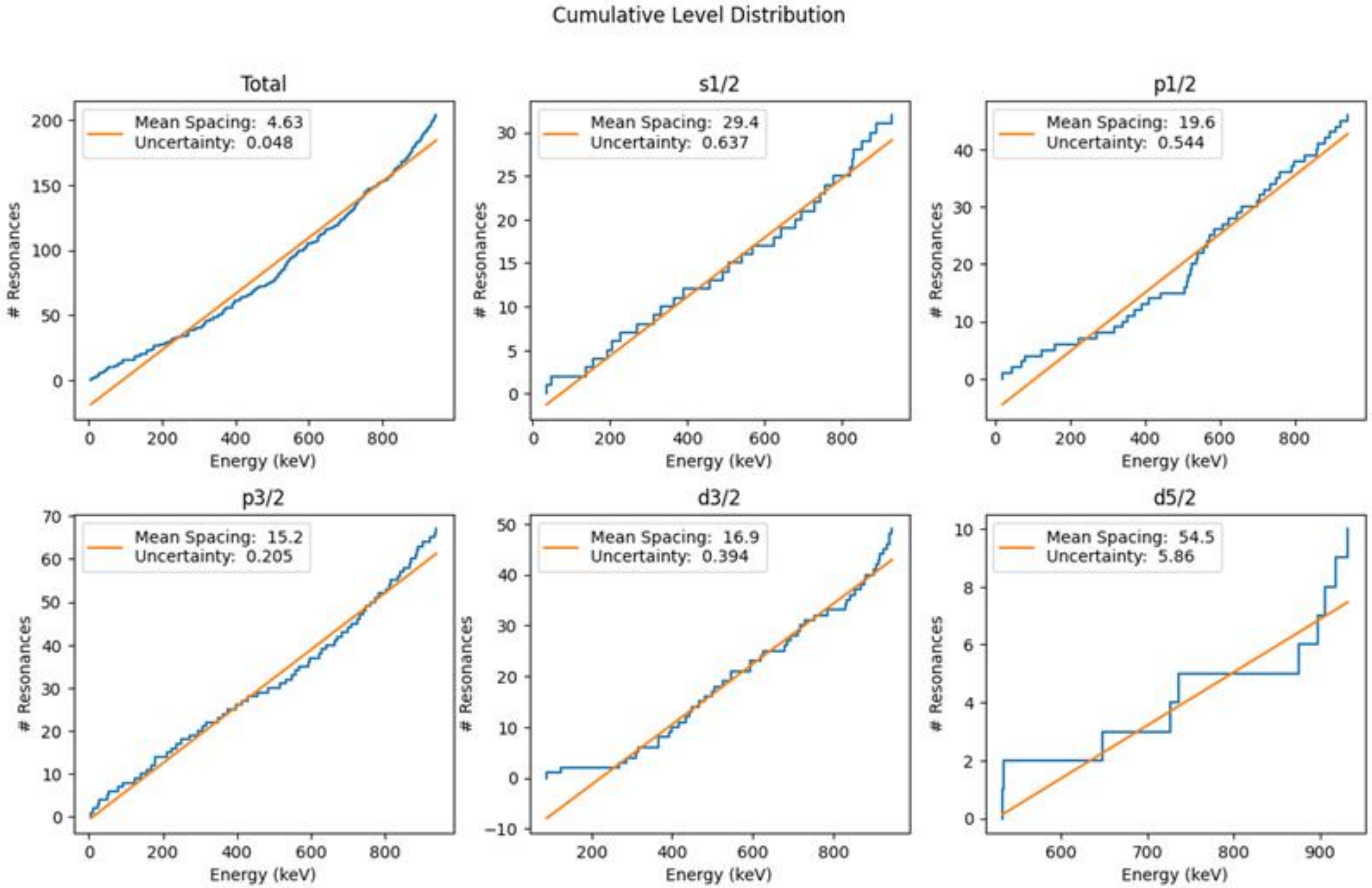
Implicit correlations: LD of each SG adds up to total LD

Implies sumrules:

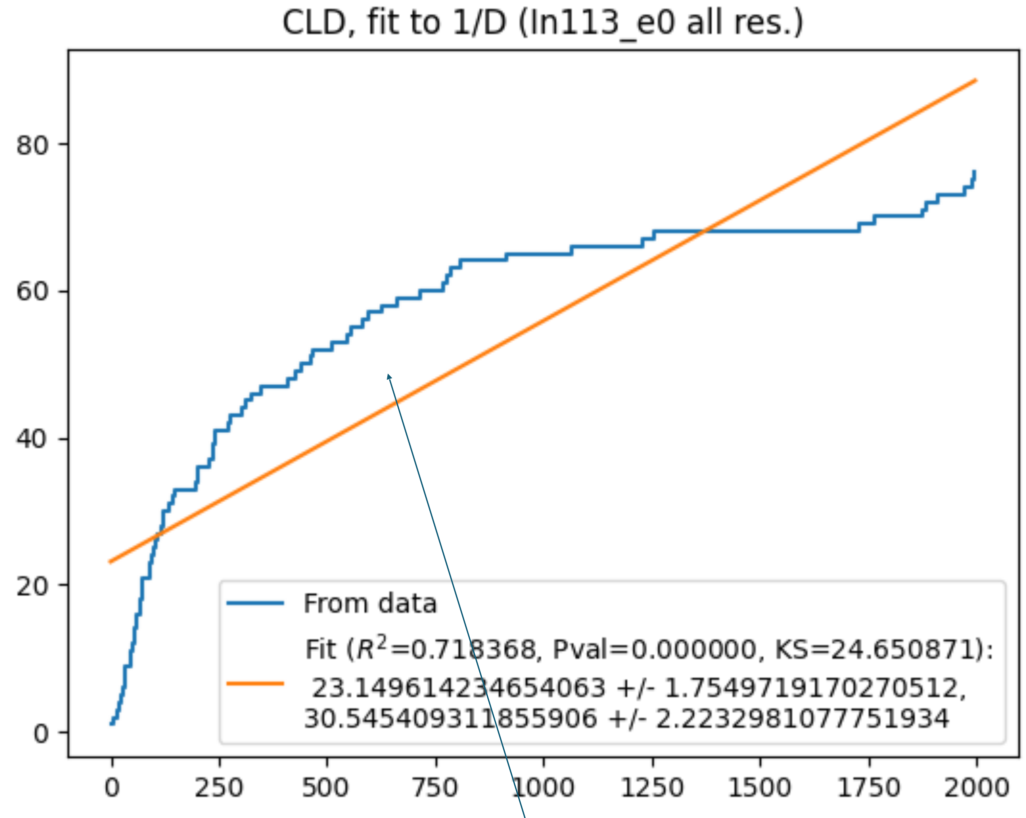
$$\frac{1}{D} = \sum_L \frac{1}{D_L}$$

$$\frac{1}{D_L} = \sum_J \frac{1}{D_{LJ}}$$

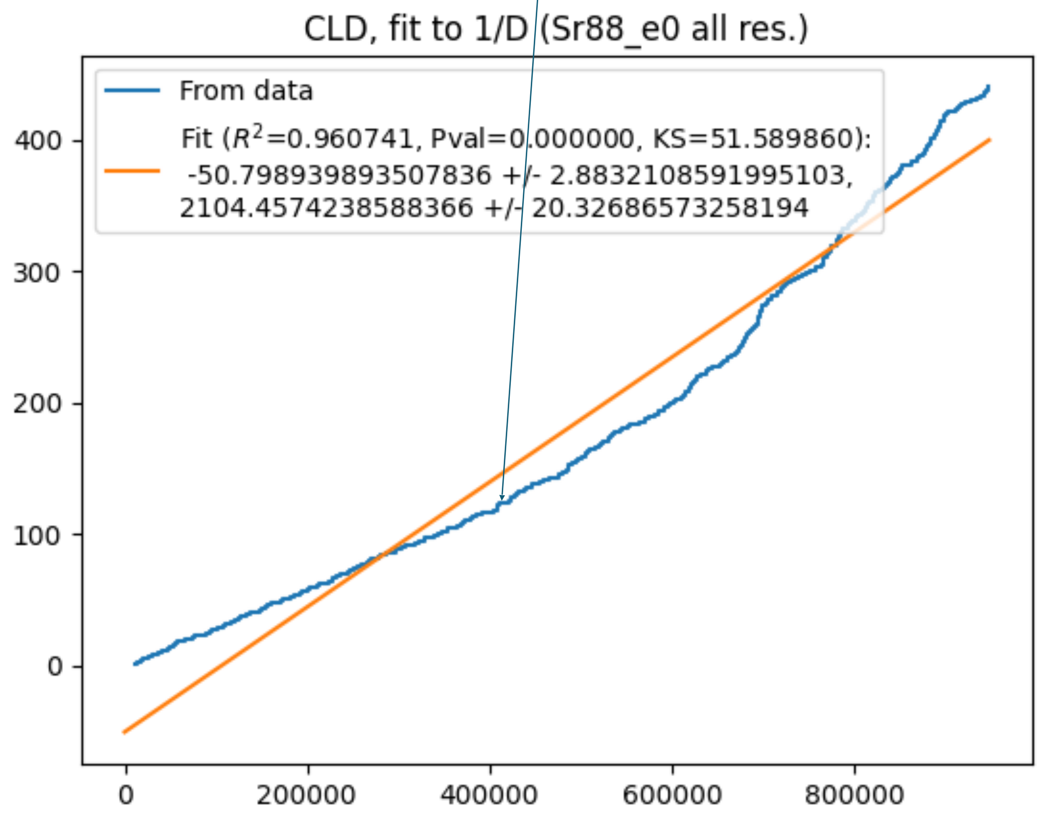
(these rules couple the fit slopes, but the intercepts are correlated too!)



Strange features in real-life CLD’s

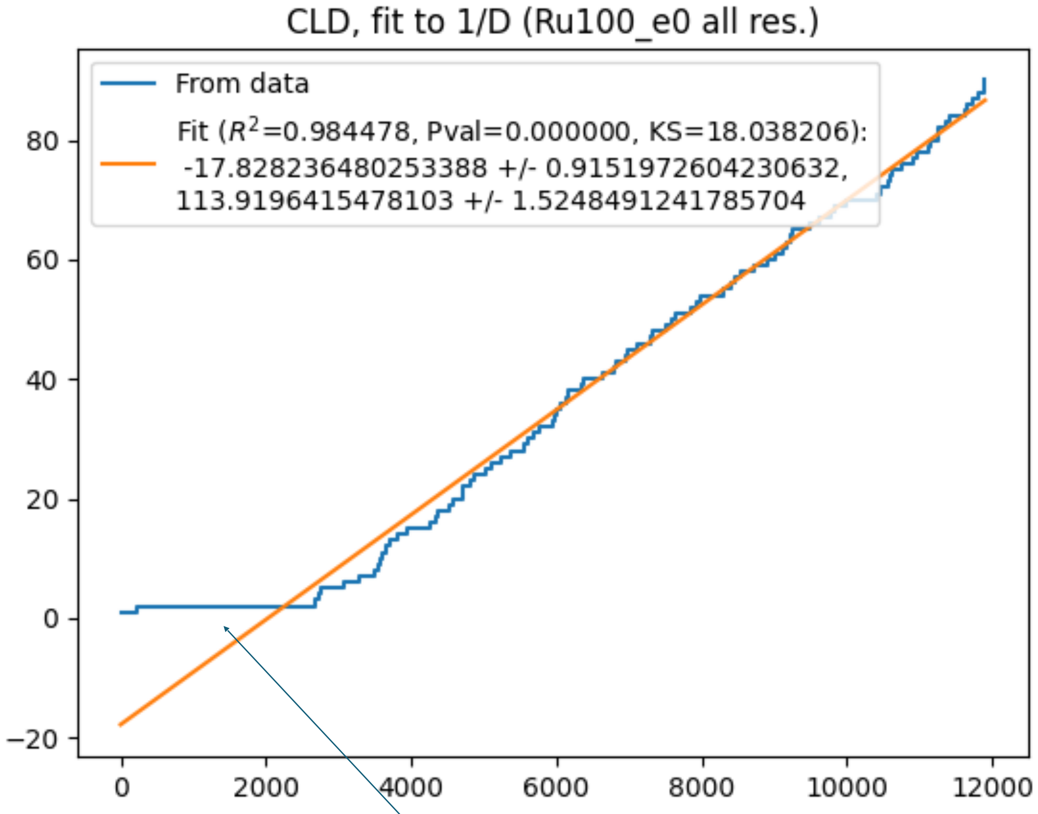


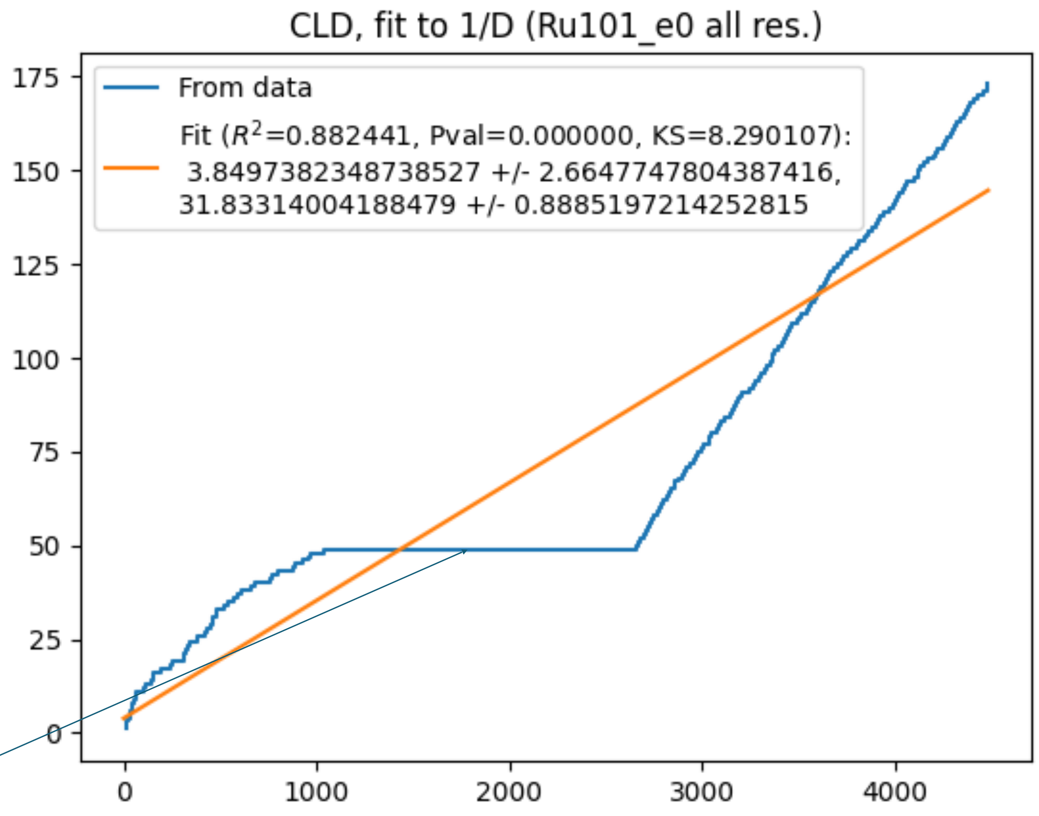
Mughabghab ignores upturn and gets much bigger spacing than we do



This strangeness caused by poor statistics in L=1

More strange features in real-life CLD's

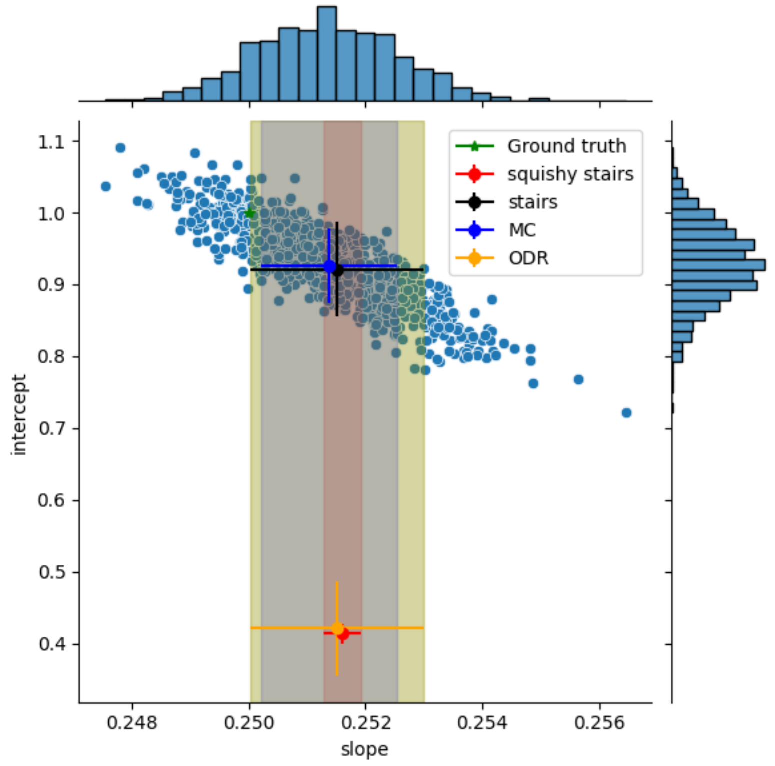


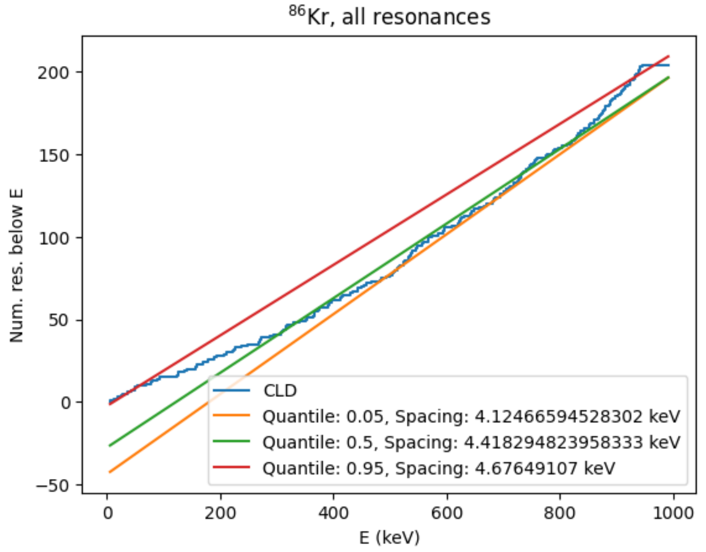


Why the gap?

Our try-everything approach

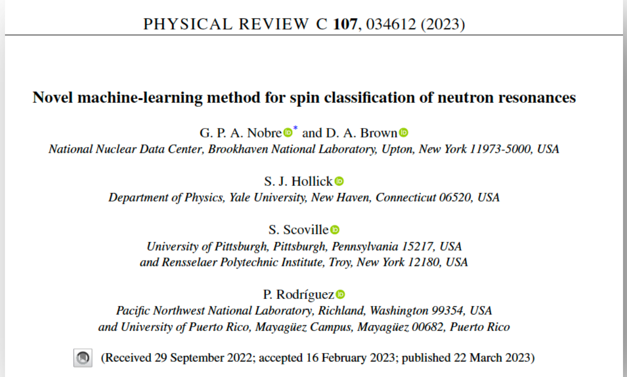
- Built generative model to test approaches
  - Model used to develop BRR (so can use ML to reassign spingroups)
  - Benchmarked variety of regression approaches including: GLQR, CGLSR,ODR, MC-MC, Quantile Regression
  - Also looked at full Empirical CDF of spacings
  - Generative model needs more real-life features
- Quantile regression is best (most robust and statisticians' favorite)
  - Need multivariate, correlated version





Bayesian Resonance Reclassifier

- A machine-learning method for resonance spin re-classification
- First article on the method has been published in FY23
- It is shaping up to be a great tool to assist in resonance evaluations



PHYSICAL REVIEW C **107**, 034612 (2023)

Novel machine-learning method for spin classification of neutron resonances

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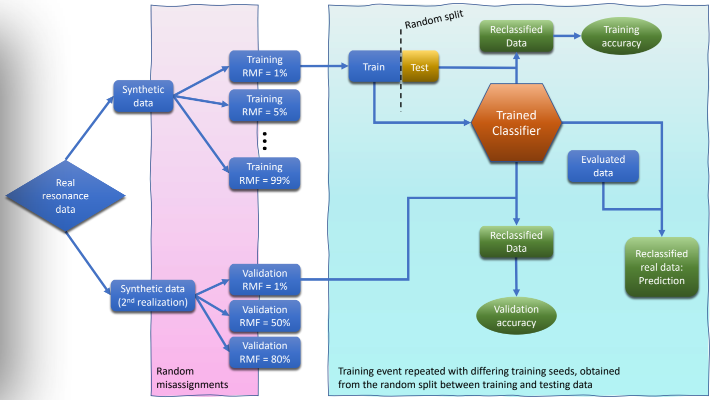
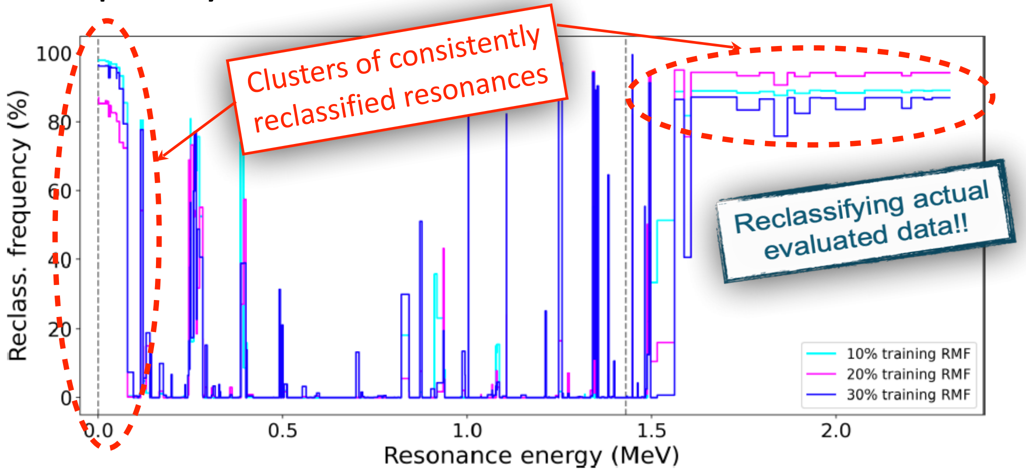
(Received 29 September 2022; accepted 16 February 2023; published 22 March 2023)

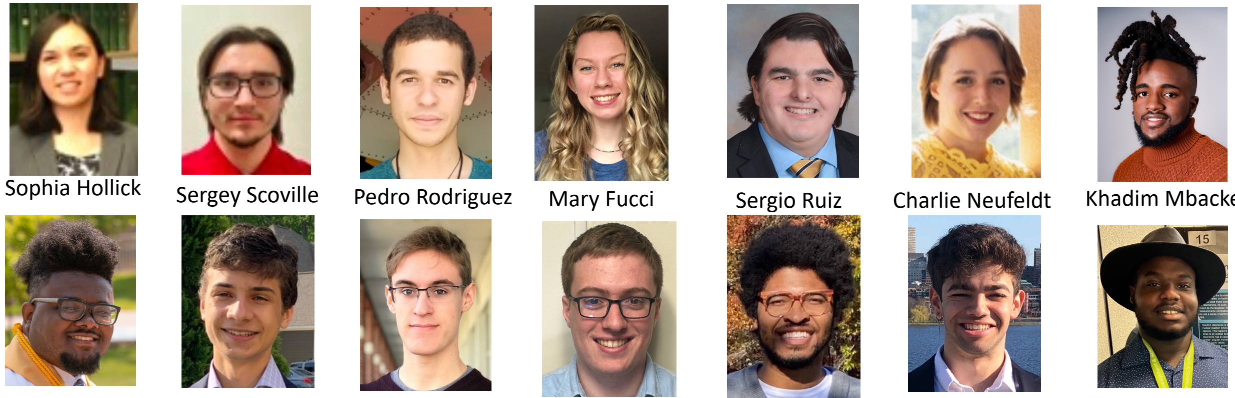


These mis-assignments in resonance evaluations can potentially impact many reactor applications!

- Work done mainly with undergraduate interns
- Interns presented CEU posters at 2022/2023 DNP Meetings
- Past interns went on to grad school or staff positions

Frequency of reclassification of resonances in ^{52}Cr





Sophia Hollick, Sergey Scoville, Pedro Rodriguez, Mary Fucci, Sergio Ruiz, Charlie Neufeldt, Khadim Mbacke

Marcus McLaurin, Nicholas Fritsch, Ian Snider, Ethan Richards, Ayman Abdullah-Smoot, Isaac Broussard, Kwame Bennett

Project goals

- Decide best automated approach to compute mean spacings
- Apply to Atlas of Neutron Resonances
- Publish to ANDT
- Keep exploring and expanding BRR
- Enlist help of summer students

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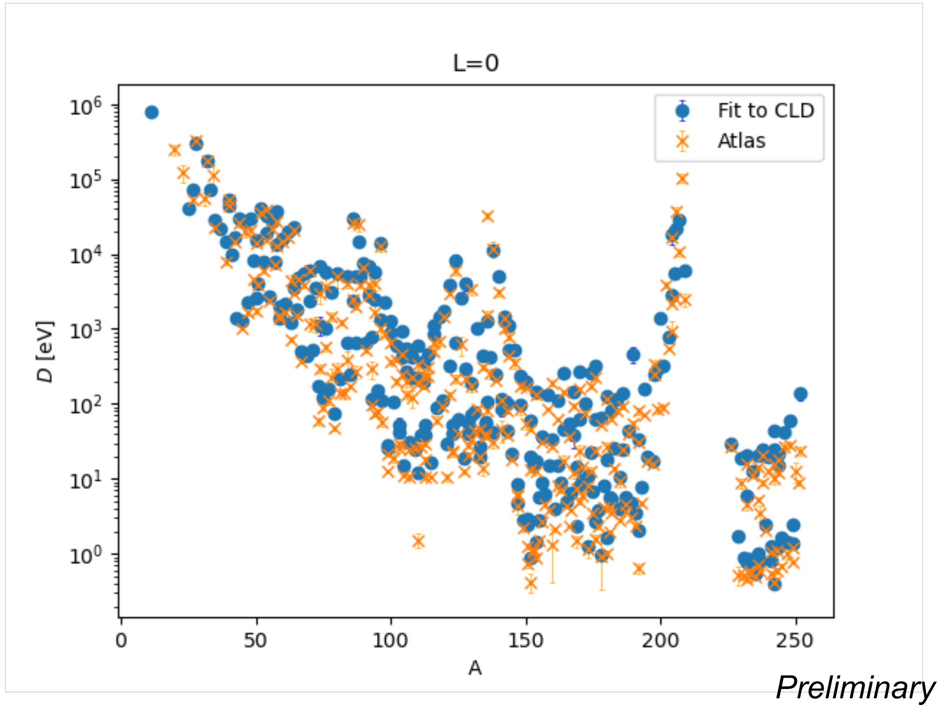

Bottom line:

Experimental resonances spacings D_λ are not as well-known or well-determined as would be desired for unequivocally pinning NLD measurements!

Even if you do have reliable D_0 & D_1…

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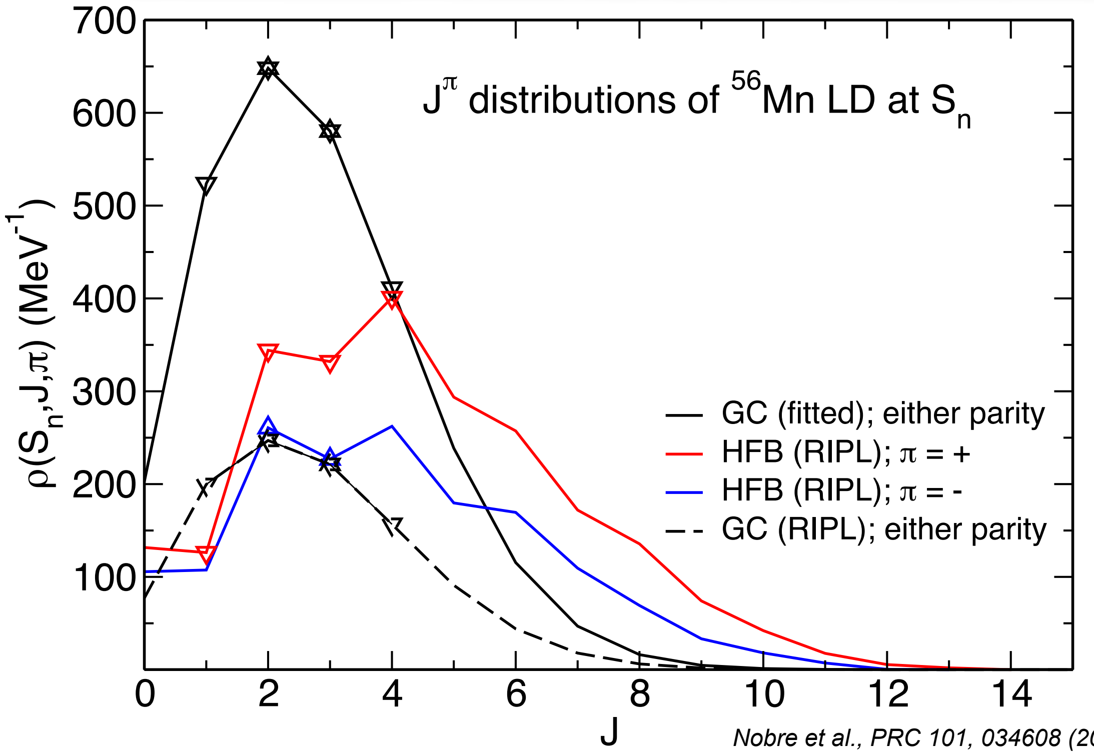
- That only constrains the LD at certain spins and parities and CANNOT uniquely define the total LD

- For ^{56}Mn, there are D_0 & D_1 available
- Ground state of ^{55}Mn is $I_0 = 5/2^-$
- D_0 constrains $J^\pi = (2^-, 3^-)$
- D_1 constrains $J^\pi = (1^+, 2^+, 3^+, 4^+)$



Nobre et al., PRC 101, 034608 (2020)

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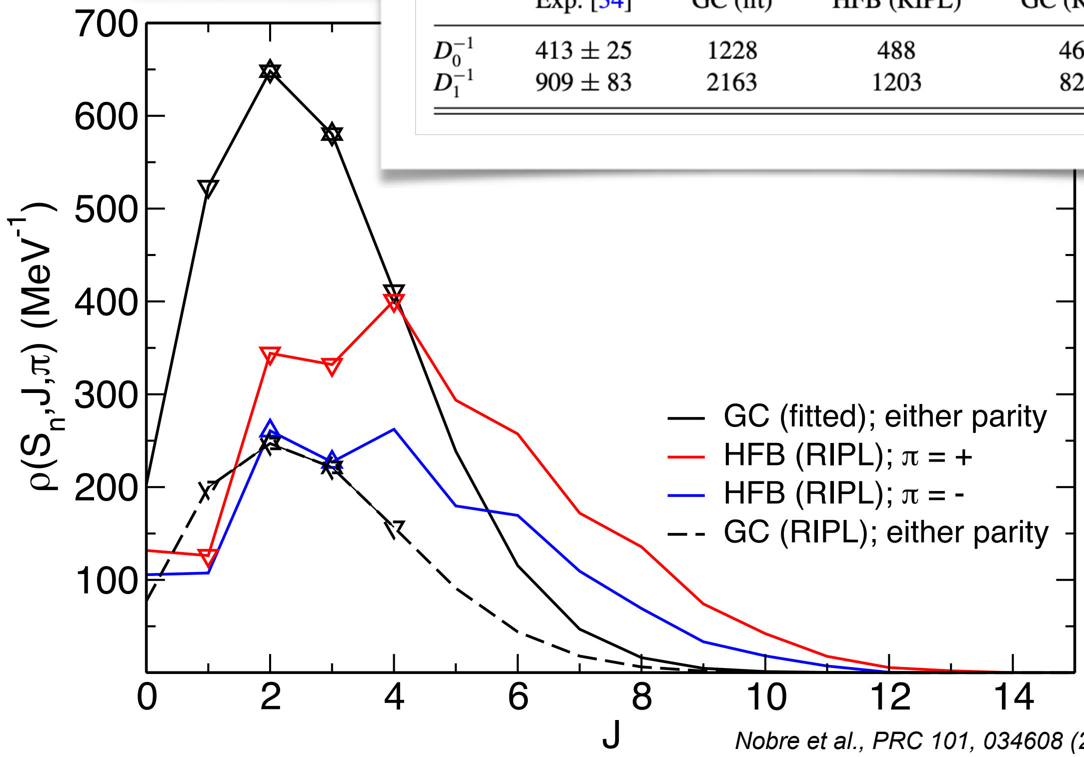
TABLE I. Comparison between the experimental D_0^{-1} and D_1^{-1}, in units of MeV^{-1} with values obtained from ^{56}Mn level density.

	Exp. [34]	GC (fit)	HFB (RIPL)	GC (RIPL)
D_0^{-1}	413 ± 25	1228	488	468
D_1^{-1}	909 ± 83	2163	1203	824



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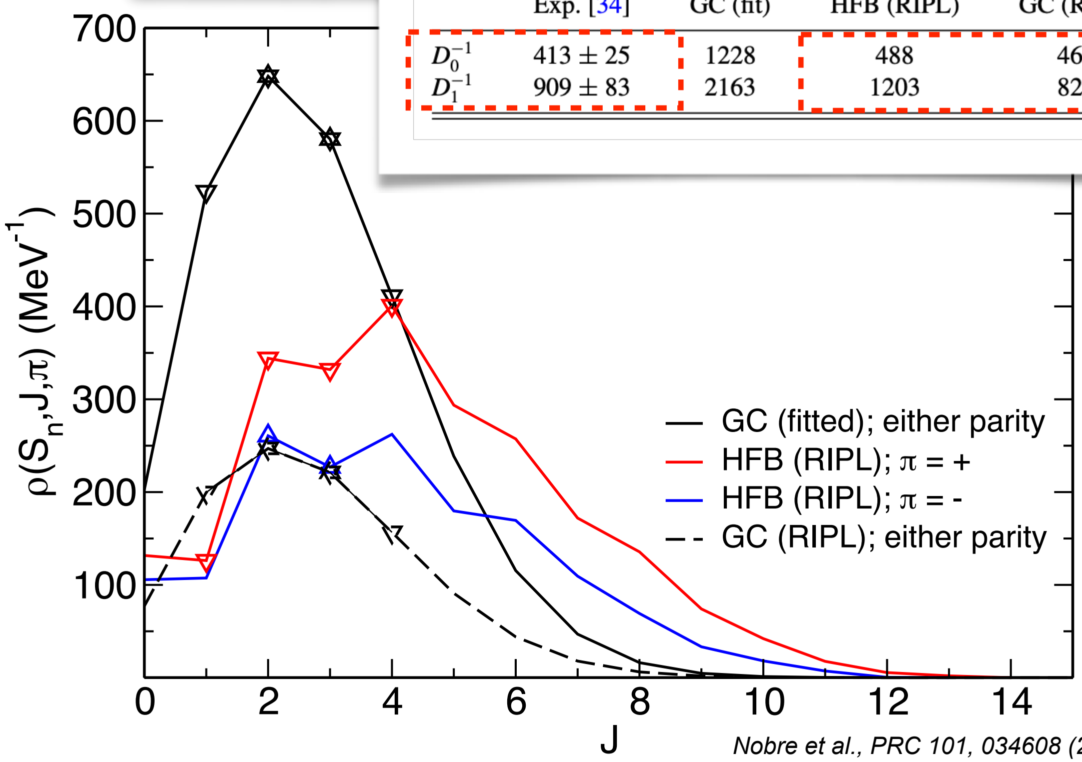

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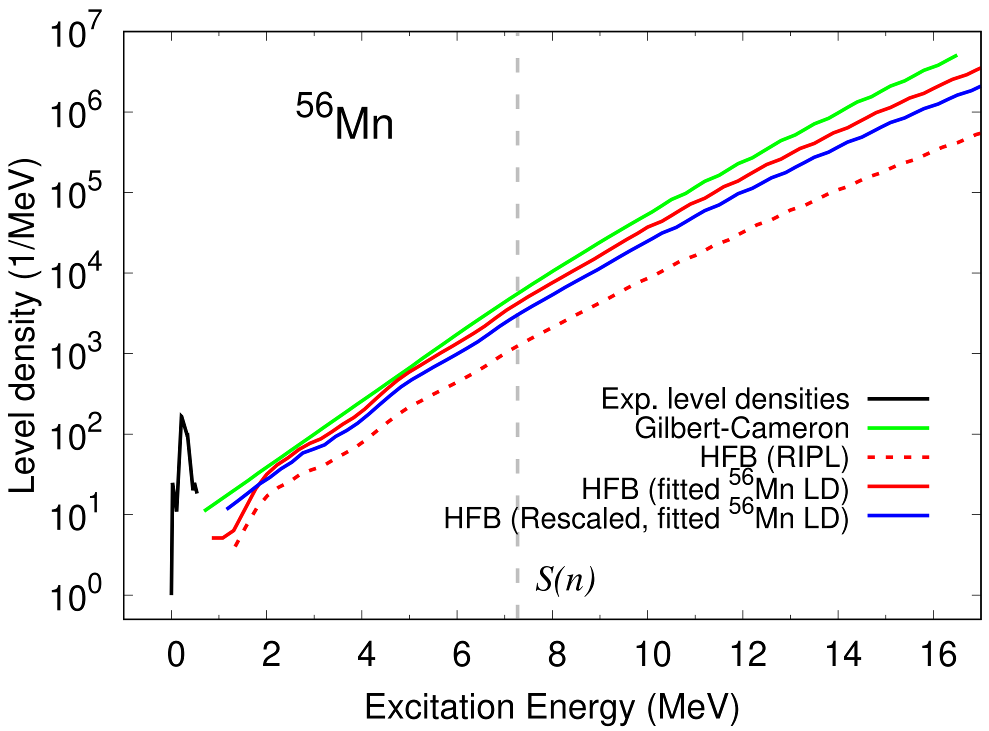

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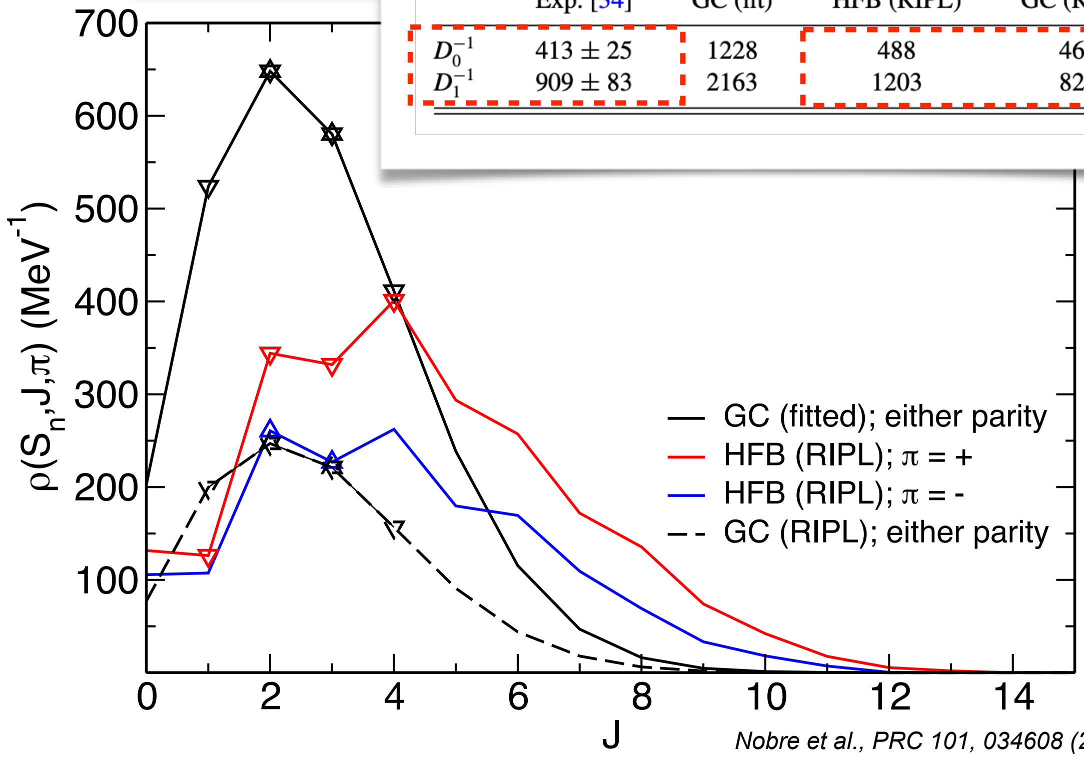

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- That only constrains the LD at certain spins and parities and CANNOT uniquely define the total LD
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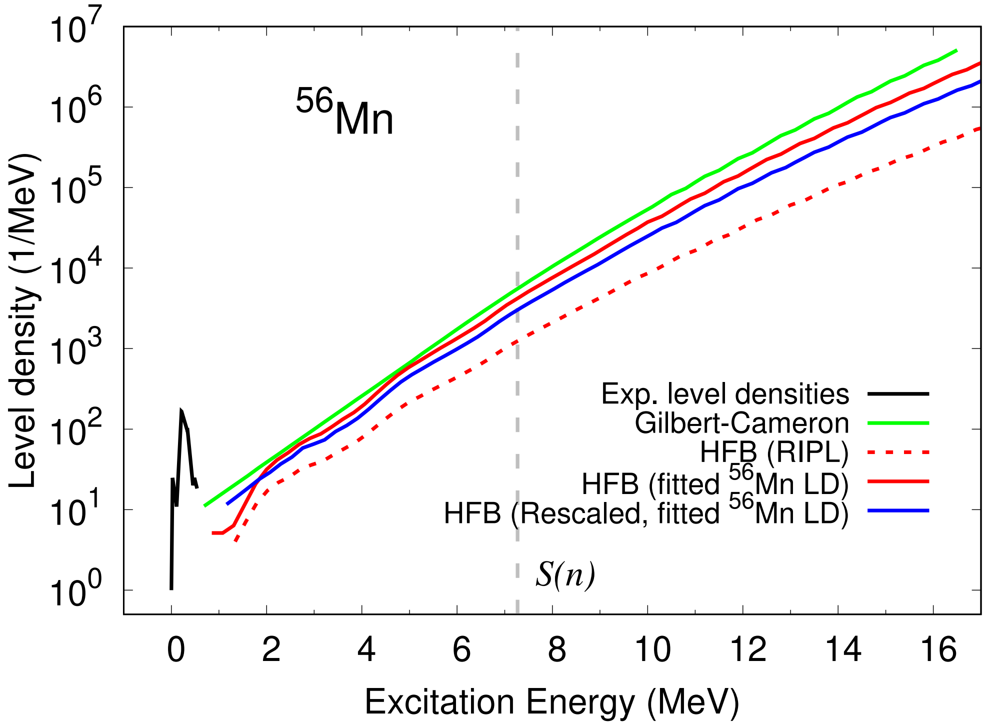
- So, agreeing with normalized total NLD measured data **does not** necessarily mean agreeing with the actual measurements: Dependent on model assumptions!



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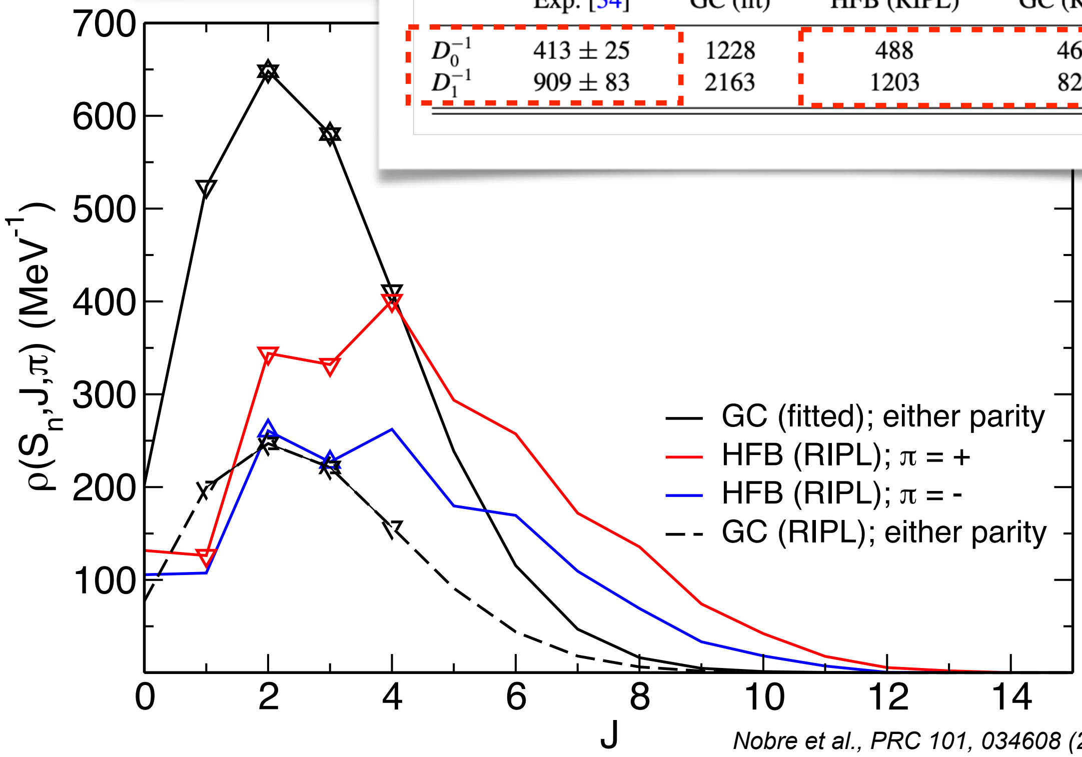

Nobre et al., PRC 101, 034608 (2020)

Another example…

- Ref. [1] reports great work using Oslo method to measure ^{56,57}Fe NLD
- They make generally reasonable assumptions
- But how realistic is some of them?

$$\rho(S_n) = \frac{2\sigma^2}{D_0} \cdot \frac{1}{(J_t + 1)\exp[-(J_t + 1)^2/2\sigma^2] + J_t \exp[-J_t^2/2\sigma^2]}, \tag{5}$$

assuming equally many positive- and negative-parity states. Here, J_t is the ground state spin of the target nucleus in the neutron-resonance experiment and σ is the spin cutoff parameter. We make use of the phenomenological spin cutoff parameter suggested in [40]:

$$\sigma^2(E) = 0.391A^{0.675}(E - 0.5Pa')^{0.312}. \tag{6}$$

Brookhaven National Laboratory

[1] A.C. Larsen et al., J. Phys. G: Nucl. Part. Phys. **44** (2017) 064005

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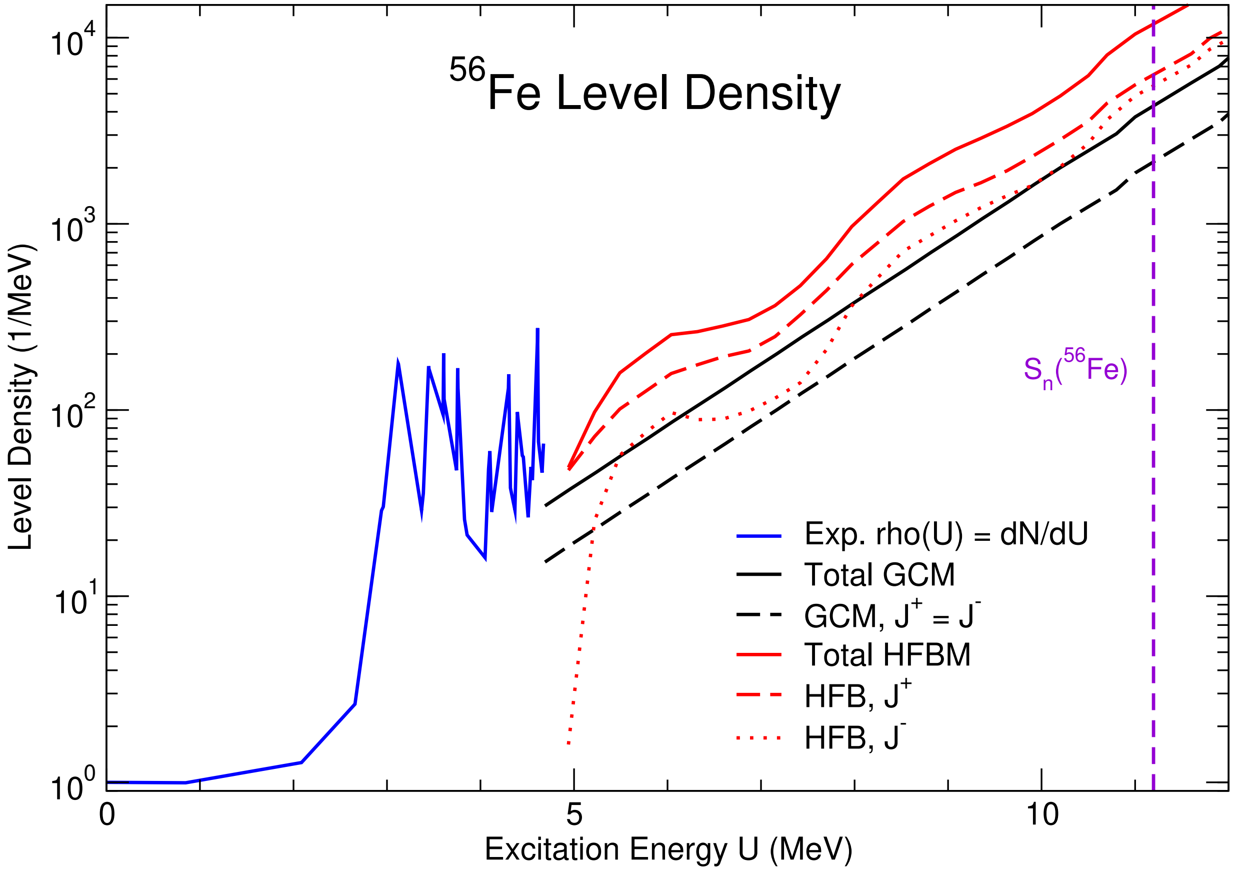

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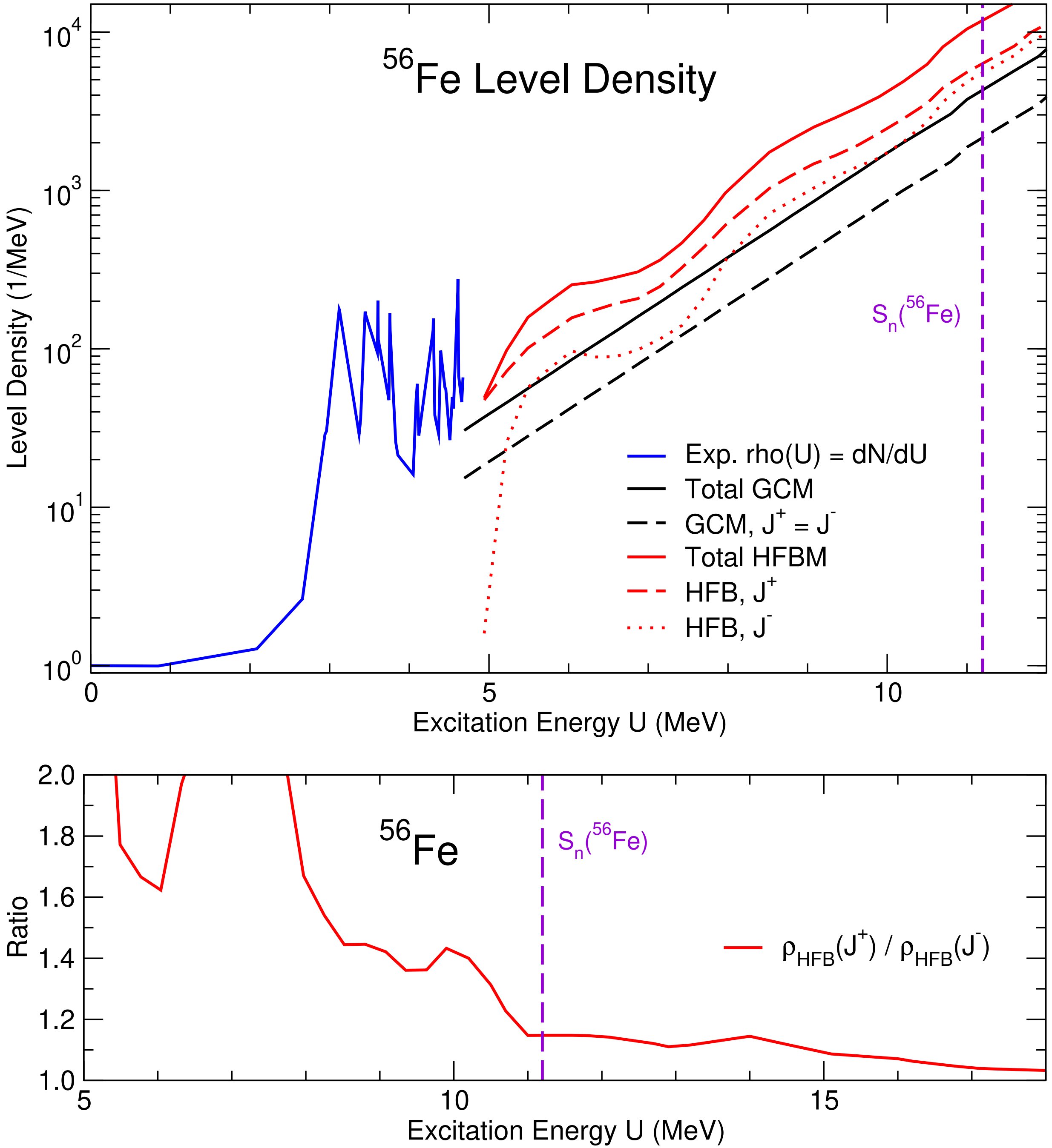
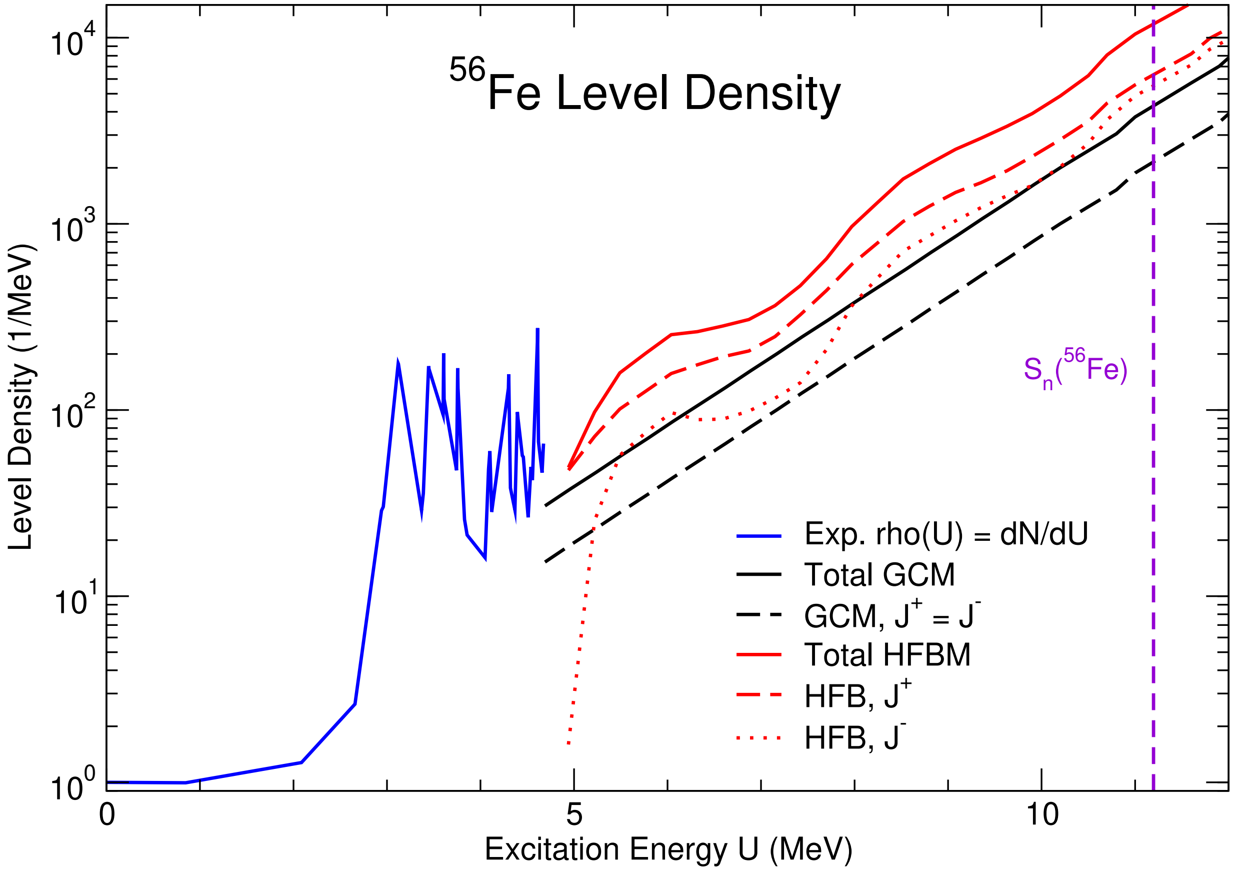
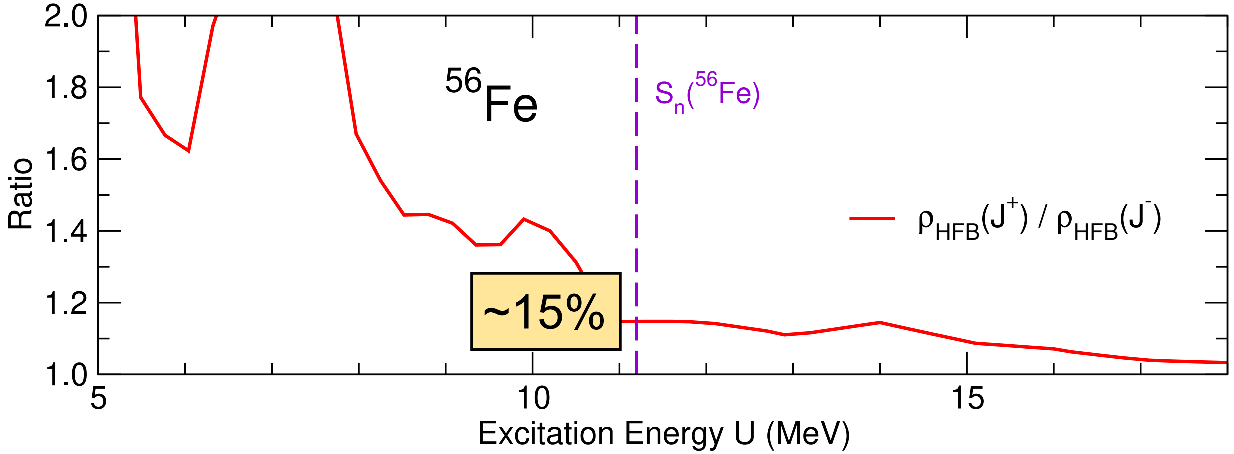


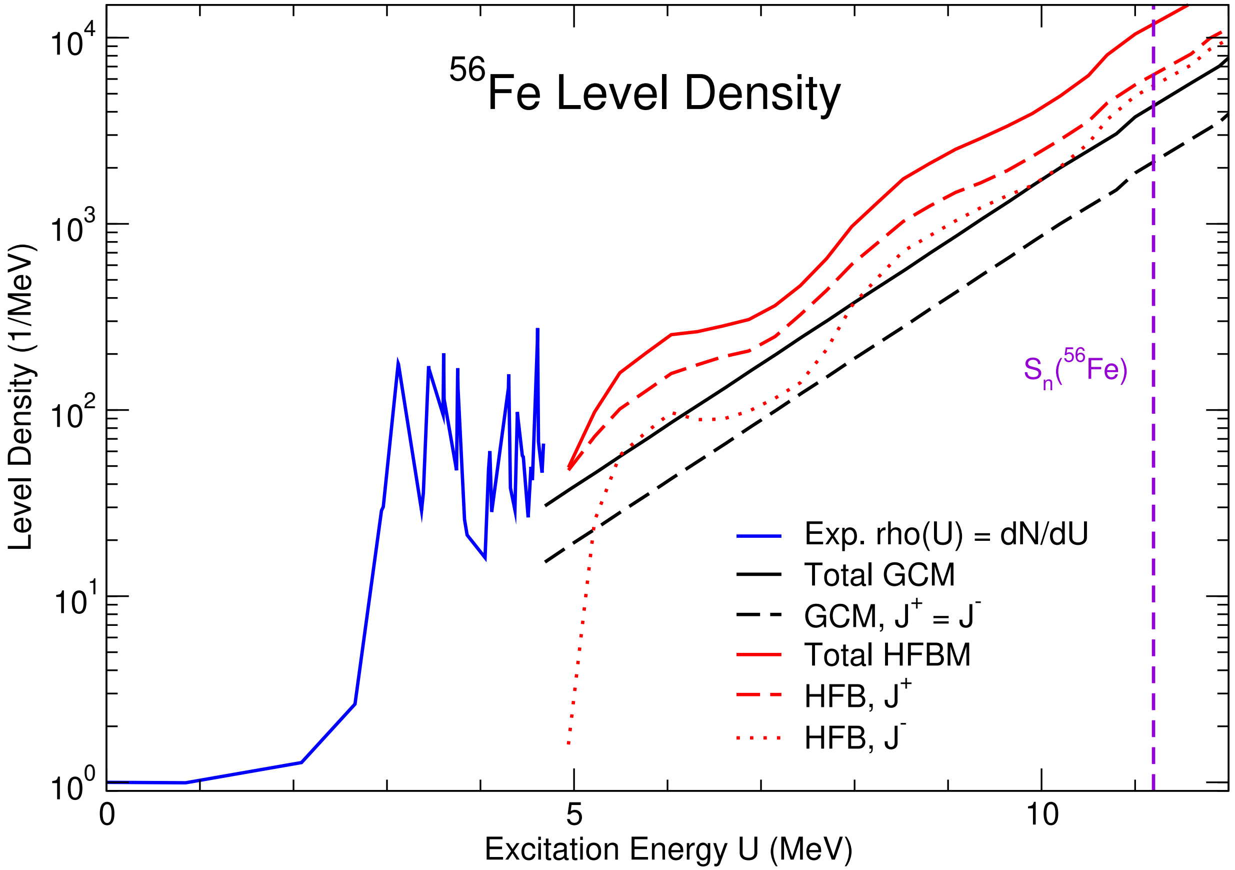
56Fe Level Density
Level Density (1/MeV)
Excitation Energy U (MeV)
Exp. rho(U) = dN/dU
Total GCM
GCM, J+ = J-
Total HFBM
HFB, J+
HFB, J-
Sn(56Fe)
56Fe
Ratio
ρHFB(J+) / ρHFB(J-)



^{56}Fe Level Density
Level Density (1/MeV)
Excitation Energy U (MeV)
$S_n(^{56}Fe)$
Exp. rho(U) = dN/dU
Total GCM
GCM, $J^+ = J^-$
Total HFBM
HFB, J^+
HFB, J^-



^{56}Fe
Ratio
Excitation Energy U (MeV)
$S_n(^{56}Fe)$
$\rho_{HFB}(J^+) / \rho_{HFB}(J^-)$
~15%



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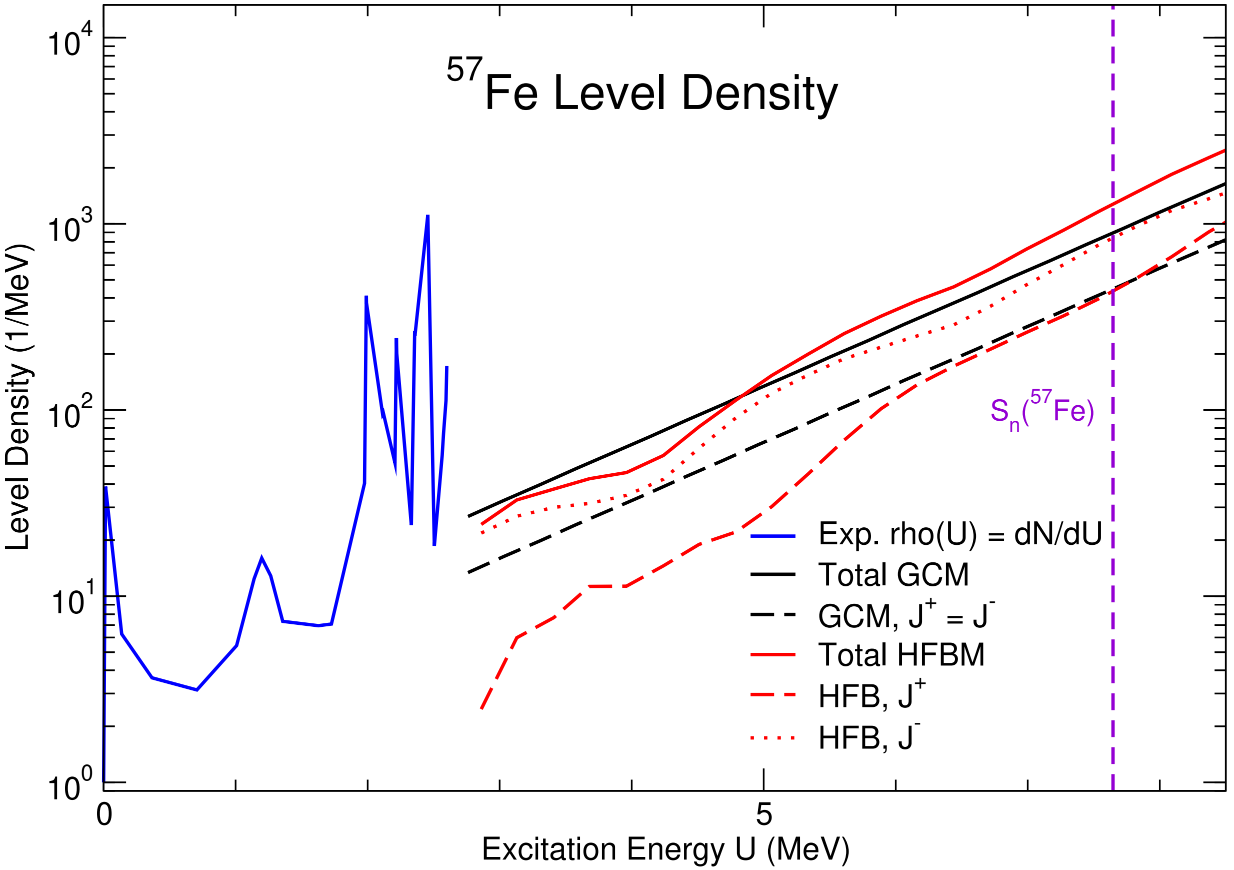

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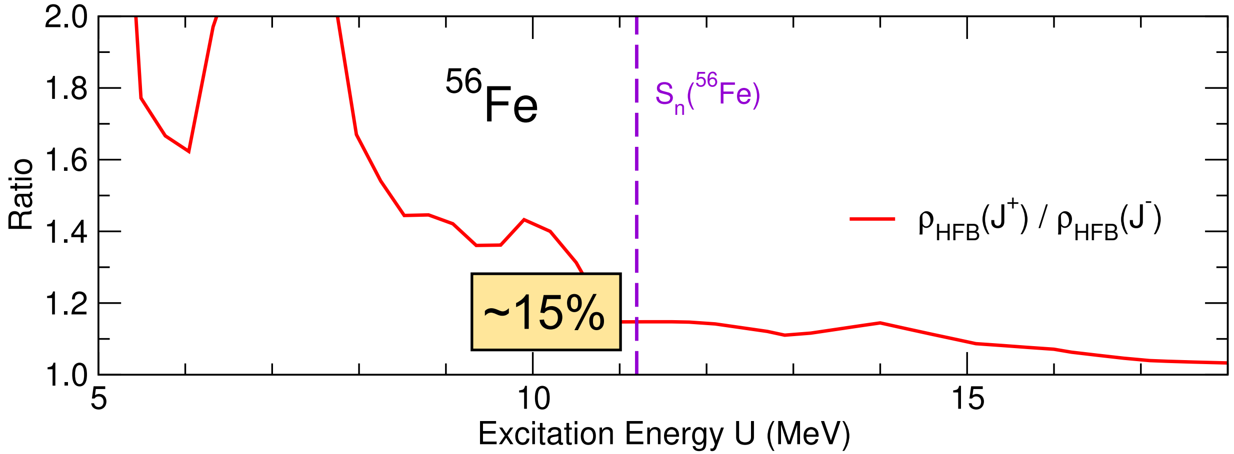

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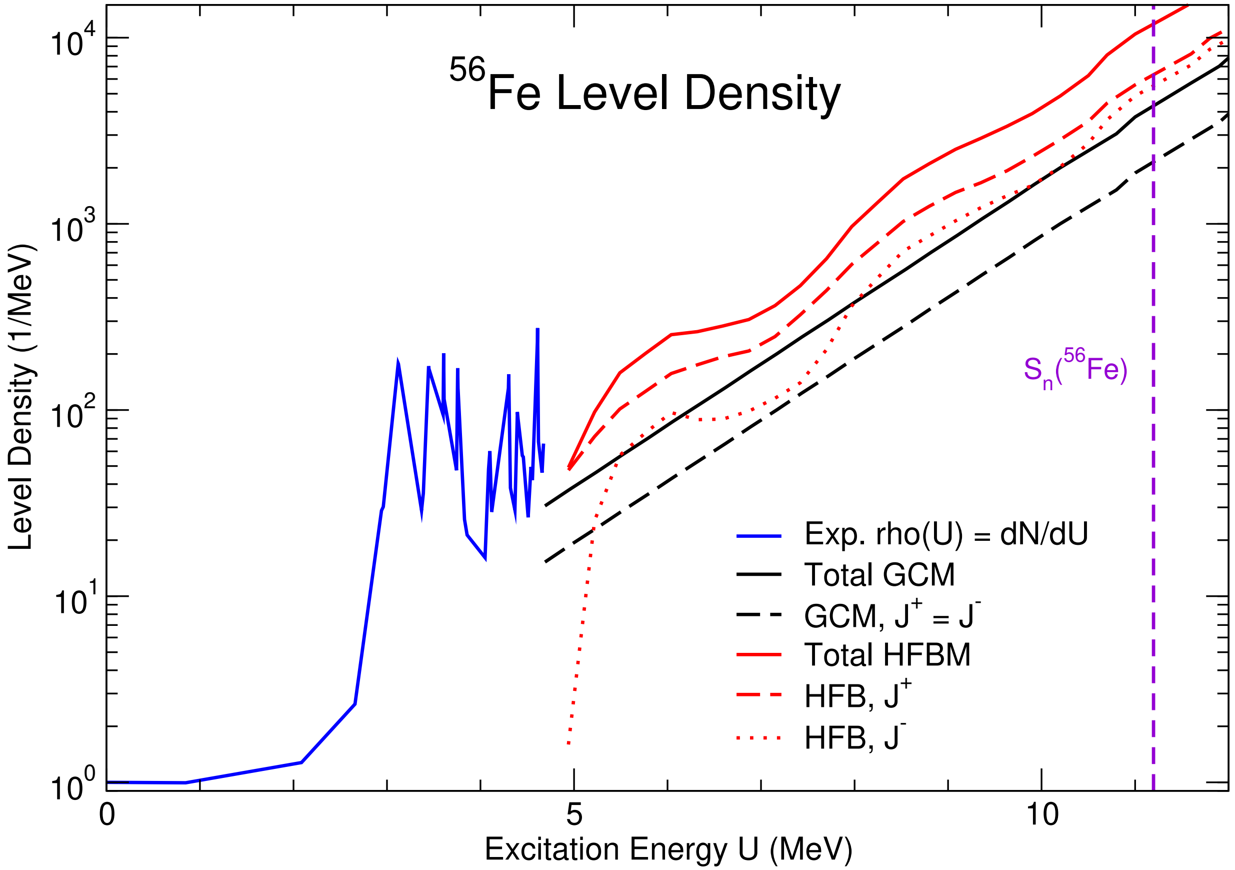
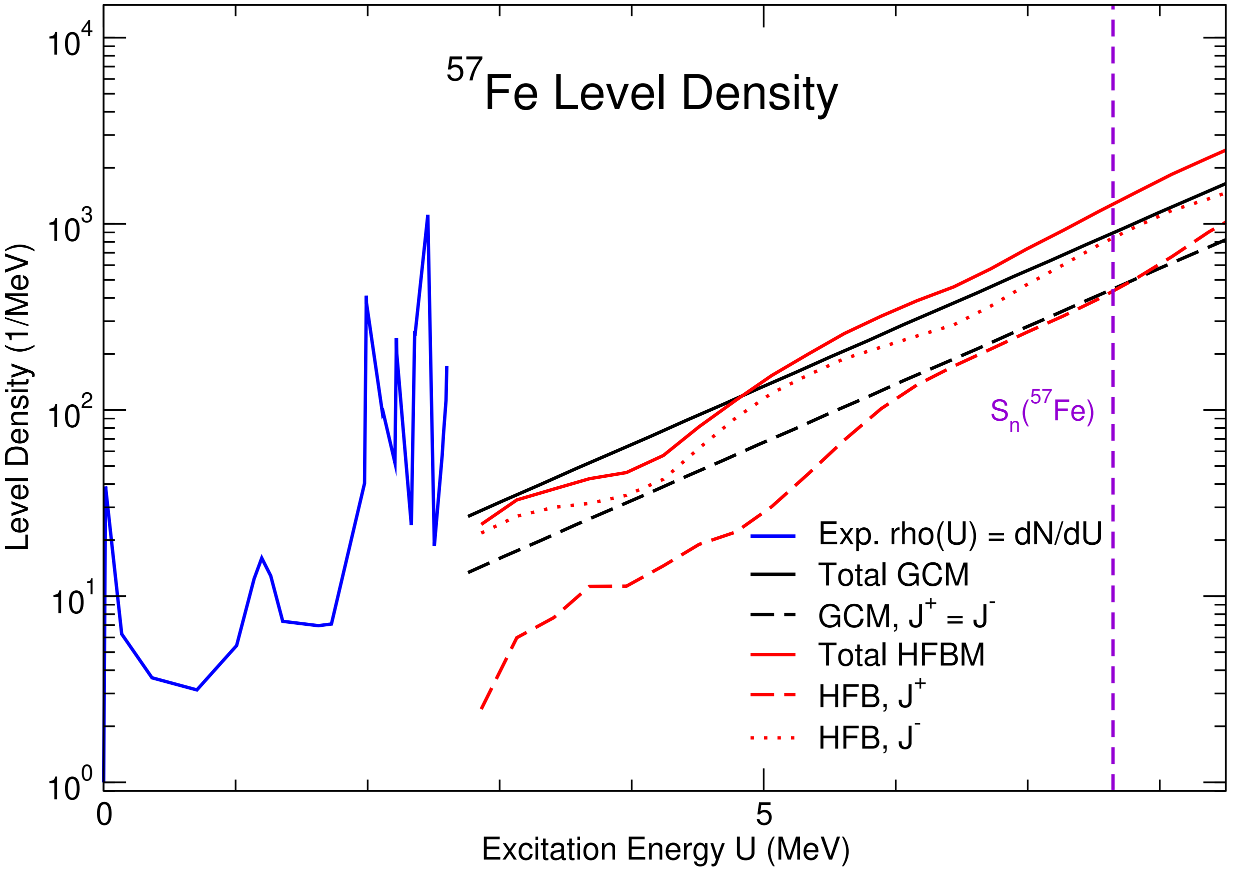


56Fe Level Density
Level Density (1/MeV)
Excitation Energy U (MeV)
Sn(56Fe)
Exp. rho(U) = dN/dU
Total GCM
GCM, J+ = J-
Total HFBM
HFB, J+
HFB, J-



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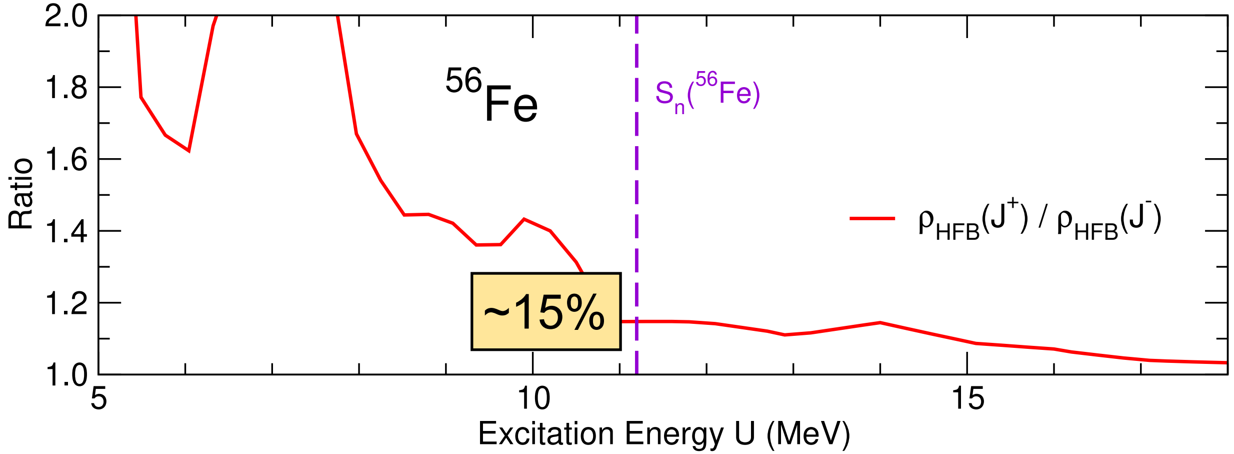

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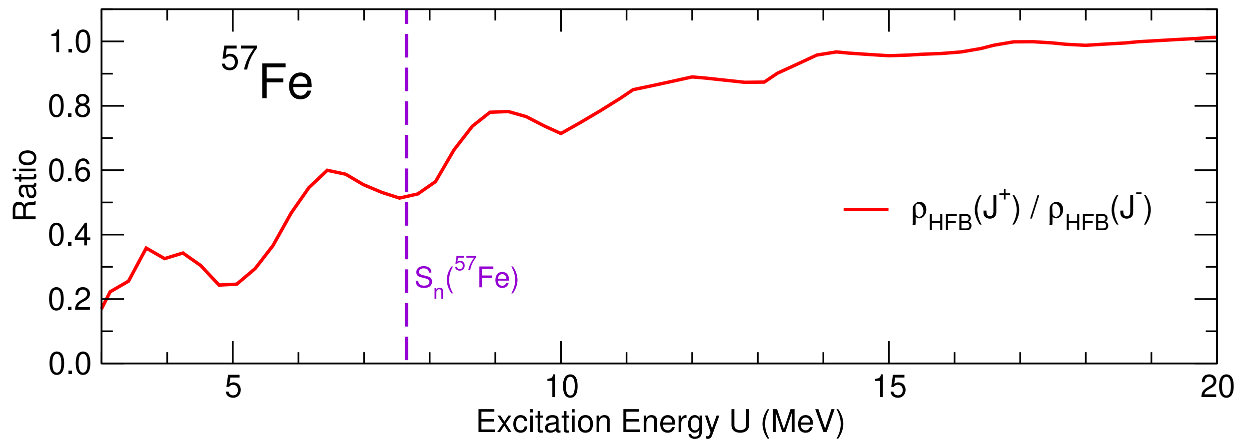
Excitation Energy U (MeV)



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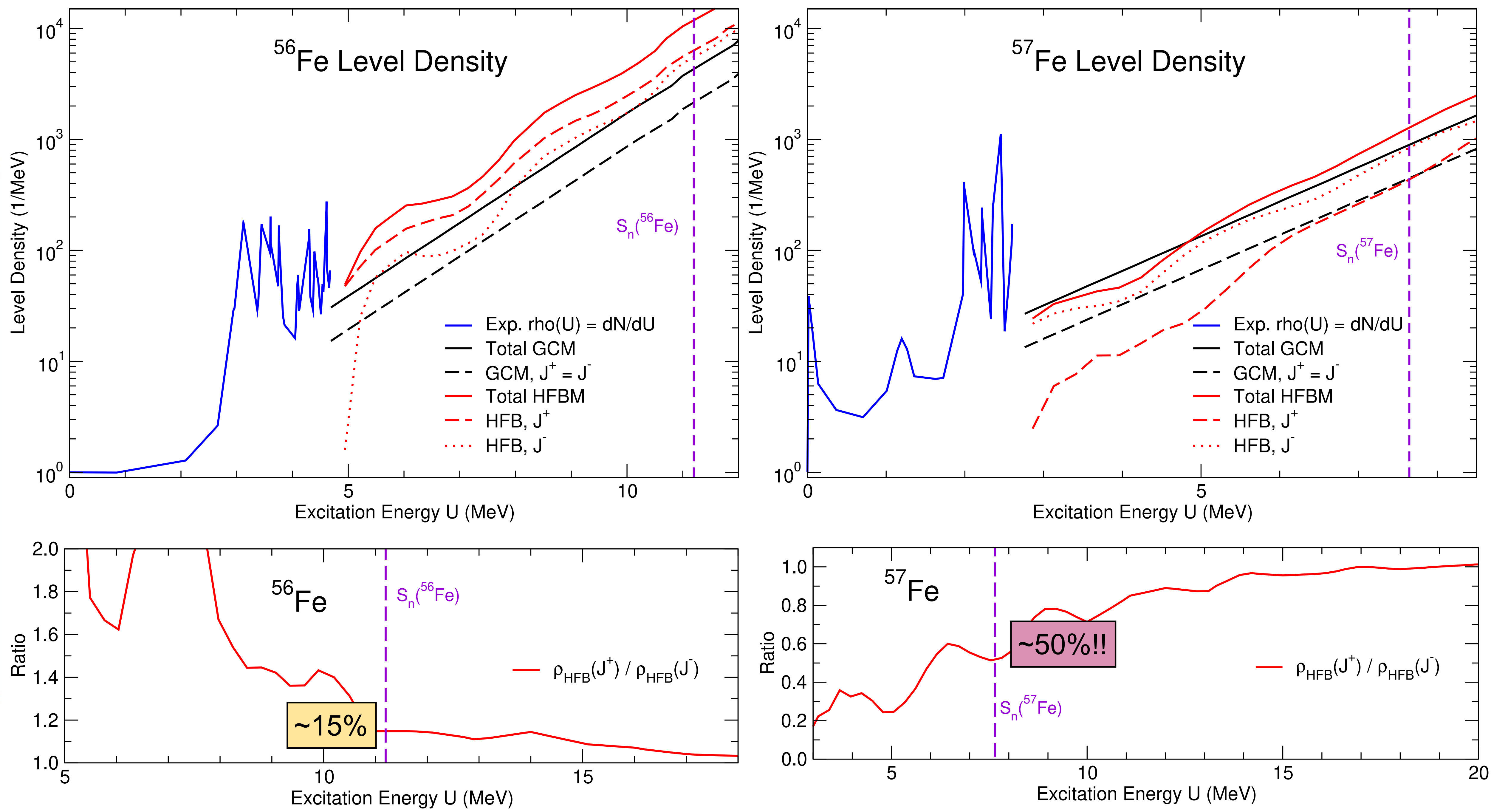

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GCM, J+ = J-
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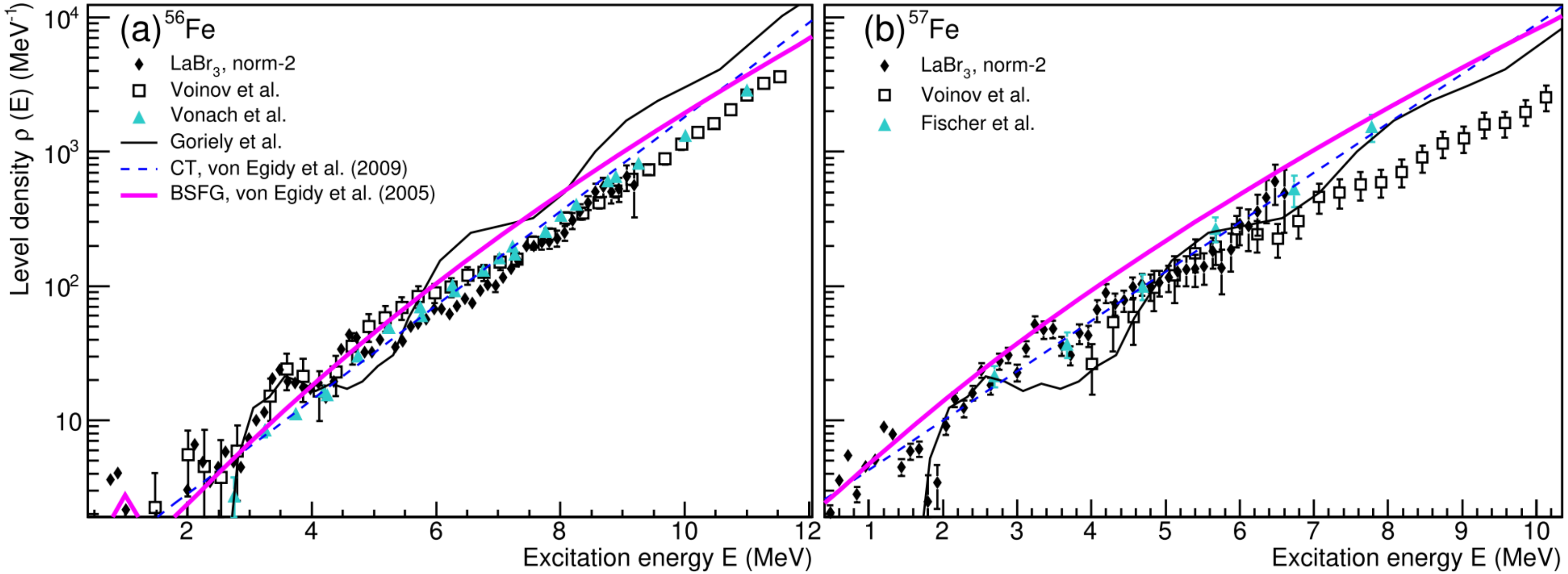
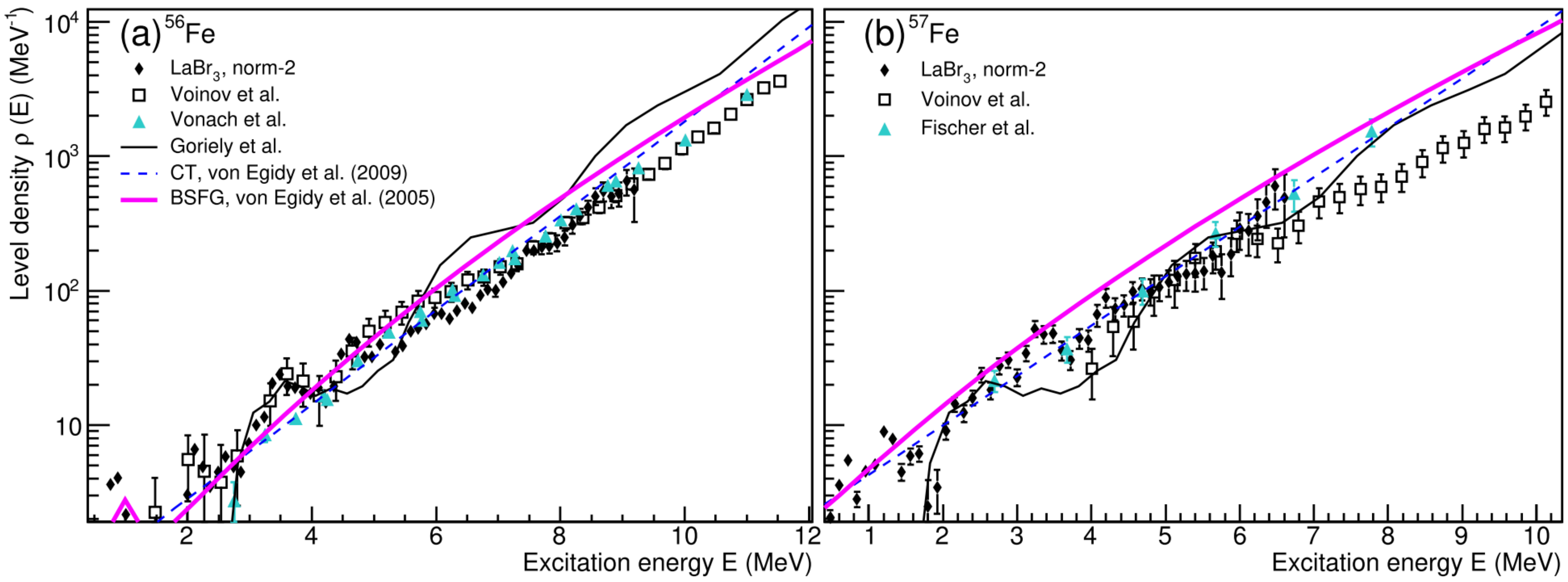
HFB, J+
HFB, J-
56Fe
57Fe
Ratio
ρHFB(J+) / ρHFB(J-)
~15%
~50%!!



3.3. Comparison with theory

Although there are many phenomenological models and some more microscopic calculations available, they typically deviate considerably both in shape and magnitude. In figure 12 a selection of frequently used models are compared to the data. Note that we have used the global parameterization for the NLD models of [40, 41] to test their predicitve power. For the NLD, none of the models reproduce the data over the full energy range. Clearly, only the microscopic approach is able to grasp some of the structures seen in the experimental results. Apparently, all the NLD models overshoot the data at high excitation energy. This could have severe consequences for e.g. calculations of reaction cross sections.

[1] A.C. Larsen et al., J. Phys. G: Nucl. Part. Phys. **44** (2017) 064005



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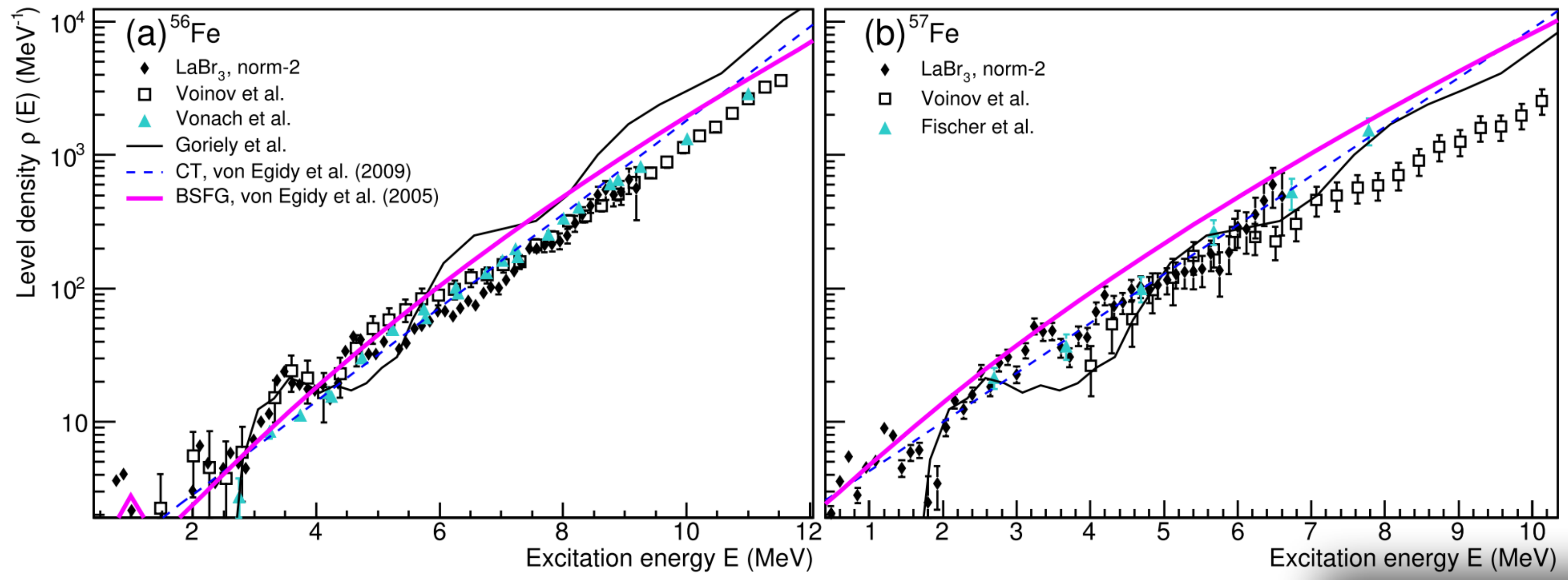

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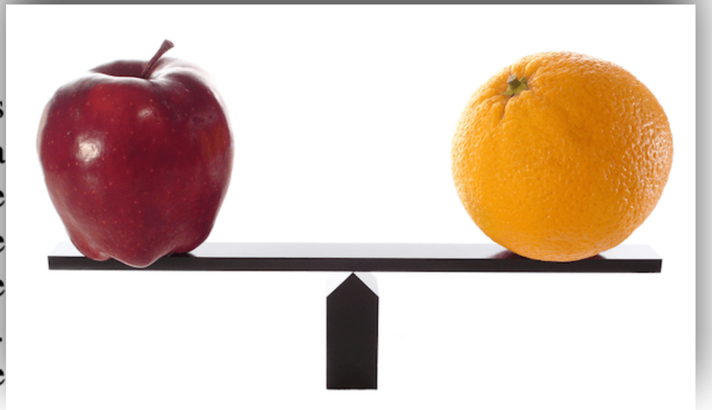

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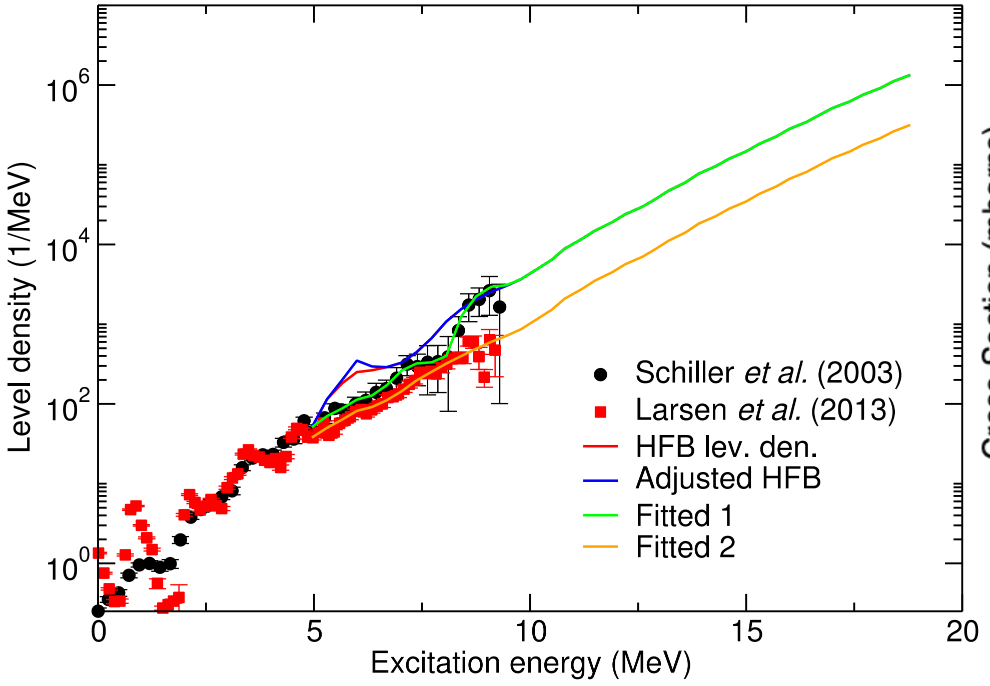
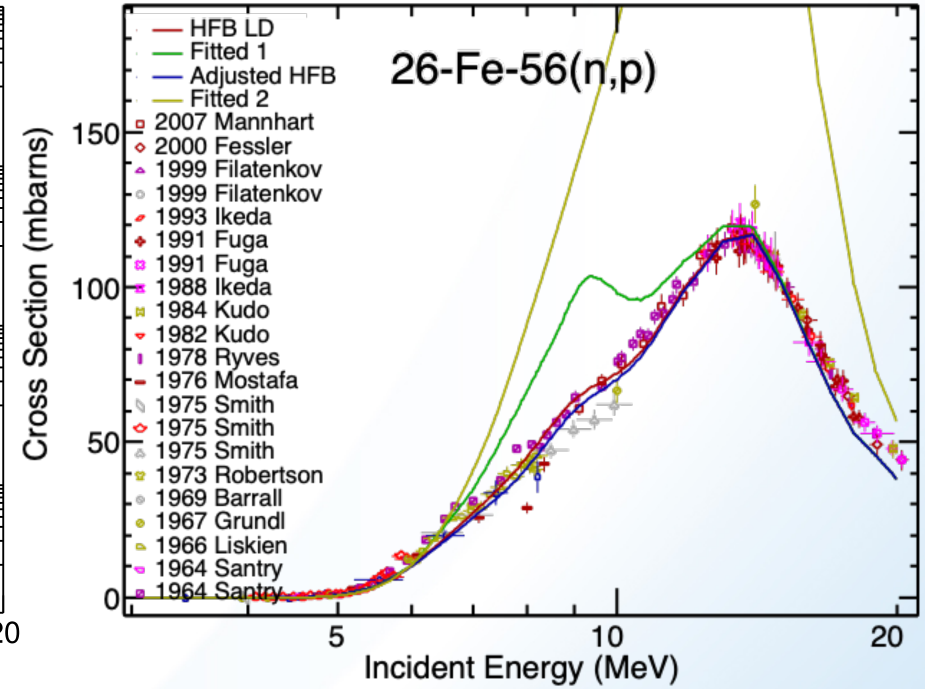
^{56}Fe(n,p) sensitivity to ^{56}Fe lev. den.

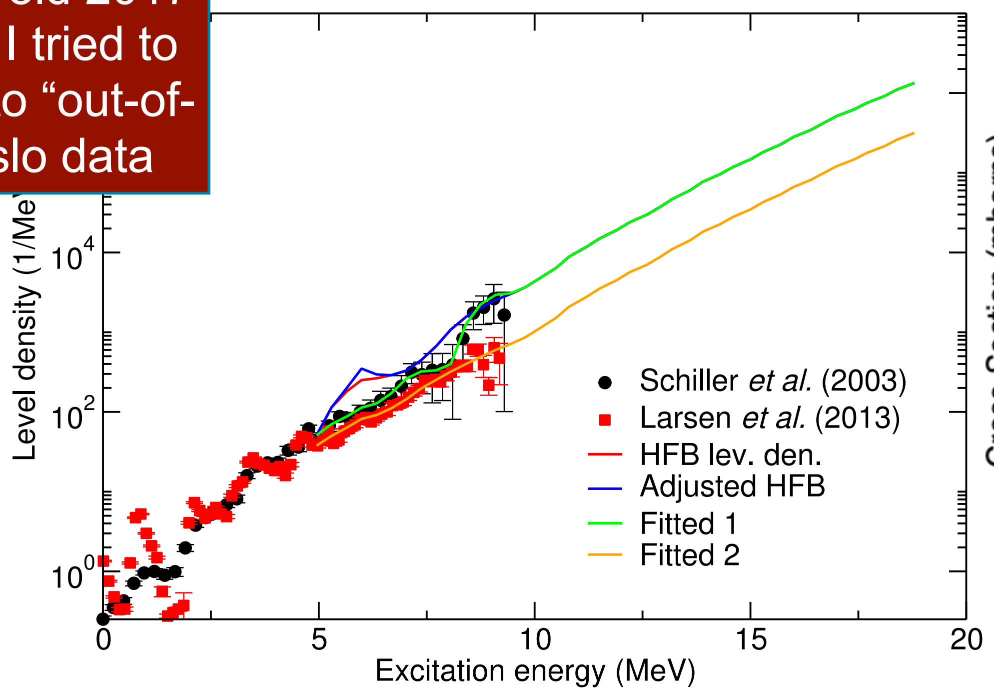


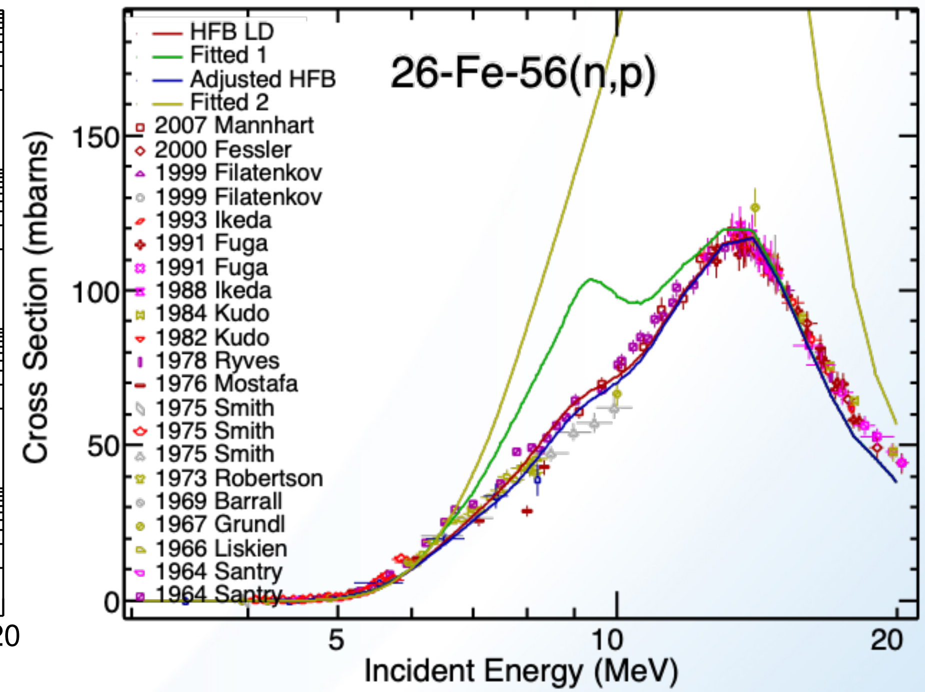


- Also incredibly sensitive to ^{56}Fe level density.
- Center of experimental LD leads to poor (n,p).
- Tweaks on LD can significantly change (n,p).

^{56}Fe(n,p) sensitivity to ^{56}Fe lev. den.

Searched an old 2017 slide, where I tried to fit HFB NLD to “out-of-the-box” Oslo data





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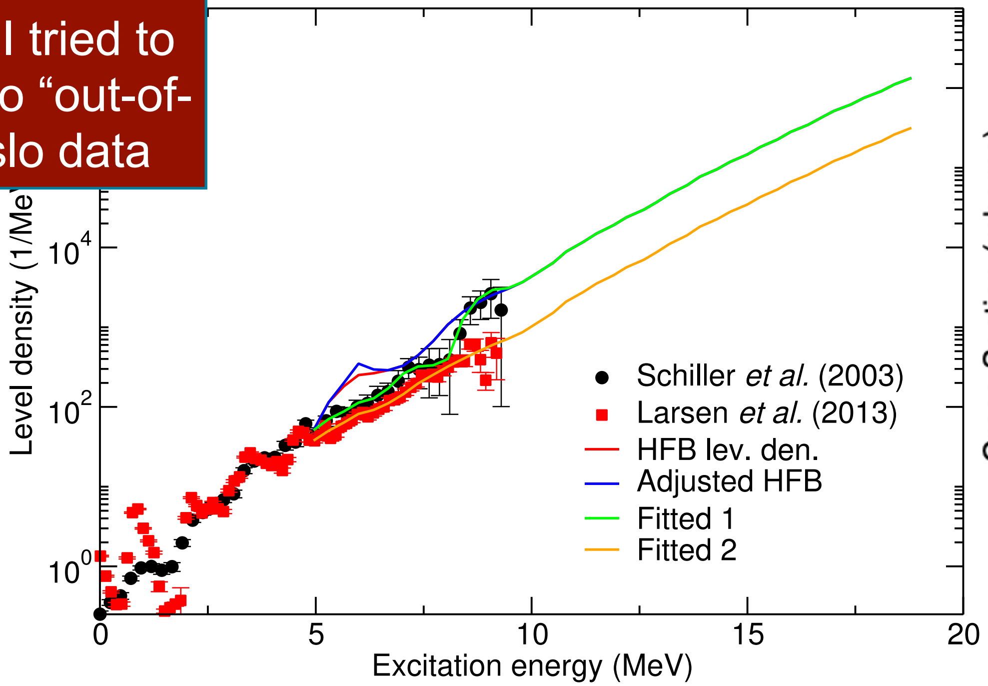

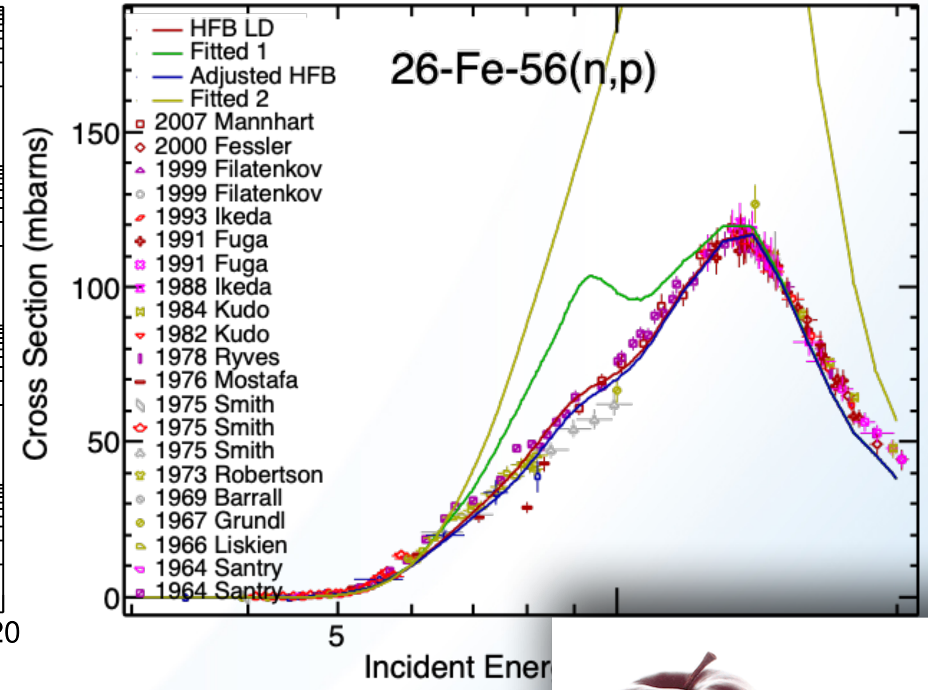

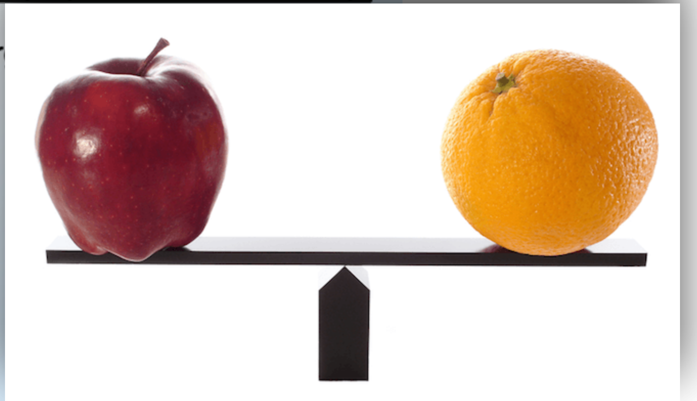

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Experimental NLD data

- There are many methods: Oslo, shape, evaporation, etc…
  - Illustrative example: The Oslo method is great!
    - Has producing a large breath of NLD exp data
    - Well-documented: The website (https://www.mn.uio.no/fysikk/english/research/about/infrastructure/ocl/nuclear-physics-research/compilation/) is a great resource for the NLD data and publications
    - The associated publications are very clear about the assumptions made in each case
    - They are all very reasonable assumptions! (… in a broad perspective.)
    - However, they should NOT be used in reaction calculations, unless the same assumptions are employed!

Nuclear Data question to be answered

What ***exactly*** is the data telling us?

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- Proposal: that we build not only a database of total NLD (which again, are only useful if spin/parity distributions and other model assumptions are consistent), but rather we store **UN**-normalized measured NLD data. This way we can tune NLD models and reaction calculations to the actual measured quantities, even if that can lead to different total NLD.

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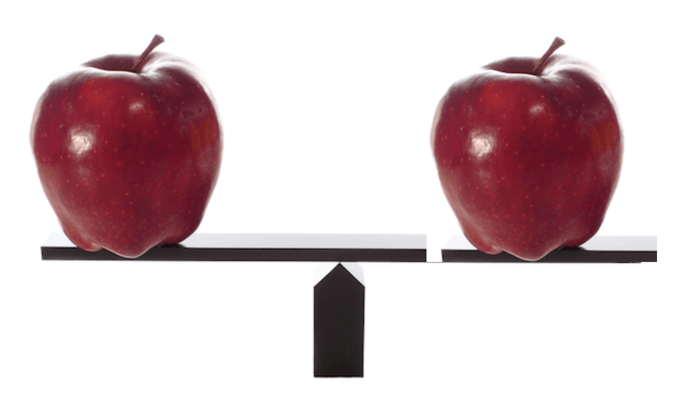

Acknowledgements

This work was supported by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the U.S. Department of Energy. Additionally, work at Brookhaven National Laboratory was sponsored by the Office of Nuclear Physics, Office of Science of the U.S. Department of Energy under Contract No. DE-SC0012704 with Brookhaven Science Associates, LLC. This project was supported in part by the Brookhaven National Laboratory (BNL), National Nuclear Data Center under the BNL Supplemental Undergraduate Research Program (SURP) and by the U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists (WDTS) under the Science Undergraduate Laboratory Internships Program (SULI).

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