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Averaging cross section data so we can fit it

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Averaging cross section data so we can fit it

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(Dated: October 23, 2014)

Make average versions of ^{56}Fe(n,tot), ^{56}Fe(n,el), ^{56}Fe(n,γ) and ^{56}Fe(n,n') cross sections, with some notion of uncertainty estimates.

I. INTRODUCTION

The ^{56}Fe cross section we are interested in have a lot of fluctuations. We would like to fit the average of the cross section with cross sections calculated within EMPIRE [1].

EMPIRE, being a Hauser-Feshbach theory based nuclear reaction code, essentially requires cross sections to be smoothed using a Lorentzian profile. Indeed, most textbooks describing Hauser-Feshbach theory derive it using such a smoothing profile [2]:

$$L(E,E') = \frac{1}{\pi}\frac{I}{(E'-E)^2+I^2}. \tag{1}$$

With this, functions which are analytic in the upper half of the complex E-plane can be averaged with a little bit of complex analysis:

$$\begin{aligned}\langle f(E)\rangle &= \int_{-\infty}^{\infty} dE' L(E,E') f(E') \\ &= f(E+iI)\end{aligned} \tag{2}$$

Here, we will explore various smoothing profiles and demonstrate their practical interchangeability and we will compute the smoothed ^{56}Fe cross sections, with uncertainties.

We plan to fit EMPIRE to these cross sections in the fast region only (say above 500 keV), but use only the part of the EMPIRE calculations above the resolved resonance region. We may also use the angular distributions from EMPIRE through the resonance region provided they behave themselves.

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II. SPECTRUM WEIGHTING

Given a weighting spectrum $\phi(E)$, we intend to average a cross section as follows

$$\langle\sigma\rangle = \int_{E_{\min}}^{E_{\max}} dE\ \phi(E)\sigma(E) \tag{3}$$

In this note, weighting spectrum is really a smoothing profile of some sort. We assume the weighting spectrum is normalized over the integration region defined here so

$$\int_{E_{\min}}^{E_{\max}} dE\ \phi(E) = 1 \tag{4}$$

To compute the uncertainty, we resort to the basis function expansion of the covariance as follows:

$$\Delta^2\sigma(E,E') = \sum_{ij} \Delta^2\sigma_{ij} B_i(E) B_j(E') \tag{5}$$

In the ENDF format, all covariances are assumed to be grouped in energy so the basis functions are simple window functions:

$$B_i(E) = \begin{cases} 1 & E_i \le E \le E_{i+1} \\ 0 & \text{otherwise} \end{cases} \tag{6}$$

This basis is an orthogonal basis, with the inverse being $B_i^{-1}(E) = (E_{i+1}-E_i)^{-1} B_i(E)$.

With this, the uncertainty of the average cross section is

$$\begin{aligned}\delta\langle\sigma\rangle &= \sqrt{\int dE dE' \phi(E)\phi(E')\Delta^2\sigma(E,E')} \\ &= \sqrt{\textstyle\sum_{ij} \Delta^2\sigma_{ij} \langle B_i\rangle \langle B_j\rangle}\end{aligned} \tag{7}$$

In general, the covariance between two different weighting spectra (e.g. the smoothing function evaluated at too different energies) can also be computed, but as it can not be currently used in the fitting in Sam's code, we won't compute it here.

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Lorentzian:	$L(E,E') = \frac{1}{\pi}\frac{I}{(E'-E)^2+I^2}$
Gaussian:	$G(E,E') = \frac{1}{I\sqrt{2\pi}}\exp\left[-\frac{(E-E')^2}{2I^2}\right]$
Window:	$W(E,E') = \begin{cases} 1/I & \lvert E-E'\rvert \le I \\ 0 & \text{otherwise} \end{cases}$

TABLE I. Smoothing profiles considered in this work.

III. INSENSITIVITY TO SMOOTHING PROFILE

We now use the results from the previous section to smooth cross sections. We consider the three separate smoothing profiles in Table I. All of these profiles are normalized over the entire real axis. Only positive valued of energy are physically relevant. Furthermore, the data tables we intend to average only span a limited range of energies. However, all of the smoothing profiles are very narrow so truncating the averaging integrals over a finite range much larger than each smoothing profiles intrinsic length scale I is a reasonable approximation. Fig. 1 shows the smoothed capture cross section for ^{56}Fe showing the good agreement between smoothing with Gaussian and Lorenzian profiles.

We also applied the smoothing to the total and elastic cross sections. Here the two smoothing profiles gave comparable results. In Fig. 2 we see the elastic cross section in the range 500 keV to 1.8 MeV. We first note that the ENDF file does not provide covariance for the cross section above 900 keV. The total cross section is shown in 3. Here the uncertainties are given over the entire cross section and the smoothed results are in excellent agreement.

Due to an undiagnosed bug in our averaging code, the window smoothing function could not be used. Since we had no intention of ever using it in practice, we have not expended the effort to get this piece of code functioning.

IV. SMOOTHING CROSS SECTIONS FROM CIELO STARTER FILE

The CIELO starter file from Luiz Leal includes a resolved resonance region given using the LRF=7 option, that is, using the R-matrix limited format. It includes resonances for (n,γ), $(n,$,el), $(n$,tot) and (n,n_1') up to 2 MeV. Given that there are 20 resonances within each 200 keV window in the region from 500 keV-2 MeV, we think it is reasonable to shrink the averaging width to $I = 100$ keV. This will allow us to approach the discontinuity in the capture cross section as well as the thresholds in the inelastic cross sections.

V. OVERVIEW OF THE GEEL INELASTIC SCATTERING DATA

We now compare the Geel results to the CIELO starter file. Figs 4–6 show the total inelastic cross section. Clearly the ENDF file compares favorably to the Geel data. The ENDF file also appears to correctly represent the pre-equilibrium contribution to the cross section as we see from agreement with other data at the 14 MeV point. Figs. 7–8 compare the cross sections for the first few excited states. Clearly good agreement is maintained for these levels. Curiously there is a gap in the Geel data in that there is apparently not an MT=56 file corresponding to the sixth excited state. Figs. 9 compare the seventh through the eleventh excited state cross sections. Here the impressive agreement between the Geel data and ENDF breaks down.

In an effort to diagnose the source of the large disagreement, we queried the ENSDF database [8]. The sixth excited state of ^{56}Fe has $E_6 = 3.0762$ MeV, $J^\Pi = 3^-$ and has an unknown lifetime. It was not included in the ENDF evaluation and it was not measured in the Geel data. It is then reasonable to assume that the MT indexing in the Geel data should be shifted down by one unit starting with MT=57. Fig. 10 shows what happens when we do this shift. Overall, the agreement between the Geel data and ENDF is now quite impressive.

VI. SMOOTHING THE GEEL INELASTIC SCATTERING DATA

We now turn to producing smoothed versions of the inelastic cross section data. This is problematic because of the presence of a threshold (see the carton in Fig. 11). In the figure, the solid line is meant to represent the actual cross section near threshold. Were we to average this, two things would happen:

- Above but very close to threshold, the low energy Lorenzian (or Gaussian) tail would be averaged with zero, lowering the average cross section needlessly.

- Below but very close to threshold, the high energy Lorenzian (or Gaussian) tail would be averaged with the non-zero above threshold cross section, leading to a non-zero and unphysical cross section below threshold.

This is illustrated in the dotted line in Fig. 11. A similar problem exists at the end of the Geel datasets as the smoothing will attempt to average the cross section with the off-the-end-of-the-table cross section.

This is not a problem in Hauser-Feshbach theory since only OMP things are averaged (in this case, the absorption cross section and transmission coefficients). The transmission coefficients go to zero at $E = 0$, but are shifted in argument up to the threshold of a reaction to

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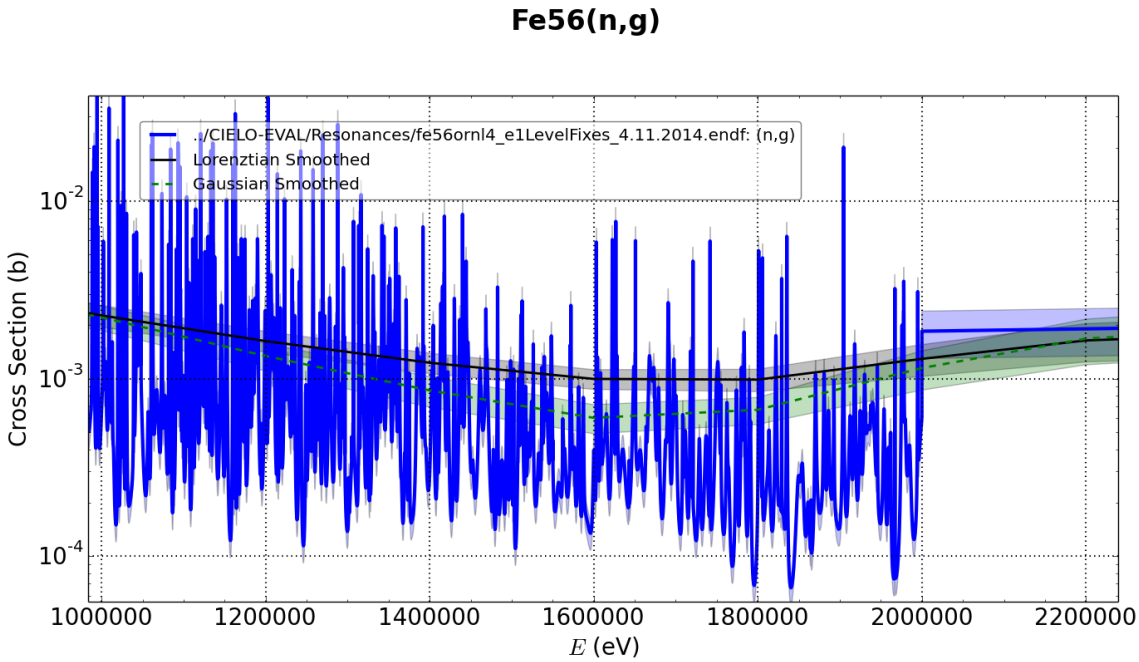

FIG. 1. Comparison of the effects of various smoothing profiles. In all cases, the intrinsic smoothing scale I is set to 200 keV. Note that both smoothing profiles are non-local in that they have large tails. This accounts for the slow relaxation to the average cross section in the region 800 keV to 2 MeV.

ensure that the correct threshold behavior is given. In this way, they are both smoothed correctly and are zero at threshold. Starting from Geel data or from the ENDF file itself, we do not have this luxury.

To combat this problem, we will not smooth the threshold cross sections within the vicinity of the threshold, as denoted by the exclusion zone in Fig. 11. To determine the smoothed cross section near the threshold, we resort to physical reasoning and common sense. In Ref. [3], Satchler argues that the near threshold cross section for inelastic scattering should be proportional to the outgoing neutron velocity. Therefore, we expect

$$\sigma(E) \propto (E - E_{th})^{1/2} \tag{8}$$

So, as a practical solution, we will match the constant of proportionality in Eq. (8) to the smoothed cross section at the upper energy cut off of the exclusion zone. In this way, we will have a smooth cross section down to the threshold. We also have an estimate of the uncertainty in the constant of proportionality from the smoothing procedure itself.

We choose the energy cut off to be at least $2I$ from the threshold (or other dangerous feature, like the end of the dataset). There is a mathematical motivation for this choice. Namely, inserting energies $E = E' + nI$ into a Lorenzian centered at E', we find:

$$L(E = E' + nI, E') = \frac{1}{\pi} \frac{I}{(E' + nI - E')^2 + I^2} \tag{9}$$

$$= \frac{1}{\pi I^2 (n^2 + 1)} \tag{10}$$

so for $n = 2$, the height of the Lorenzian has dropped by a factor of 5. Going at least $3I$ from features means the Lorenzian would be down by a factor of 10, but the Geel data doesn't span a large enough energy range to make this practical. See Fig. 12 for a sample of results using Lorenztian smoothing on these threshold reactions. We note that for higher levels, the energy window of usable experimental data is shrinking so the Lorentzian tails are being averaged with zeros, lowering the entire curve. This is especially noticeable with the I=200 keV cause as it has the longest tails.

Gaussians are maybe a better choice since their tails are not as long as a Lorenzian. Indeed, with a Gaussian, moving $2I$ out means the smoothing function has dropped to 13% of the peak value and moving to $2.5I$, the function drops to 5% of the peak. Fig. **??** shows the results with Gaussian smoothing and these results seem quite acceptable.

VII. SMOOTHING THE ENDF MT=51 INELASTIC SCATTERING DATA

So that we have a set of data directly from the ENDF file resonance region for MT=51, I averaged it too.

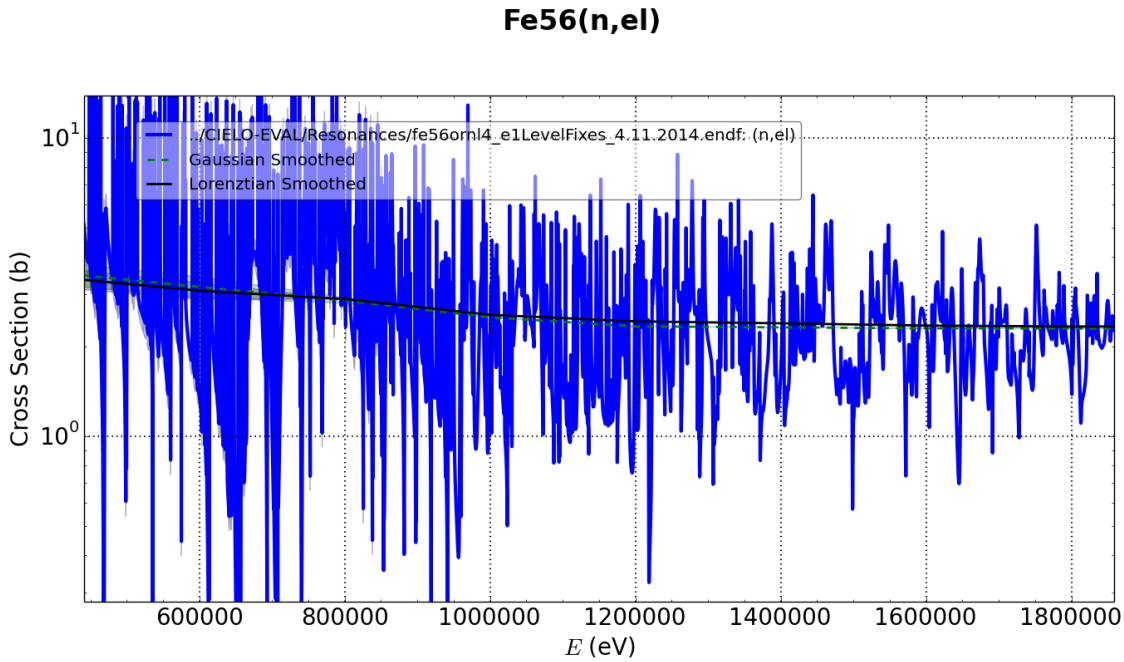

FIG. 2. Comparison of the effects of various smoothing profiles on the elastic cross section. In all cases, the intrinsic smoothing scale I is set to 200 keV.

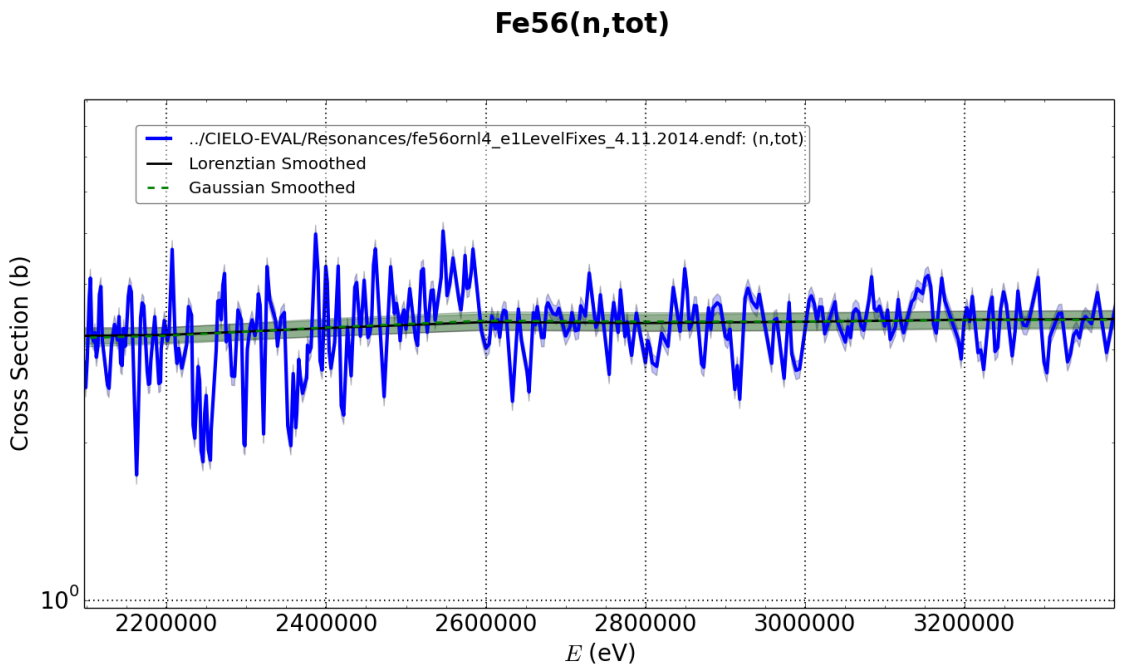

FIG. 3. Comparison of the effects of various smoothing profiles on the total cross section. In all cases, the intrinsic smoothing scale I is set to 200 keV.

VIII. SMOOTHING ANGULAR DISTRIBUTIONS

It is recognized that the angular distributions of both the elastic and first few inelastic cross sections have a large impact on neutron leakage. In the CIELO starter ENDF file, the resonances are given in the LRF=7 format, so they contain enough information to reconstruct the entire neutron angular distributions for MT=2 and 51.

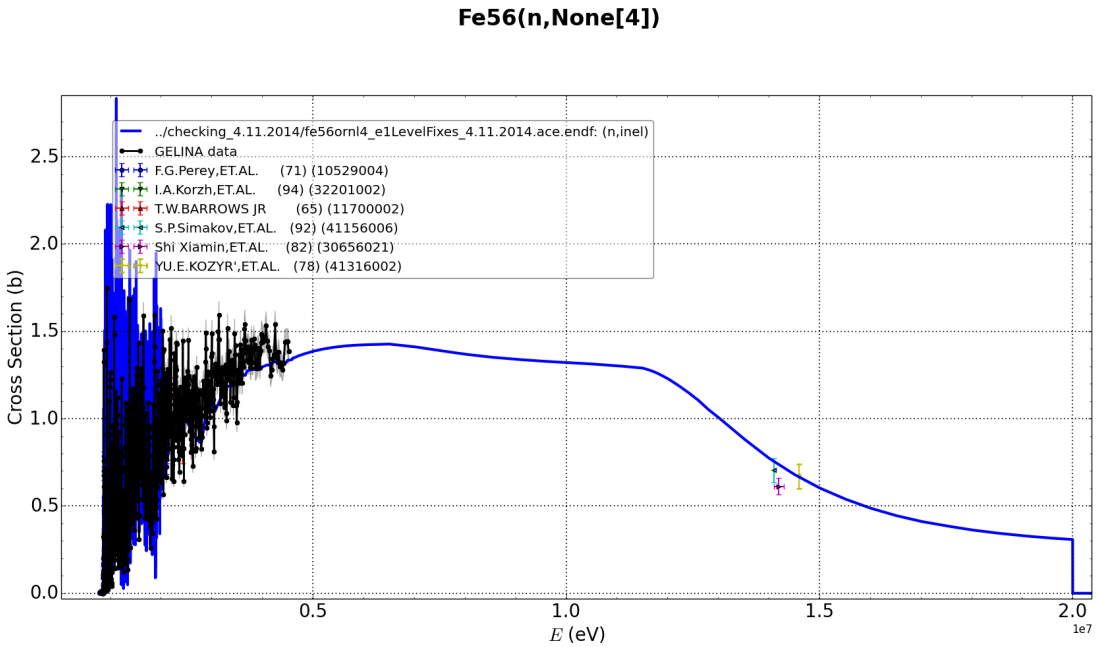

FIG. 4. Comparison of ENDF total inelastic cross section to that inferred by the Gelina experiment.

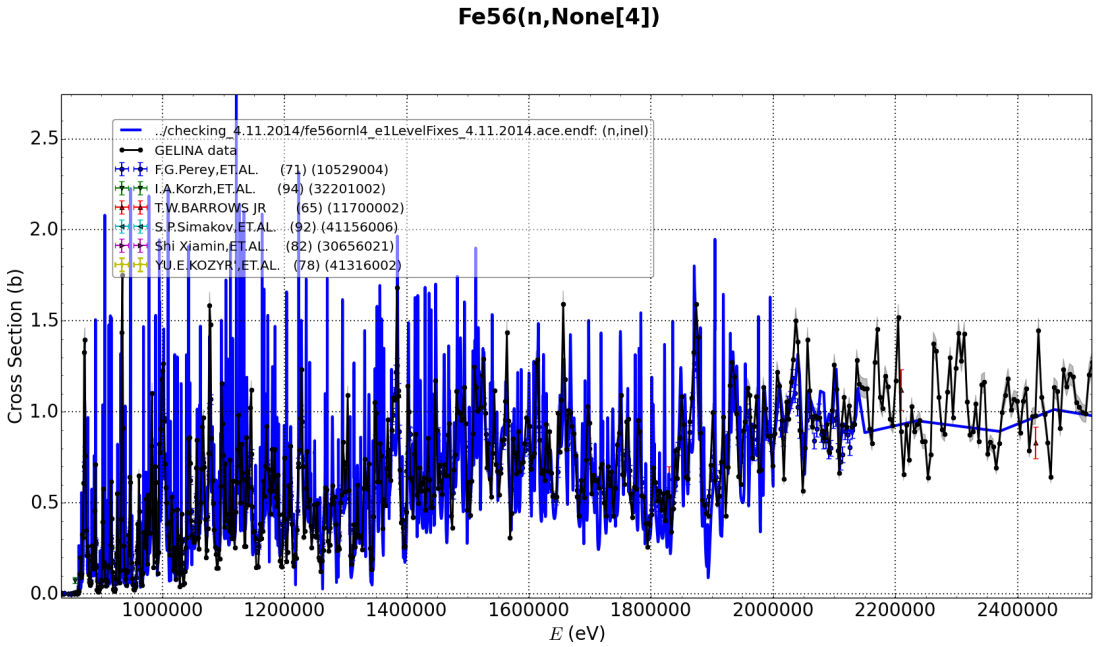

FIG. 5. Zoomed view of the comparison of ENDF total inelastic cross section to that inferred by the Gelina experiment.

We have asked Luiz Leal (ORNL) and Skip Kahler (LANL) to provide the angular distributions as computed by NJOY2012 (and SAMMY?). Unfortunately, both files are impractically large (17 Mb in one case), all due to the large number of incident energies needed to store the angular distributions with the same fidelity as the reconstructed resonance cross sections. It is unclear whether this high a resolution angular distributions are needed in practice and, more importantly for our modeling purposes, we cannot make a direct comparison of the reconstructed angular distributions to EMPIRE calculations. We must smooth them just as we have for the cross sections in order to compare.

The MT=4 distributions represent the angular proba-

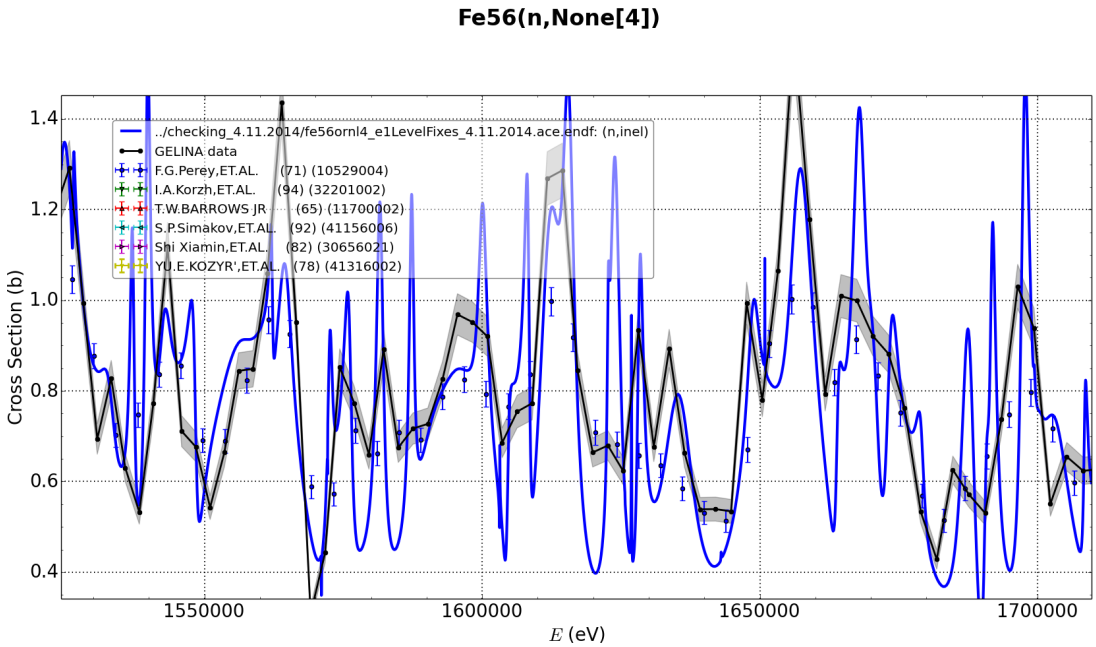

FIG. 6. Another zoomed view of the comparison of ENDF total inelastic cross section to that inferred by the Gelina experiment.

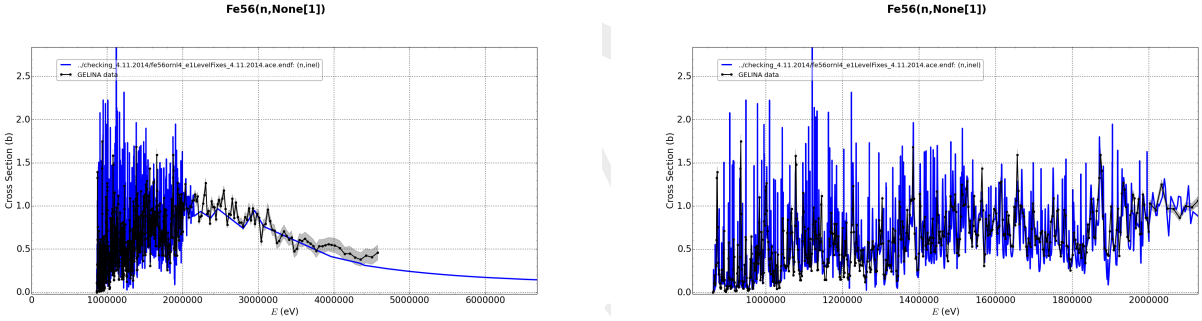

FIG. 7. Comparison of ENDF inelastic to the first excited state cross section to that inferred by the Gelina experiment. The lower panel shows a close up of the structure from 1-2 MeV.

bility distribution $P(\mu = cos(\theta)|E)$, given in the center of mass frame of the neutron-target system. In the CIELO starter files, they are expanded in Legendre moments:

$$\frac{d\sigma(E)}{d\Omega} = \frac{1}{4\pi}\sigma(E)P(\mu|E) = \frac{\sigma(E)}{4\pi}\sum_{L=0}^{\infty} P_L(\mu)C_L(E) \tag{11}$$

To smooth these distributions, we do

$$\left\langle \frac{d\sigma(E)}{d\Omega} \right\rangle = \frac{1}{4\pi}\sum_{L=0}^{\infty} P_L(\mu)\left\langle \sigma(E)C_L(E)\right\rangle \tag{12}$$

We assume that the smoothed cross section and angular distribution factorize:

$$\left\langle \frac{d\sigma(E)}{d\Omega} \right\rangle \approx \frac{\langle\sigma(E)\rangle}{4\pi}\sum_{L=0}^{\infty} P_L(\mu)\left\langle C_L(E)\right\rangle \tag{13}$$

This allows us to smooth the individual MT=4 Legendre moments as a function of incident energy. Note, the $L = 0$ term is trivial as $C_{L=0} = 1$.

As with the cross section data, we must take care new thresholds and at the end of the data tables. In the CIELO starter files, the MT=4 distributions end at the end of the resolved resonance region, at 2 MeV. Within $2I$ of 2 MeV, the smoothing gives meaningless results. Since the angular distributions must be isotropic exactly at threshold, all of the smoothed distributions must approach zero within $2I$ of inelastic threshold. Therefore, we remove all values from the smoothed tables below $2I$ of the threshold and linear interpolate from this cut-off point down to threshold. Figs. 15–fig:MT51AngleDist show the results of this smoothing exercise using the Gaussian smoothing profile and $I = 100$ keV.

In examining these figures, a few things are apparent. First, due to the couplings of the angular momenta of the

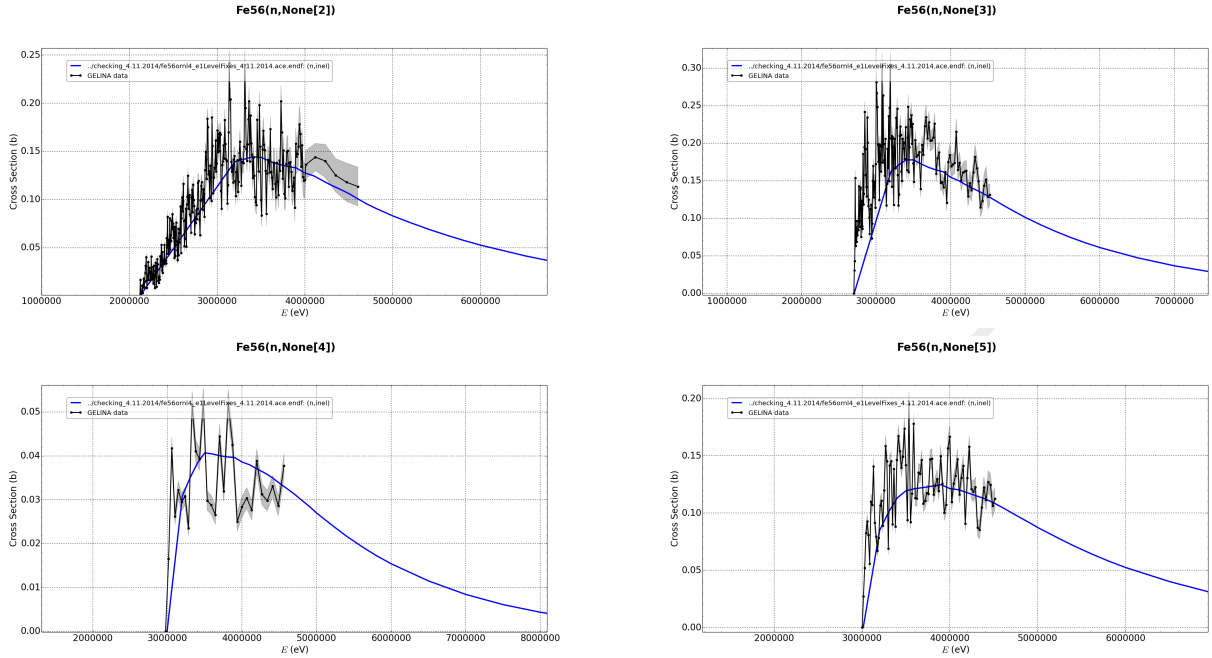

FIG. 8. Comparison of ENDF inelastic to the second through fifth excited state cross sections to that inferred by the Gelina experiment.

resonances, we find angular moments only up to $L = 6$. Second, the even L angular moments should be directly comparable to the EMPIRE calculations as compound nuclear reactions only generate forward-backward symmetric distributions. Looking at the MT=51 curves, they are already nearly isotropic on average and clearly the even L moments are larger than the nearest odd ones. For the MT=2 curves, the situation is not so straightforward. While we see a neat ordering of coefficients going from $L = 1$ to $L = 6$, clearly the odd moments are comparable to the even ones so the reaction will not be neatly described by the compound elastic results. Hopefully the shape elastic angular distributions will take care of ensuring proper agreement.

IX. RECOMMENDED FILES

Here I'll list the recommended files for fitting with EMPIRE.

For the (n, γ), $(n,$,el) and $(n,$tot) reactions, which have a mostly smooth envelope and sharp features, I recommend using the Lorentzian averaged values with $I = 100$ keV. This is the most mathematically correct way of averaging (as far as the optical model is concerned). The files are as follows:

- `endf_MT1_100keV_lorentzian.xydy.dat`: The smoothed total cross section, smoothed with a Lorentzian profile and $I = 100$ keV
- `endf_MT2_100keV_lorentzian.xydy.dat`: The smoothed elastic cross section, smoothed with a Lorentzian profile and $I = 100$ keV
- `endf_MT102_100keV_lorentzian.xydy.dat`: The smoothed capture cross section, smoothed with a Lorentzian profile and $I = 100$ keV

Note: do not use these data below roughly $2 * I = 200$ keV as the average will have a lot of "pollution" from the thermal region.

For fitting the discrete level excitation data, I do not recommend using any of the Lorentzian averaged data. The tails are too long and result in odd average behavior on either end of the fitting interval. I recommend instead using the Gaussian averaged versions. Whether we should use the $I = 100$ keV or 200 keV versions really depends on the threshold behavior and how much structure in the data should be resolved. My recommendations are:

- `geel_smoothed_200keV_MT51_846keV.xydy.dat`: The smoothed MT=51 inelastic cross section, smoothed with a Gaussian profile and $I = 200$ keV
- `geel_smoothed_200keV_MT52_2085keV.xydy.dat`: The smoothed MT=52 inelastic cross section, smoothed with a Gaussian profile and $I = 200$ keV
- `geel_smoothed_100keV_MT53_2657keV.xydy.dat`: The smoothed MT=53 inelastic cross section, smoothed with a Gaussian profile and $I = 100$ keV
- `geel_smoothed_200keV_MT54_2941keV.xydy.dat`: The smoothed MT=54 inelastic cross section, smoothed with a Gaussian profile and $I = 200$ keV

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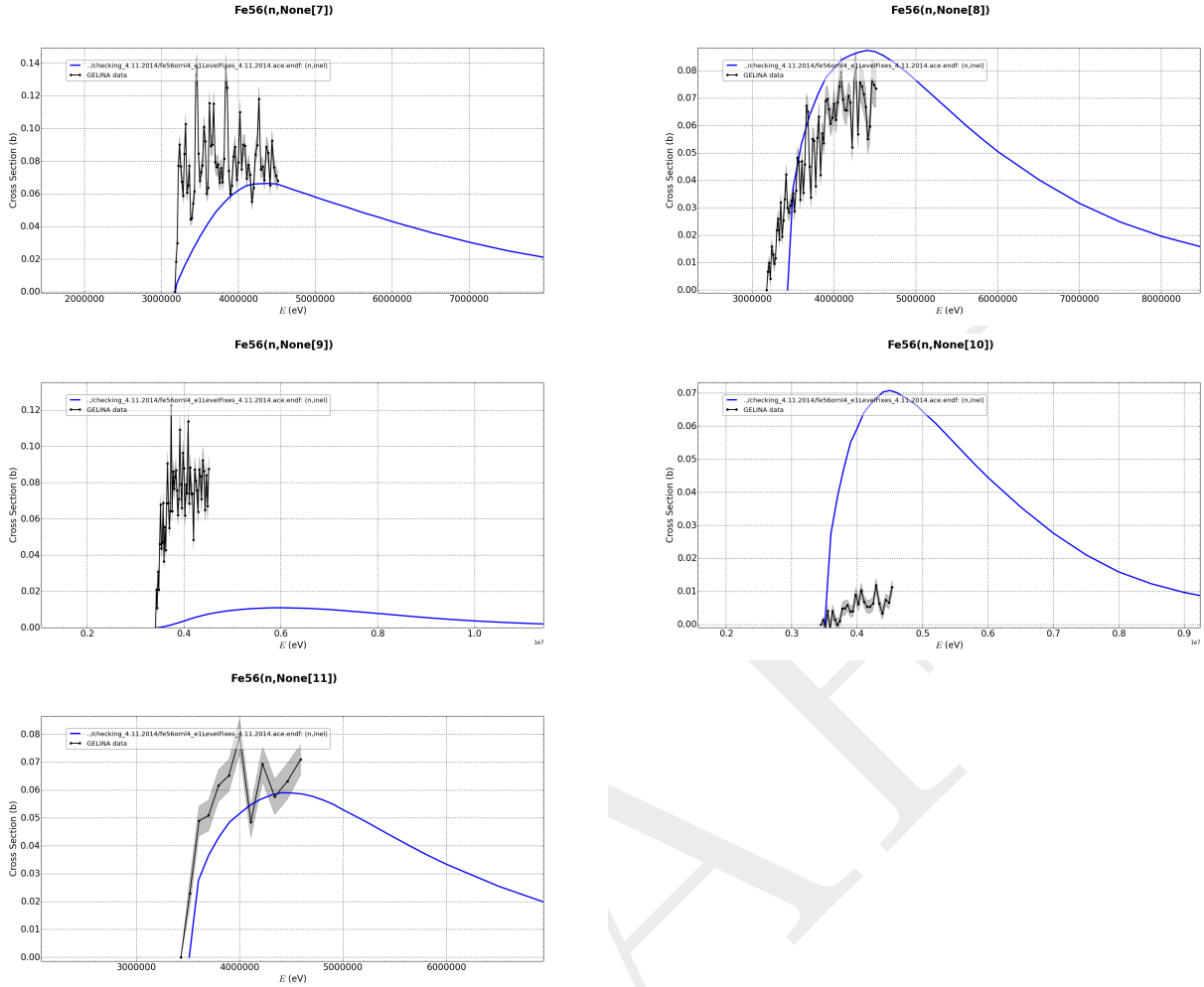

FIG. 9. Comparison of ENDF inelastic to the seventh through eleventh excited state cross sections to that inferred by the Gelina experiment.

- `geel_smoothed_100keV_MT55_2959keV.xydy.dat`: The smoothed MT=55 inelastic cross section, smoothed with a Gaussian profile and $I = 100$ keV
- `geel_smoothed_100keV_MT56_3120keV.xydy.dat`: The smoothed MT=56 inelastic cross section, smoothed with a Gaussian profile and $I = 100$ keV
- `geel_smoothed_200keV_MT57_3122keV.xydy.dat`: The smoothed MT=57 inelastic cross section, smoothed with a Gaussian profile and $I = 200$ keV
- `geel_smoothed_100keV_MT58_3369keV.xydy.dat`: The smoothed MT=58 inelastic cross section, smoothed with a Gaussian profile and $I = 100$ keV
- `geel_smoothed_100keV_MT59_3388keV.xydy.dat`: The smoothed MT=59 inelastic cross section, smoothed with a Gaussian profile and $I = 100$ keV
- `geel_smoothed_100keV_MT60_3445keV.xydy.dat`: The smoothed MT=60 inelastic cross section, smoothed with a Gaussian profile and $I = 100$ keV

None of these files should be used past 4 MeV for two reasons: the Geel data starts being too high here and it is just before the data runs out causing problems with the smoothing.

For matching the final fitted MT=51 curve onto a smoothed version of Luiz's resolved resonances, I recommend using:

- `endf_smoothed_100keV_MT51_lorentzian.xydy.dat`: The smoothed MT=51 inelastic cross section, smoothed with a Lorentzian profile and $I = 100$ keV

The other variations of this curve are either too sensitive to the fine structure of the resonance data (`endf_smoothed_100keV_MT51_gaussian.xydy.dat` and `endf_smoothed_200keV_MT51_gaussian.xydy.dat`) or not sensitive enough (`endf_smoothed_200keV_MT51_lorentzian.xydy.dat`).

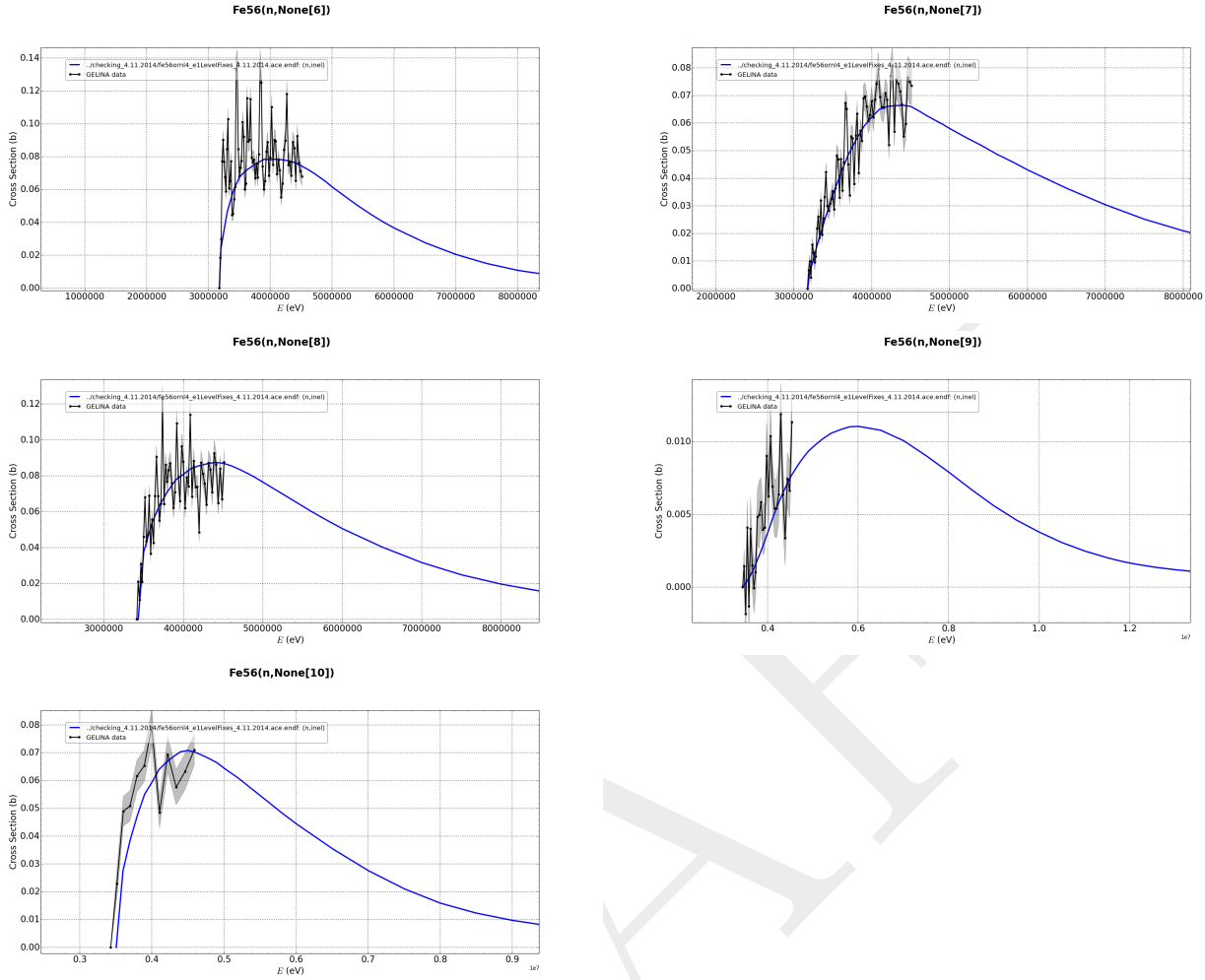

FIG. 10. Comparison of ENDF inelastic to the seventh through eleventh excited state cross sections to that inferred by the Gelina experiment, after reindexing the MT values of the Gelina files.

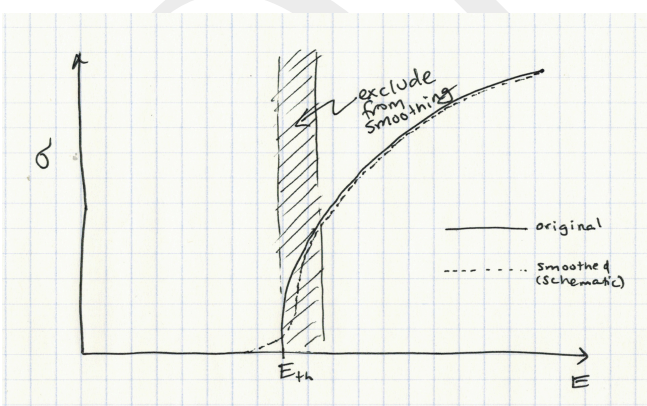

FIG. 11. Strategy for smoothing an inelastic cross section. Here we exclude fitting near the threshold so as to avoid the behavior of the smoothed cross section in the dotted curve.

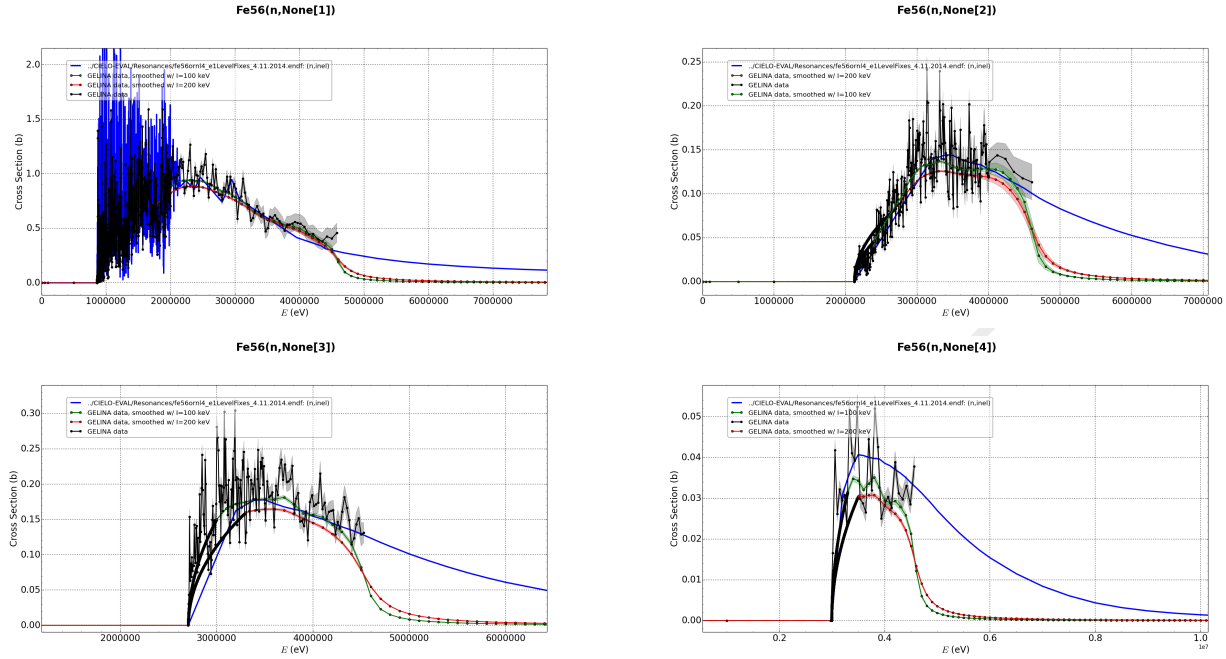

FIG. 12. Smoothing the Geel data with Lorenzians width 100 keV and 200 keV.

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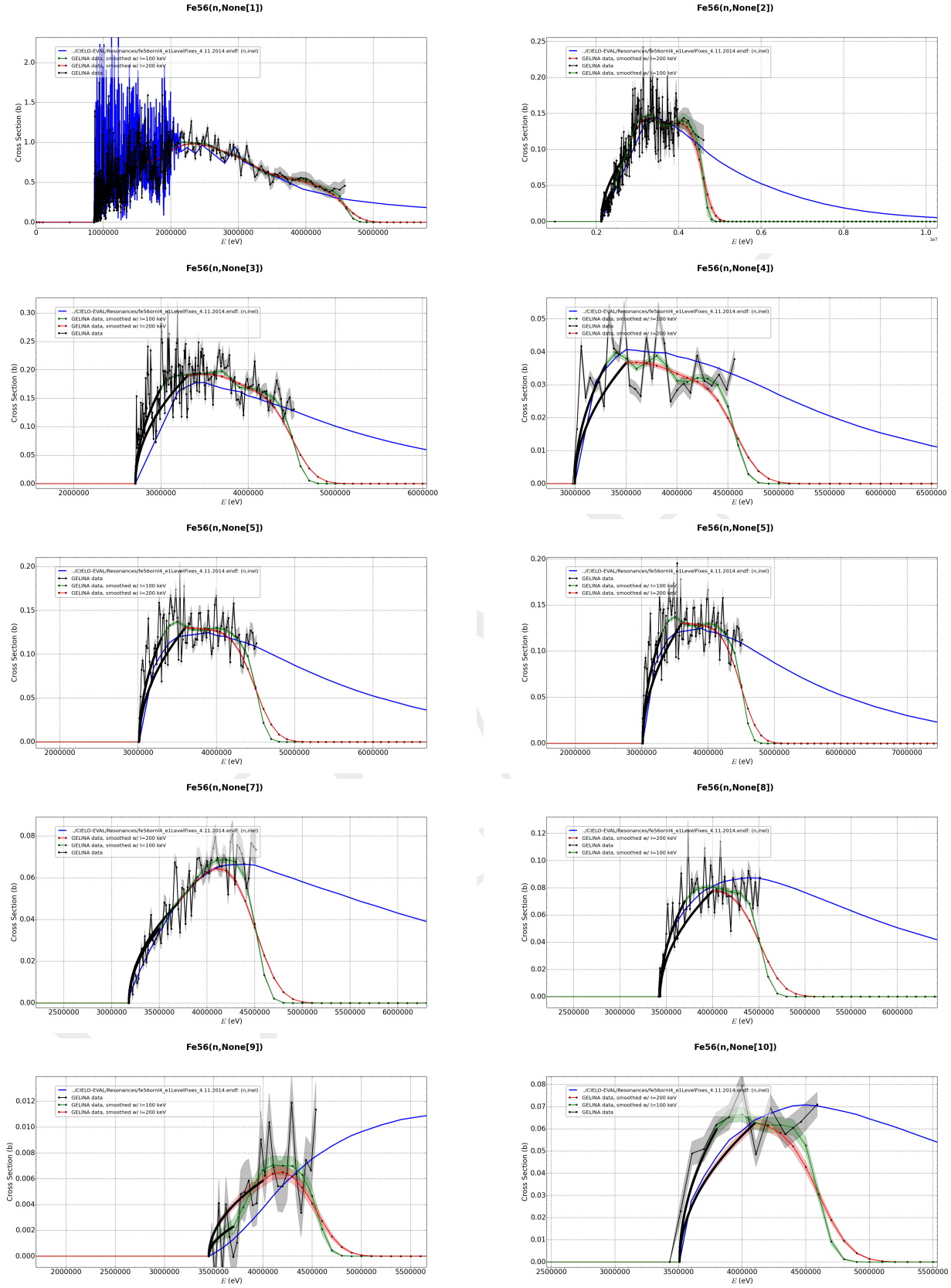

FIG. 13. Smoothing the Geel data with Gaussian width 100 keV and 200 keV.

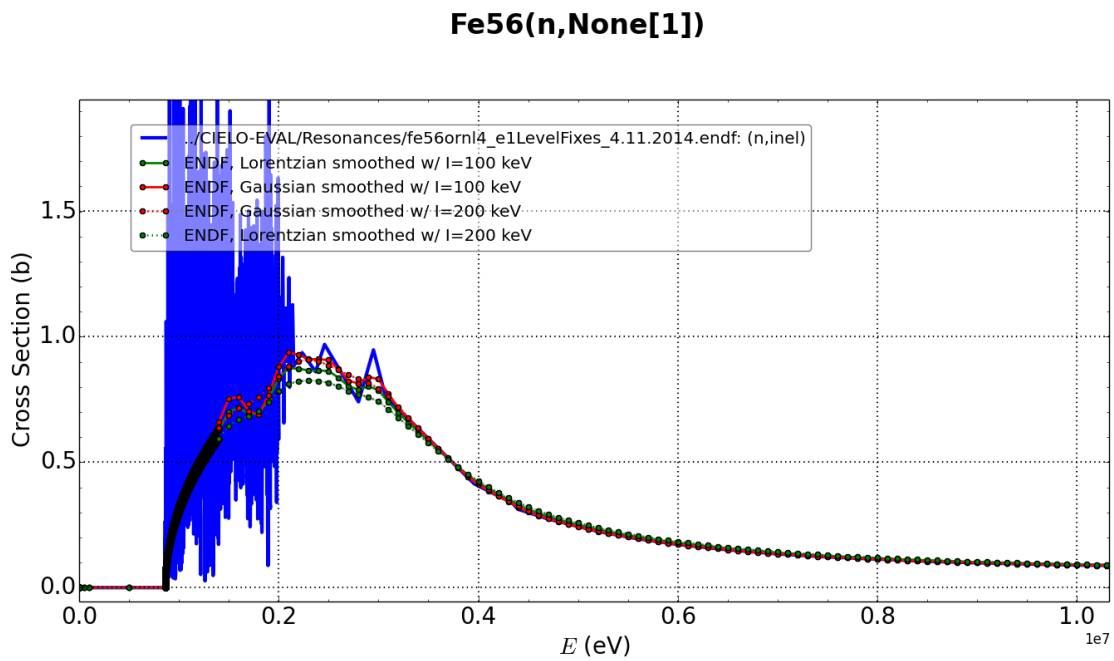

FIG. 14. ENDF file resonance region for MT=51, smoothed a bunch of different ways.

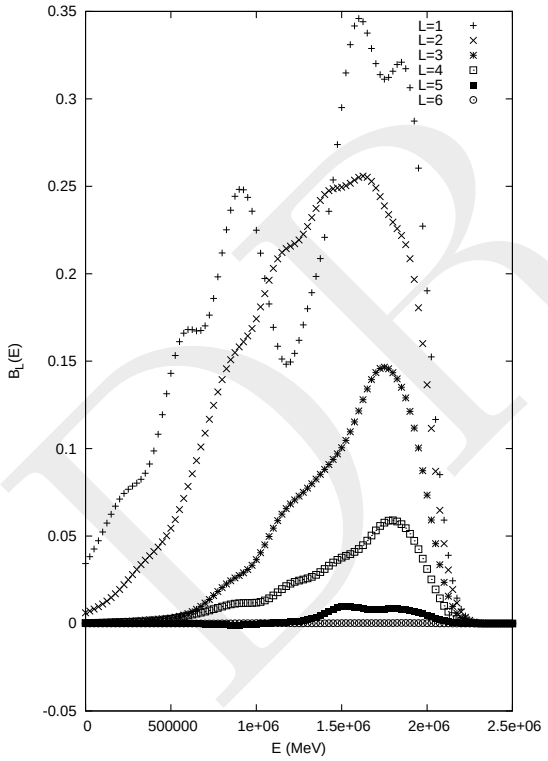

FIG. 15. Results of smoothing the (n,el) angular distribution from the CIELO starter file using a Gaussian smoothing profile with $I = 100$ keV.

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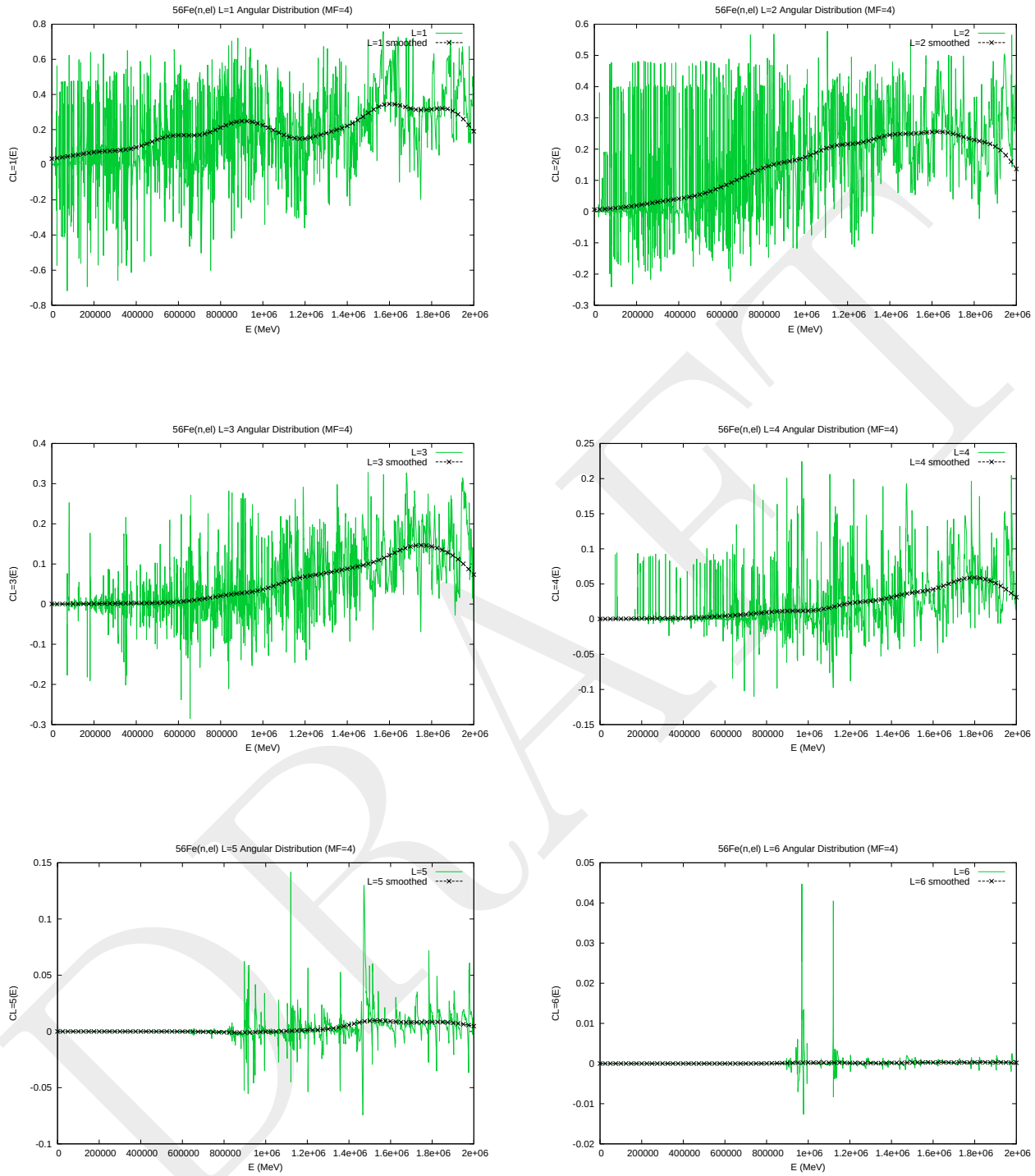

FIG. 16. Results of smoothing the (n,el) angular distribution from the CIELO starter file, compared to the original reconstructed resonance angular distribution.

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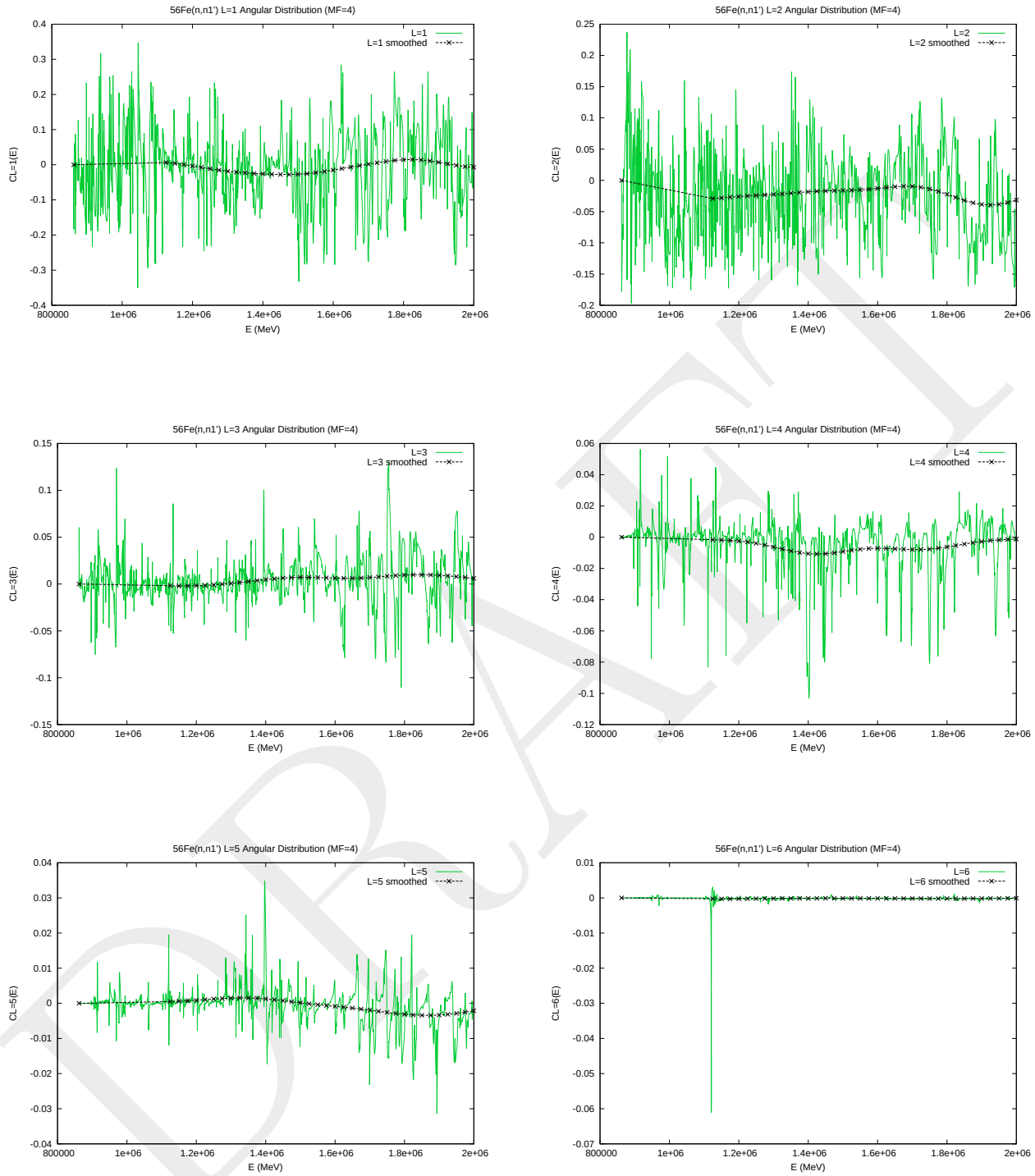

FIG. 17. Results of smoothing the (n,n$'_1$) angular distribution from the CIELO starter file, compared to the original reconstructed resonance angular distribution.

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