Possible agenda for systematic code-comparison to resolve RAC/EDA differences

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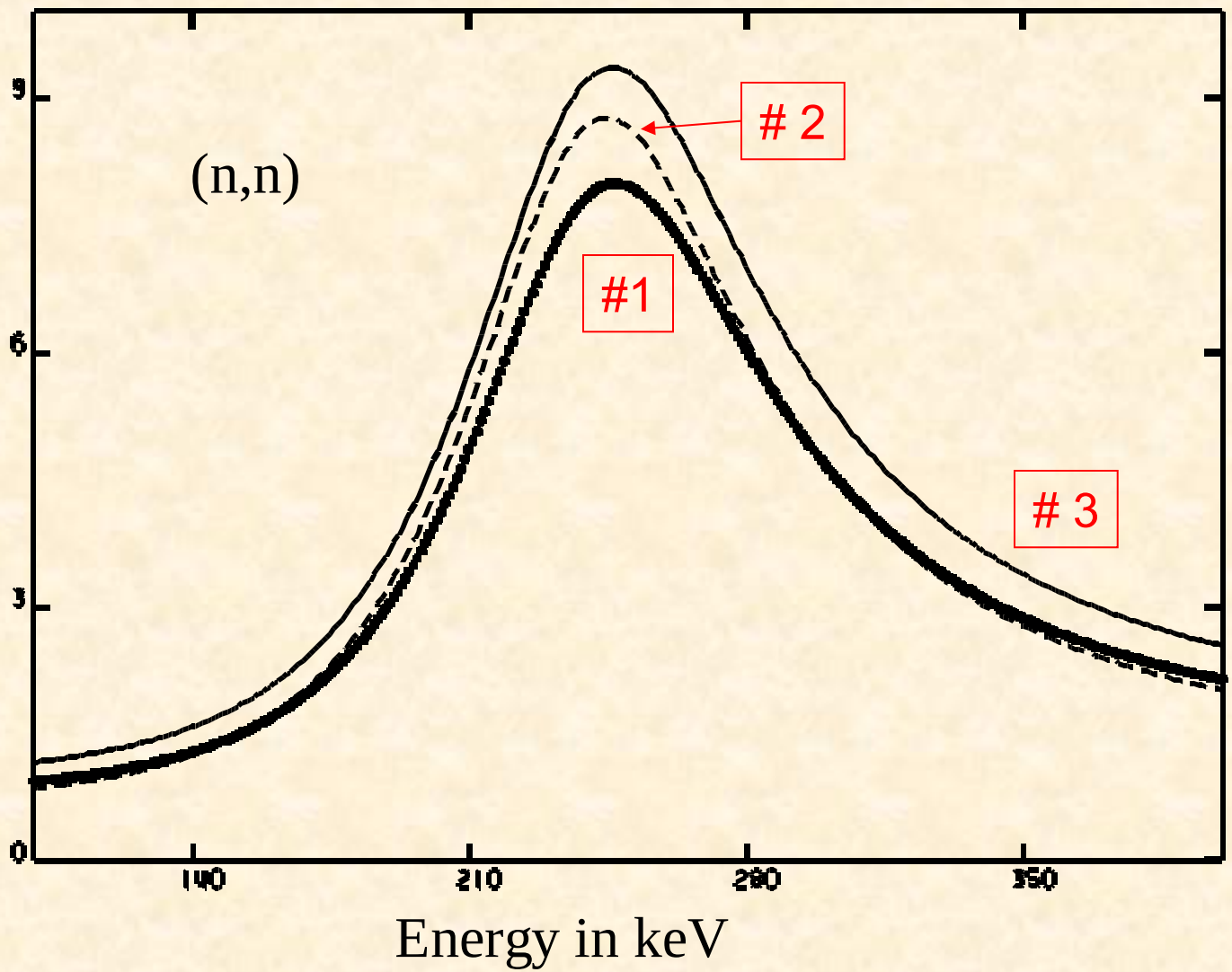
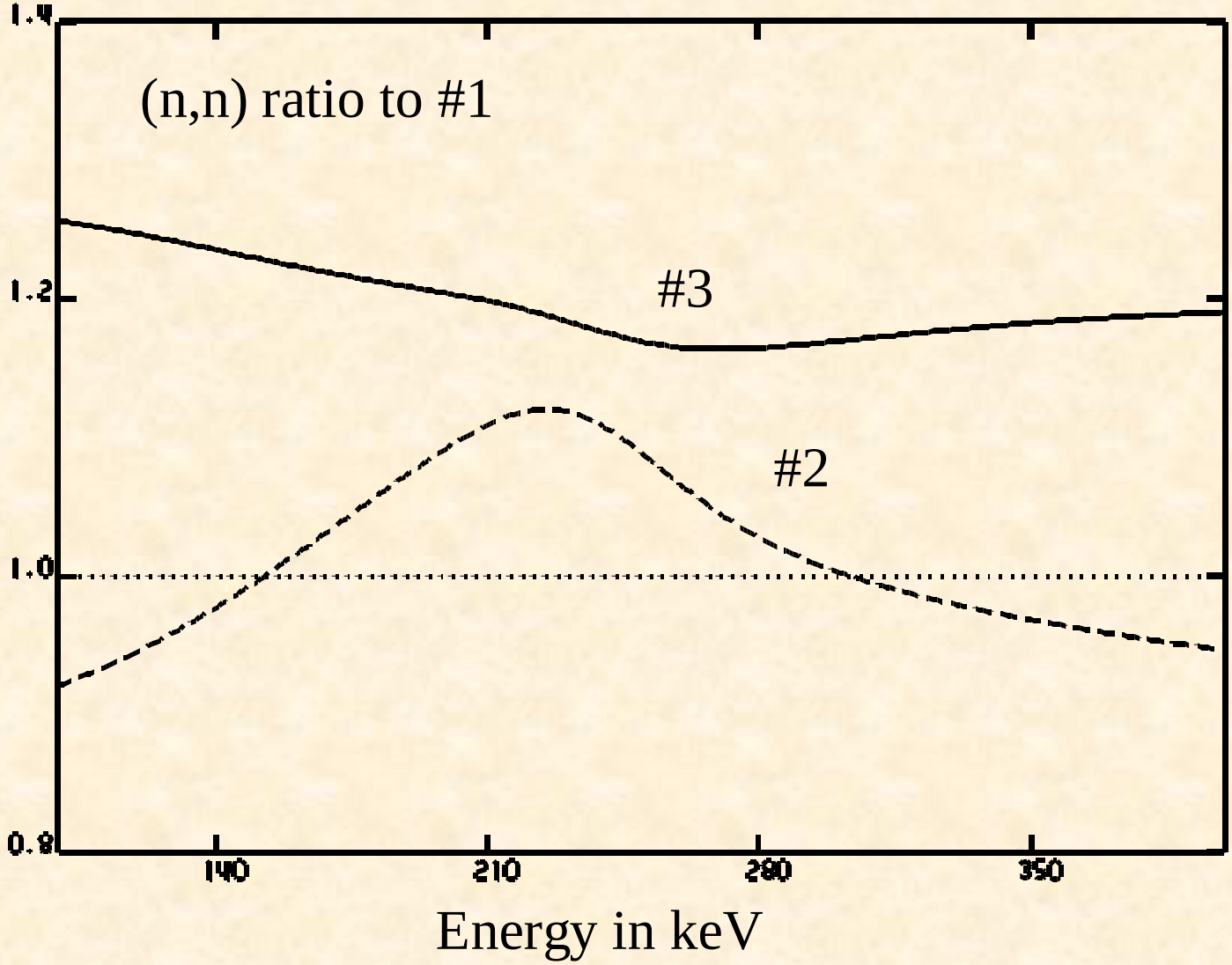
SAMMY fitting to Gerry Hale's test case on ^{6}Li(n,t), ^{6}Li(n,n), and ^{6}Li(n,all)

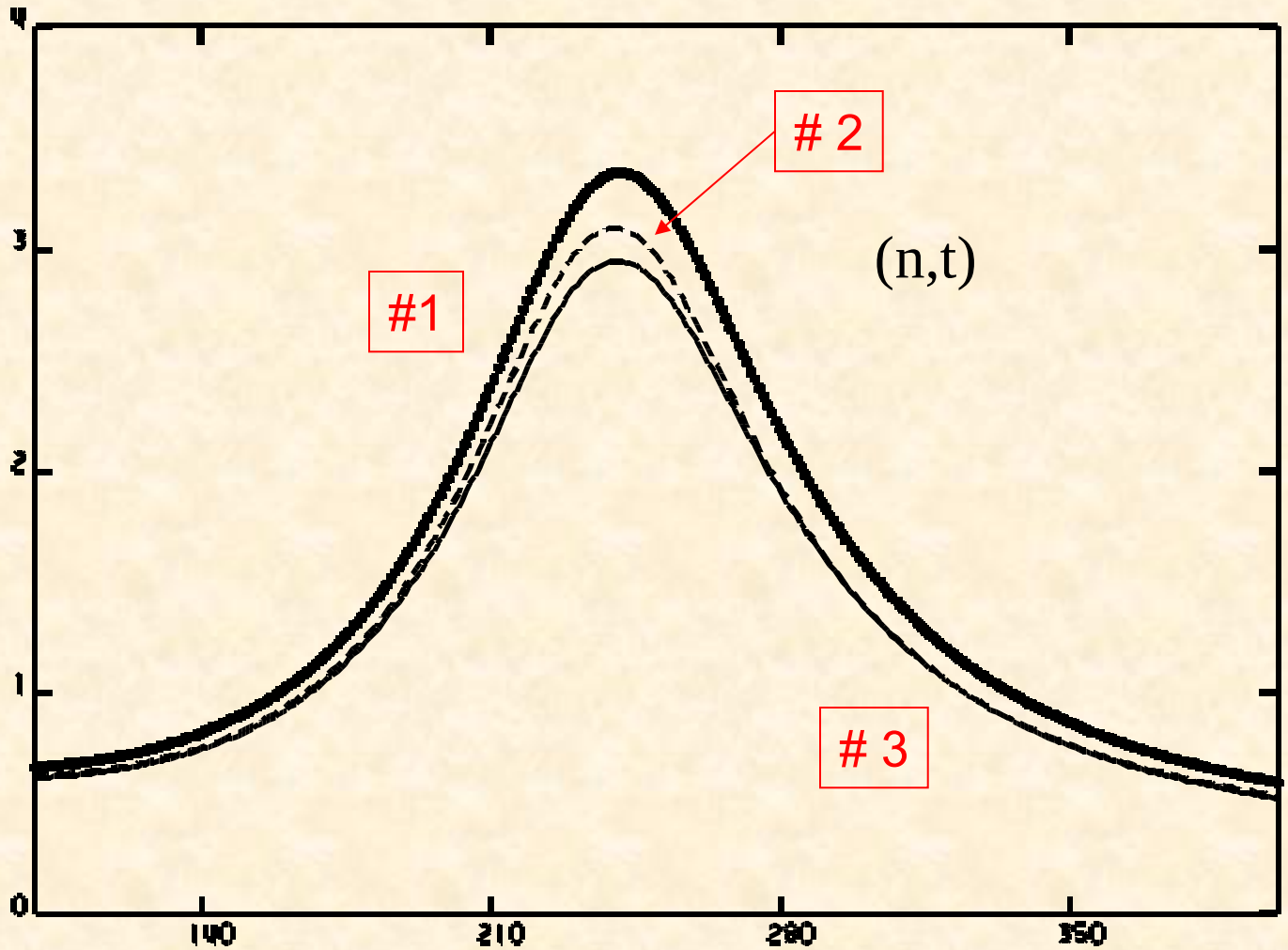
- **Tried a few dozen different methods …**
- **Results? A few dozen slightly-different cross sections**
- **Shown on following slides:**
  - **1. Include normalization on (n,t) data sets only** + + +
  - **2. Exclude Harv75 data; norm on (n,t) only** - - -
  - **3. Include normalization on (n,n) and total also; include Harv75 data** solid

details ...

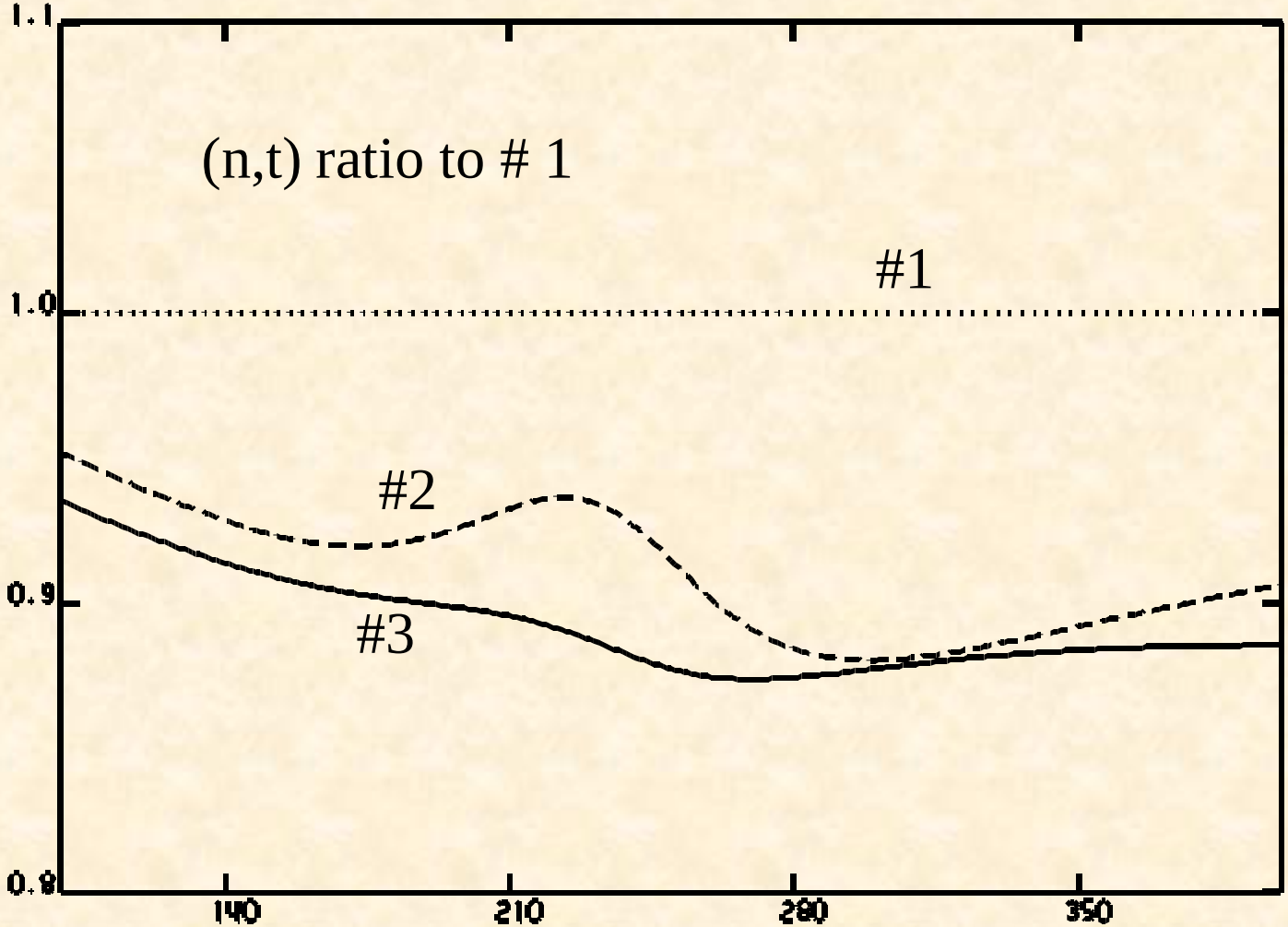
- **Normalization was included as "propagated uncertainty parameter"**
  - **i.e., as data covariance matrix, but with sensitivities calculated at the theoretical cross section rather than at the experimental values**
- **Uncertainty on normalization was arbitrarily assigned at 100%**
  - **Obviously unrealistic**
  - **However, results with 10% look similar**
- **All data analyzed simultaneously**
  - **(not so easy in SAMMY – usual mode is sequential)**
- **No iteration for non-linearities**


(n,n)
2
#1
3
9
6
3
0
140
210
280
350
Energy in keV

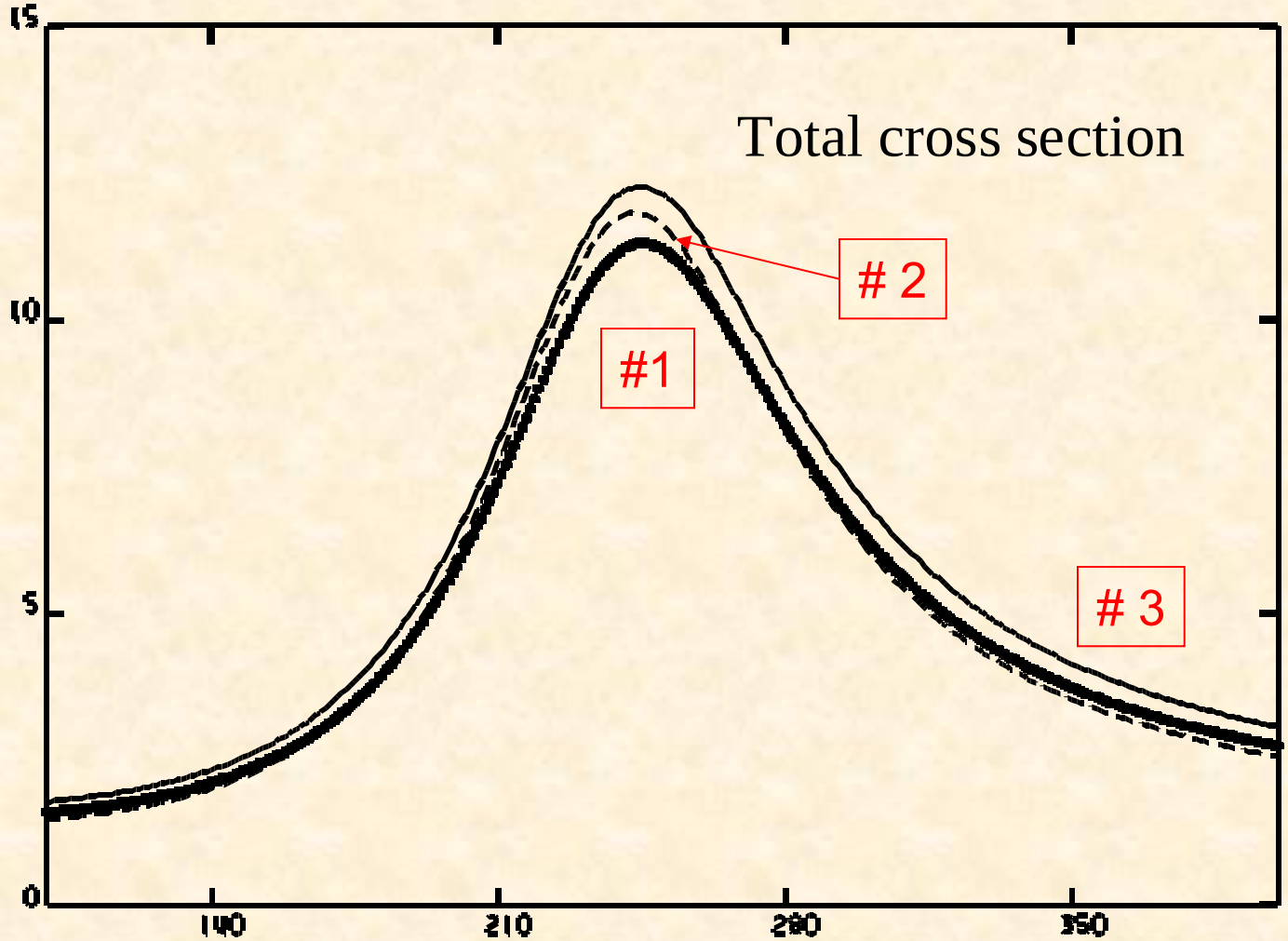

(n,n) ratio to #1
#3
#2
1.4
1.2
1.0
0.8
140
210
280
350
Energy in keV



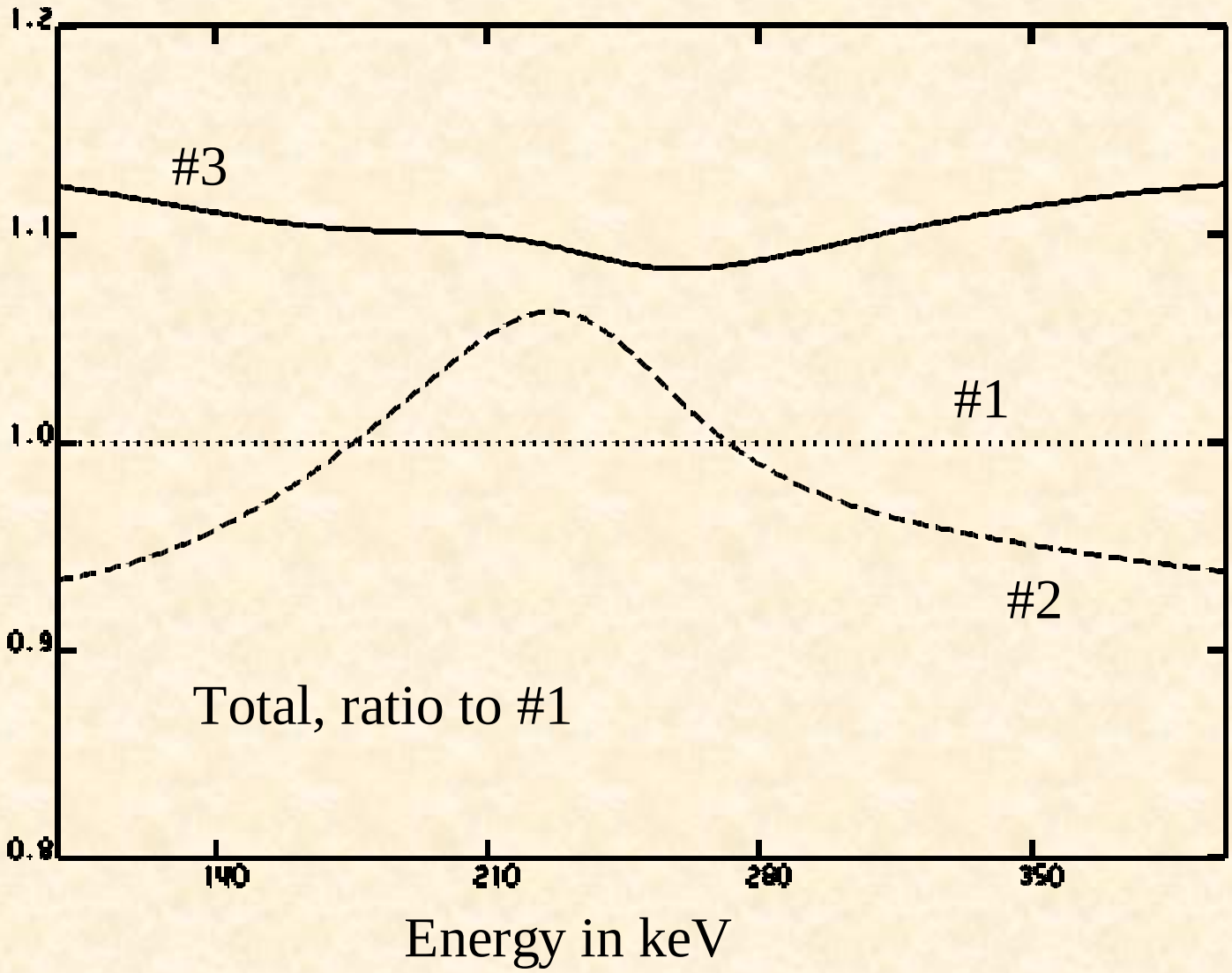
Energy in keV

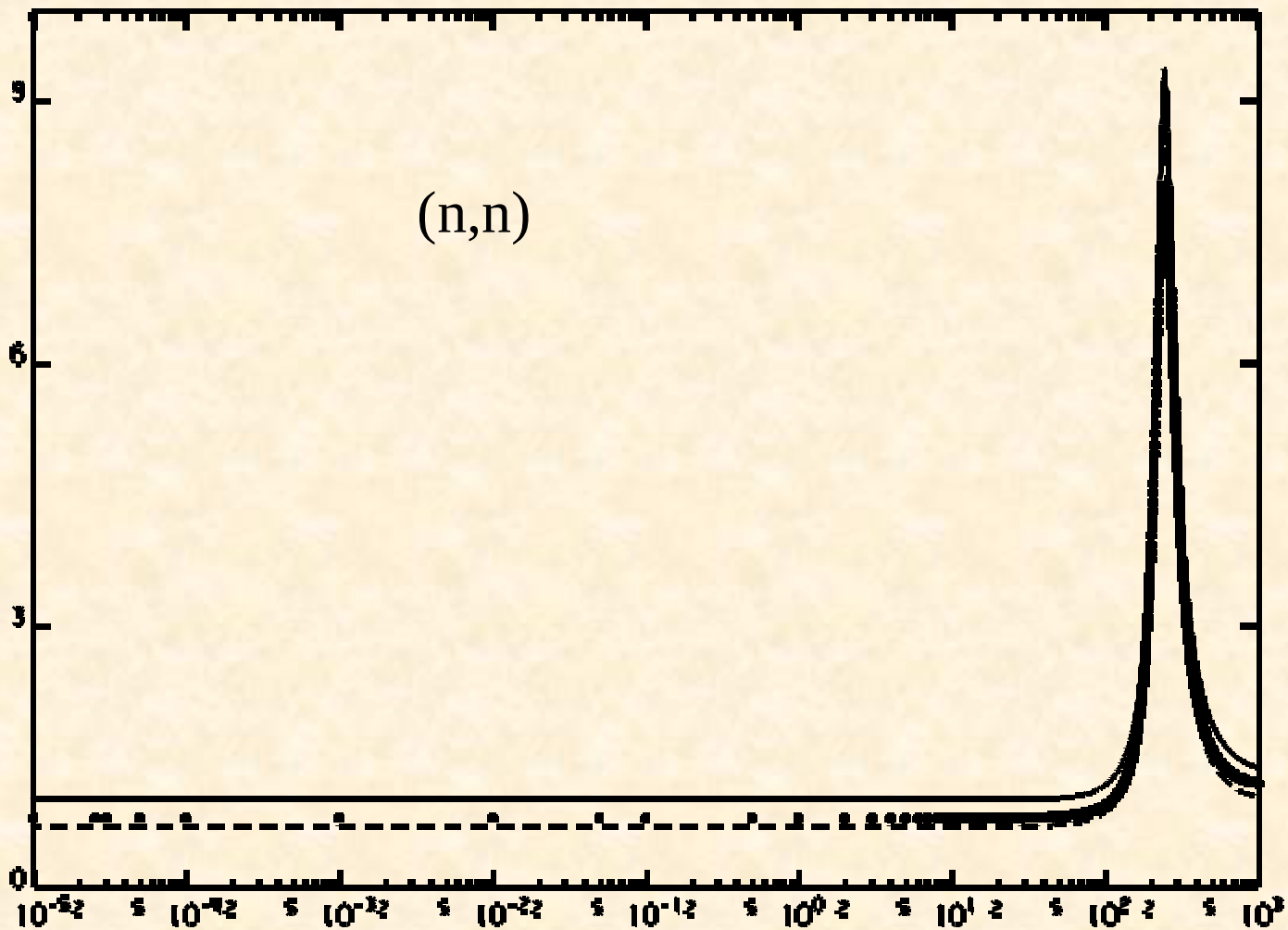


Energy in keV

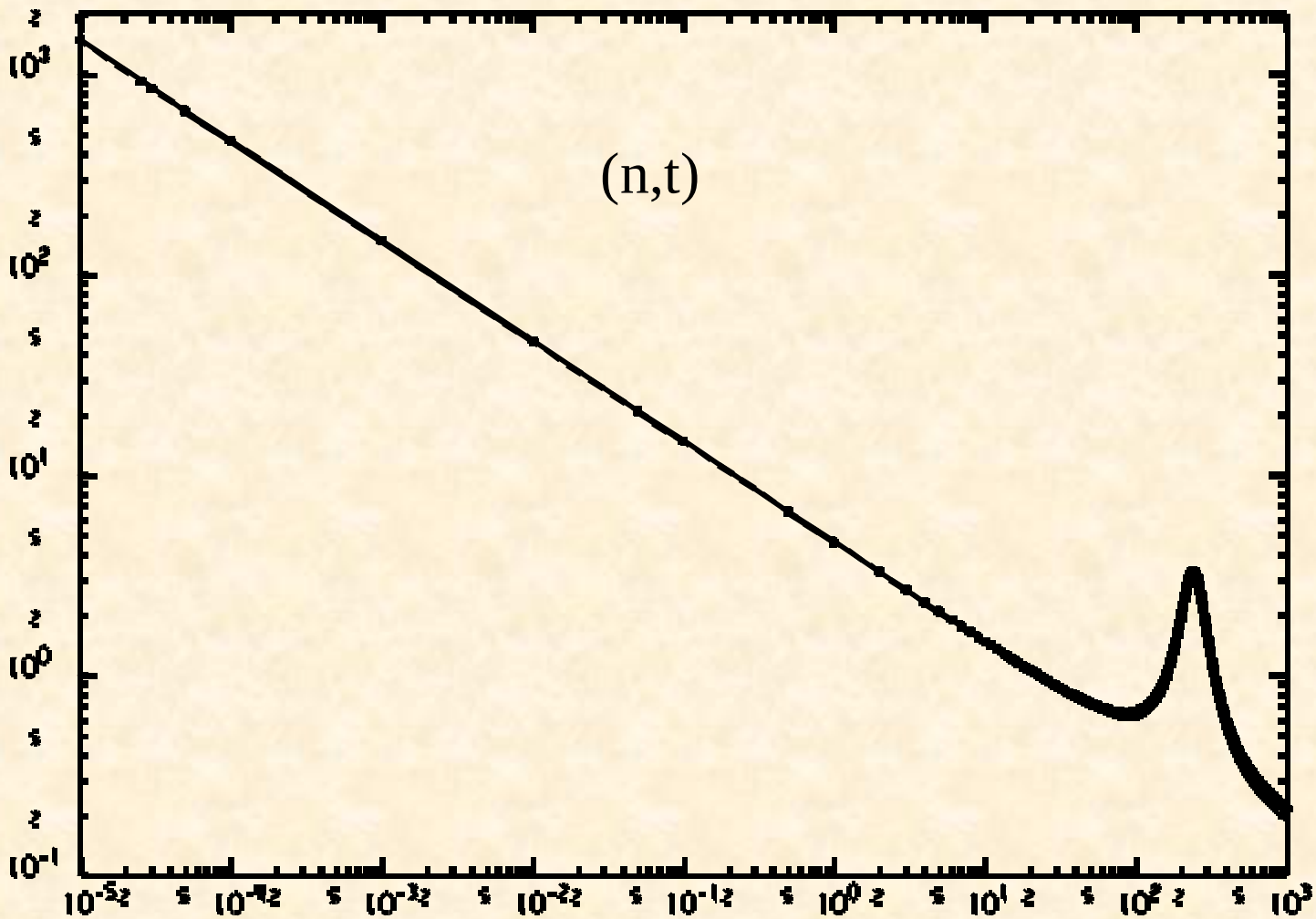


Energy in keV

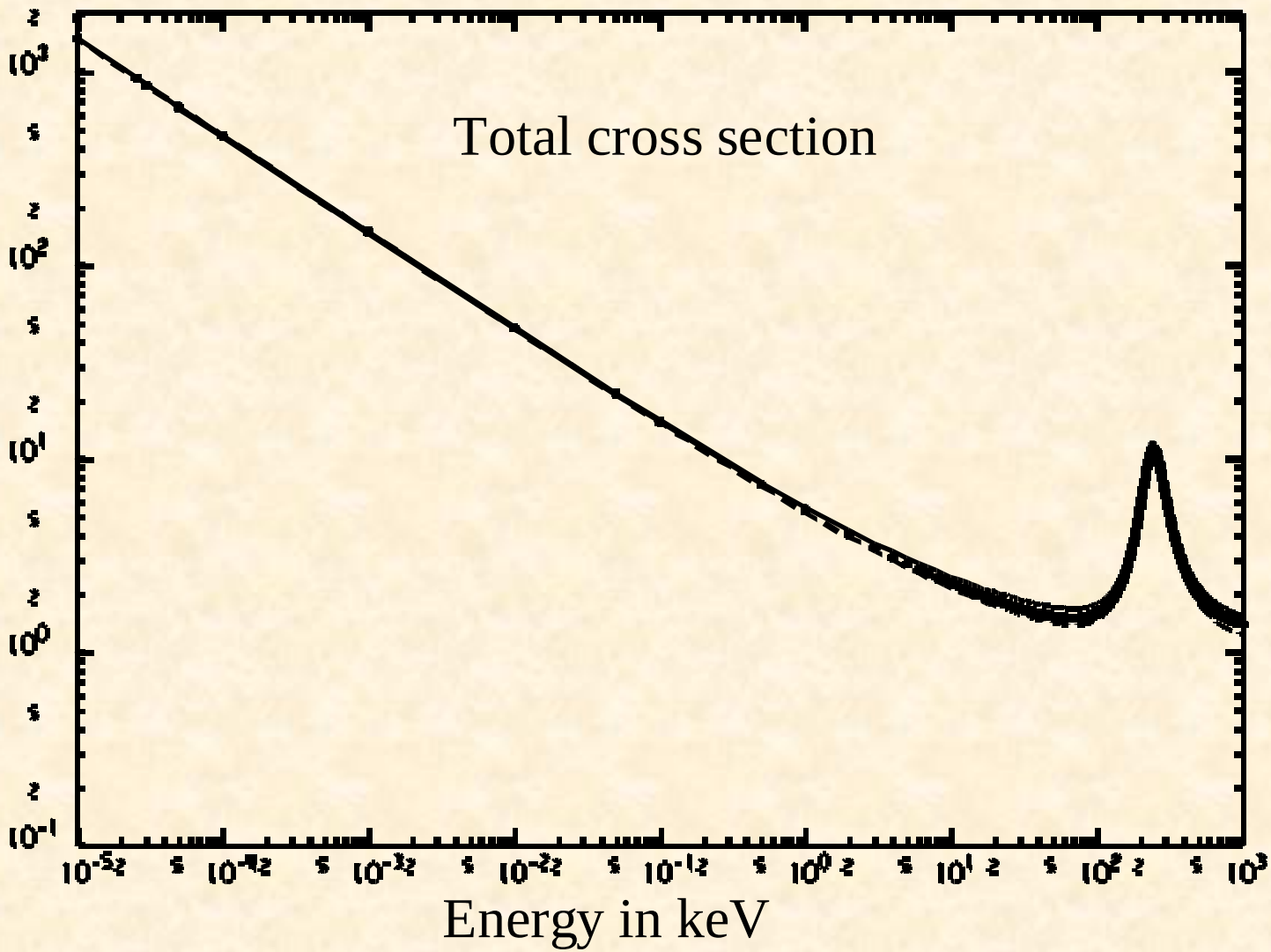

1.2
1.1
1.0
0.9
0.8
#3
#1
#2
Total, ratio to #1
140
210
280
350
Energy in keV



Wed Oct 13 17:57:39 2004



Energy in keV


Total cross section
Energy in keV

Conclusions?

- **The final result is tied very closely to**
  - **the method of treatment of uncertainties**
  - **the input values for uncertainty information**
  - **which data are included**
  - **all the details!**

The issue at hand:

- **EDA and RAC give different results when evaluating the light-element standards**
- **There are many differences between the two evaluations**
  1. **Relativity**
  2. **Data sets and energy range for each set**
  3. **Corrections for experimental conditions (resolution broadening, e.g.)**
  4. **Which uncertainties/covariances are used**
  5. **How those covariances are treated within the codes**
- **At present, we can only speculate as to which of these five is (are) important**

How to determine what's important?

- **Do three-way code comparisons (EDA, RAC, SAMMY)**
- **Start from *very simple* cases, resolve all differences before moving to more complicated cases**
- **Details coming on next slides …**

Proposed agenda: # 1

- **Given ~~identical~~ equivalent input, do the three codes calculate identical values of the cross sections?**
  - **Comparison has already been done**
  - **Result: if EDA turns off relativity, cross sections are identical**
  - **Conclusion: EDA should turn off relativity for the remainder of these comparisons**

Proposed agenda: # 2

- **Given equivalent input, do the three codes calculate identical values of the partial derivatives with respect to R-Matrix parameters?**

Comparison may not be possible, given the internal workings of the codes, but could be illuminating if it can be done.

  - **Include RAC/EDA/SAMMY for those observables which SAMMY can calculate**
  - **Include RAC/EDA for other observables**

Proposed agenda: # 1a & # 2a

- **Add resolution broadening or other experiment-related corrections**
- **# 1a: Repeat # 1**
- **# 2a: Repeat # 2**

Proposed agenda: # 3

- **First attempt at fitting data**
  - **Choose one data set** one that SAMMY can calculate, please
  - **Vary only one parameter**
  - **No iterations for non-linearities**
  - **No corrections for experimental conditions**
  - **Include statistical uncertainties but no systematic uncertainties**
    - **Data covariance matrix is diagonal**
  - **Compare fitted values from all three codes**
    - **Parameter value and uncertainty**
    - **Cross section values and covariance matrix**

Proposed agenda: # 4 & # 5

- **# 4: Repeat # 3 with different varied parameter**
- **# 5: Repeat # 3 with more-than-one varied parameter**
- **In each case, compare values from all 3 codes**
  - **Parameter values**
  - **Parameter covariances**
  - **Cross section values**
  - **Cross section covariances**

Proposed agenda: # 6, # 7, # 8

- **Repeat # 3, # 4, # 5 with iterations for non-linearities**

Proposed agenda: # 9

- **Next attempt at fitting data**
  - **Same data set as # 3; no iterations**
  - **Vary only one R-matrix parameter**
  - **Include statistical uncertainties plus normalization**
    - **Data covariance matrix is no longer diagonal**
      - **RAC → externally-calculated data covariance matrix**
      - **EDA → normalization as a fitting parameter**
      - **SAMMY 1 → RAC method**
      - **SAMMY 2 → EDA method**
      - **SAMMY 3 → SAMMY's PUP method**
  - **Compare fitted values from all five calculations**

These should be identical

These should be identical

My expectation is for small differences between these two

Proposed agenda: # 10

- **Repeat # 9 with iterations for nonlinearities**
  - **RAC ➔ externally-calculated data covariance matrix**
  - **EDA ➔ normalization as a fitting parameter**
  - **SAMMY 1 ➔ RAC method**
  - **SAMMY 2 ➔ EDA method**
  - **SAMMY 3 ➔ SAMMY's PUP method**

These should be identical

These should be identical

My expectation is for small differences between these three

Proposed agenda: # 11 & 12

- **# 11: Repeat # 9, varying another R-matrix parameter**

  # 9 = include normalization, no iterations

- **# 12: Repeat # 9, varying several R-matrix parameters**

- **Conclusions should be same as # 9**

Proposed agenda: # 13 & 14

- **# 13: Repeat # 10, varying another R-matrix parameter**

  # 10 = include normalization, with iterations

- **# 14: Repeat # 10, varying several R-matrix parameters**

- **Conclusions should be same as # 10**

Proposed agenda: # 15

- **Like # 3 but with two uncorrelated data sets**
  - **Vary only one parameter**
  - **No iterations for non-linearities**
  - **No corrections for experimental conditions**
  - **Include statistical uncertainties but no systematic uncertainties**
    - **Data covariance matrices are diagonal**
  - **Compare fitted values from all three codes**
    - **Parameter value and uncertainty**
    - **Cross section values and covariance matrix**

Proposed agenda: # 16 & # 17

- **# 16: Repeat # 15 with different varied parameter**
- **# 17: Repeat # 15 with more-than-one varied parameter**
- **In each case, compare values from all 3 codes**
  - **Parameter values**
  - **Parameter covariances**
  - **Cross section values**
  - **Cross section covariances**

Proposed agenda: # 18, etc.

- **# 18, # 19, # 20: Repeat # 15, # 16, # 17 with iterations for non-linearities**
- **# 21: Repeat # 9 with two uncorrelated data sets**
  - **Include normalization uncertainty**
- **Etc.** **Add complications *one at a time***

The next step?

- **After we've understood the *code* differences, then we need to understand the *input* differences**

It's an art, not a science

The Bottom Line

- **It is not possible to understand the source of differences between RAC & EDA evaluations until and unless detailed comparisons are made of all the processes involved.**
- **Without those detailed comparisons, our attempts to interpret the differences are speculation only.**
- **What is needed is proof, not speculation.**