Generalized Reich-Moore *R*-matrix Approximation

Goran Arbanas, ORNL

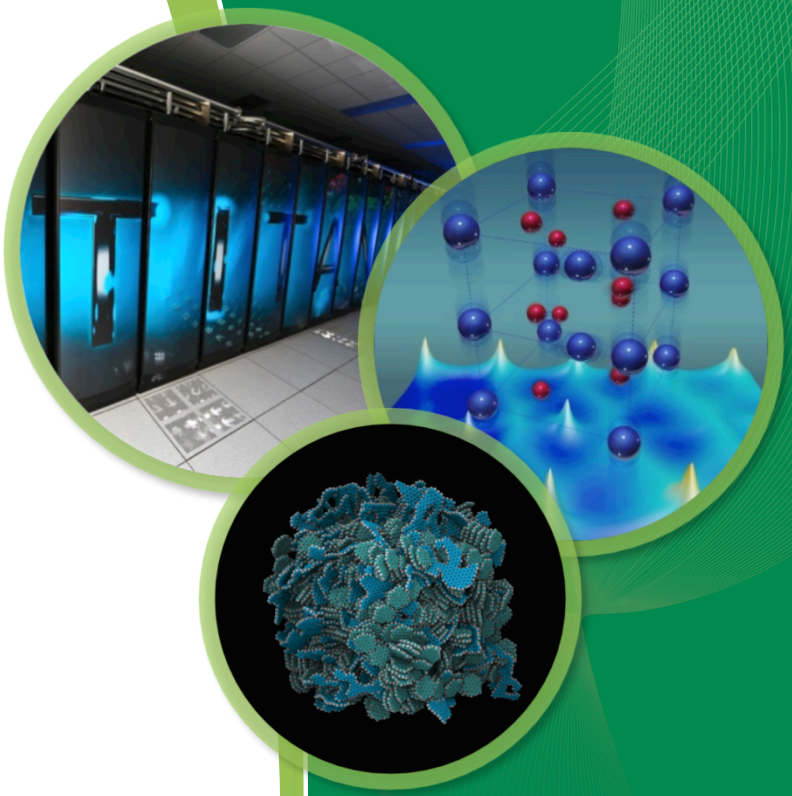
Vladimir Sobes, ORNL

Andrew Holcomb, ORNL

Pablo Ducru, MIT

Marco Pigni, ORNL

Dorothea Wiarda, ORNL



Consultant's Meeting on
R-Matrix Codes for Charged-Particle Reactions
in the Resolved Resonance Region,
IAEA Headquarters,
Vienna, Austria
December 5-7, 2016

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for the US Department of Energy

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Talk outline

- History of Reich-Moore (RM) approximation
- Motivation for generalized RM
  - Considerations of Unitarity, Brune alternative R-matrix parameters
- Derivation
  - like RM but retain level-level interference via γ-ray channels
- Implications
  - Total capture cross section fitted by fewer parameters than full R-matrix
  - Manifest Unitarity
  - Froehner's prescription
  - Insight about statistics of level-level interference via γ-channels
- SAMMY 8.1

RM History and use

Reich and Moore, Phys. Rev. 111, 929 (1958)

- Reich-Moore divides full *R*-matrix into particle and γ-ray blocks
  - Formal expressions derived for reduced R-matrix of particle channels
  - The effect of γ-ray channels on particle-channels approx. by a diagonal
    - Level-level interference among γ-ray channels neglected

F. Froehner, JEFF Report 18 (2000)

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda c'}}{E_\lambda - E - i\Gamma_{\lambda\gamma}/2} \qquad (c, c' \notin \gamma)\,, \qquad (194)$$

corresponding SLBW level matrix. Otherwise it is so exact that although the reduced collision matrix cannot be unitary - because of transitions into eliminated channels - the overall collision matrix can still be considered as unitary, i. e. as conserving probability flux, so that the capture cross section may alternatively be obtained as the difference

$$\sigma_{c\gamma} = \sigma_c - \sum_{c' \notin \gamma} \sigma_{cc'}\,, \qquad (196)$$

with σ_c calculated from the reduced collision matrix element U_{cc} according to Eq. 153.

$$\sigma_c \equiv \sum_{c'} \sigma_{cc'} = 2\pi \lambda\!\!\!^{-2}_{c} g_c (1 - \mathrm{Re}\ U_{cc})\,, \qquad (153)$$

Motivation for generalized Reich-Moore

- Conversion of RM R-matrix parameters
  - Between formal and alternative (a.k.a. physical) ones (C. Brune, 2002)
- Investigate whether Reich-Moore (RM) approx. is unitary
  - It may appear not to be as particle-channel R-matrix is complex (not real)
  - RM derivation was revisited to investigate unitarity
  - In this process a generalization of RM was found
    - This generalization is manifestly unitary
    - Corollary: Conventional RM is also unitary
    - It provides basis for Fritz Froehner's prescription used by SAMMY
- Other potential benefits Generalized RMA (gRMA)
  - May provide better fits to total capture (and other cross sections)
    - Because gRMA reproduces total cross section formally
  - May shed light on resonant-interference effects neglected by conv. RM
    - Including statistical properties of capture widths

Derivation uses full R-matrix via level-matrix A

$$\boldsymbol{A}^{-1} \quad = \quad \boldsymbol{e} - \boldsymbol{E}\mathbf{1} + \boldsymbol{\gamma}(\boldsymbol{L} - \boldsymbol{B})\boldsymbol{\gamma}^{T}$$

- Separate channel space into particle and γ-ray channels:

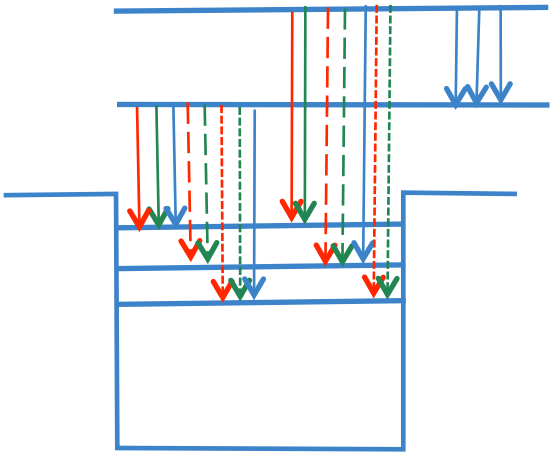
$$\boldsymbol{\gamma} \equiv (\boldsymbol{\gamma}_c, \boldsymbol{\gamma}_\gamma)$$

$$\boldsymbol{L} - \boldsymbol{B} \equiv \begin{pmatrix} \boldsymbol{L}_c - \boldsymbol{B}_c & \mathbf{0} \\ \mathbf{0} & \boldsymbol{L}_\gamma - \boldsymbol{B}_\gamma \end{pmatrix}$$

$$\boldsymbol{A}^{-1} = \boldsymbol{e} - \boldsymbol{E}\mathbf{1} + \boldsymbol{\gamma}_\gamma(\boldsymbol{L}_\gamma - \boldsymbol{B}_\gamma)\boldsymbol{\gamma}_\gamma^{T} + \boldsymbol{\gamma}_c(\boldsymbol{L}_c - \boldsymbol{B}_c)\boldsymbol{\gamma}_c^{T}$$

Full R-matrix g-ray channels

- γ-ray channels
  - defined by EM multipolarity, helicity, and final state quantum numbers
  - Selection rules based on f.s. quantum numbers, γ-ray multipolarity
  - Electric: E1, E2, E3, …
  - Magnetic: M1, M2, M3, …
- Level-level interference takes place via identical γ-ray channels
  - Use conventional approximation S-B=0
    - Or use Brune alternative R-matrix parameters for which S-B=0 always

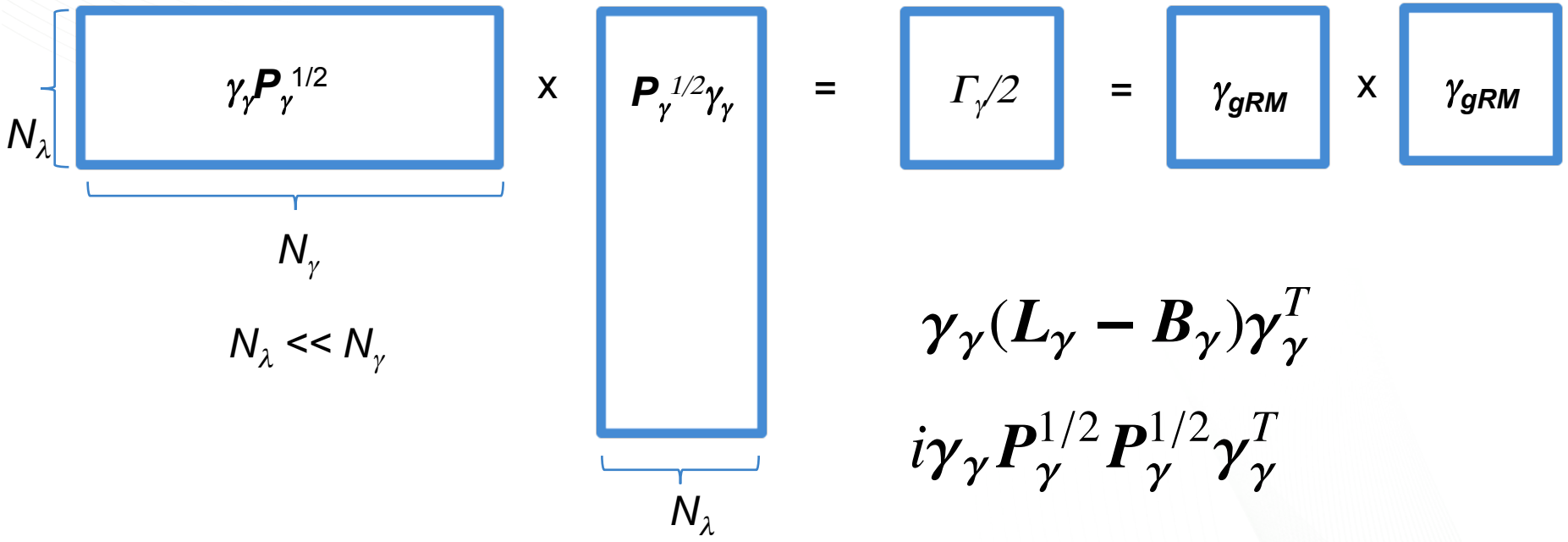


$$i\boldsymbol{\gamma}_\gamma \boldsymbol{P}_\gamma^{1/2} \boldsymbol{P}_\gamma^{1/2} \boldsymbol{\gamma}_\gamma^T$$

Generalized RM Derivation

- Consider capture-width matrix Γ_γ inside the level matrix **A**

γ_γ = N_λ x N_γ matrix of physical capture channel widths
γ_{gRM} = N_λ x N_λ matrix of gRMA capture channel widths



$N_\lambda << N_\gamma$

$$\gamma_\gamma(L_\gamma - B_\gamma)\gamma_\gamma^T$$

$$i\gamma_\gamma P_\gamma^{1/2} P_\gamma^{1/2}\gamma_\gamma^T$$

- Since *total capture* cross section depends on Γ_γ, it could be fit equally well by N_λ as it could by all N_γ capture channels
  - True for *total* capture only (individual γ-channels require full *R*-matrix)

Total capture of gRMA equals that of full R-matrix

- Working with alternative R-matrix parameters since S(E)-B=0

$$\boldsymbol{A}^{-1} = \boldsymbol{e} - E\mathbf{1} + \boldsymbol{\gamma}_\gamma(\boldsymbol{L}_\gamma - \boldsymbol{B}_\gamma)\boldsymbol{\gamma}_\gamma^T + \boldsymbol{\gamma}_c(\boldsymbol{L}_c - \boldsymbol{B}_c)\boldsymbol{\gamma}_c^T$$

$$\boldsymbol{A}^{-1} \approx \boldsymbol{e} - E\mathbf{1} + i\boldsymbol{\gamma}_\gamma \boldsymbol{P}_\gamma^{1/2}\boldsymbol{P}_\gamma^{1/2}\boldsymbol{\gamma}_\gamma^T + \boldsymbol{\gamma}_c(\boldsymbol{L}_c - \boldsymbol{B}_c)\boldsymbol{\gamma}_c^T$$

$$= \boldsymbol{e} - E\mathbf{1} + i\boldsymbol{\Gamma}^{(\gamma)}/2 + \boldsymbol{\gamma}_c(\boldsymbol{L}_c - \boldsymbol{B}_c)\boldsymbol{\gamma}_c^T$$

- The total capture cross section is proportional to:

$$\boldsymbol{U}_{c\gamma}\boldsymbol{U}_{c\gamma}^{*T} = \boldsymbol{\Omega}_c \boldsymbol{P}_c^{1/2}\boldsymbol{\gamma}_c^T \mathbf{A}\boldsymbol{\gamma}_\gamma \boldsymbol{P}_\gamma^{1/2}\boldsymbol{\Omega}_\gamma\boldsymbol{\Omega}_\gamma^*\boldsymbol{P}_\gamma^{*1/2}\boldsymbol{\gamma}_\gamma \mathbf{A}\boldsymbol{\gamma}_c^T\boldsymbol{P}_c^{*1/2}\boldsymbol{\Omega}_c^*$$

$$= \boldsymbol{\Omega}_c \boldsymbol{P}_c^{1/2}\boldsymbol{\gamma}_c^T \mathbf{A}(\boldsymbol{\gamma}_\gamma \boldsymbol{P}_\gamma^{1/2}\boldsymbol{P}_\gamma^{1/2}\boldsymbol{\gamma}_\gamma^T)\mathbf{A}\boldsymbol{\gamma}_c^T\boldsymbol{P}_c^{*1/2} \quad (14)$$

$$= \boldsymbol{\Omega}_c \boldsymbol{P}_c^{1/2}\boldsymbol{\gamma}_c^T \mathbf{A}(\boldsymbol{\Gamma}^{(\gamma)}/2)\mathbf{A}\boldsymbol{\gamma}_c^T\boldsymbol{P}_c^{*1/2}\boldsymbol{\Omega}_c^* \quad (15)$$

- → since $\boldsymbol{\Gamma}^{(\gamma)}$ is the same for full R-matrix and gRMA

Full R-matrix vs. conventional RM: total capture

- full R-matrix equivalent to gRMA; 2-level SAMMY example:

Table II B2.1. Parameter values used to illustrate Reich-Moore vs. full R-matrix calculations

	λ	Energy (MeV)	$\bar{\Gamma}_{\lambda\gamma}$ (eV)	$\Gamma_{\lambda n}$ (eV)	Sign $\times \Gamma_{\lambda\gamma}$ (eV)[a]
Reich Moore	1	1.0	1.0	10000.	
	2	1.1	1.1	11000.	
Pseudo-full R-matrix # 1	1	1.0	10^{-8}	10000.	1.0
	2	1.1	10^{-8}	11000.	1.1
Pseudo-full R-matrix # 2	1	1.0	10^{-8}	10000.	1.0
	2	1.1	10^{-8}	11000.	−1.1

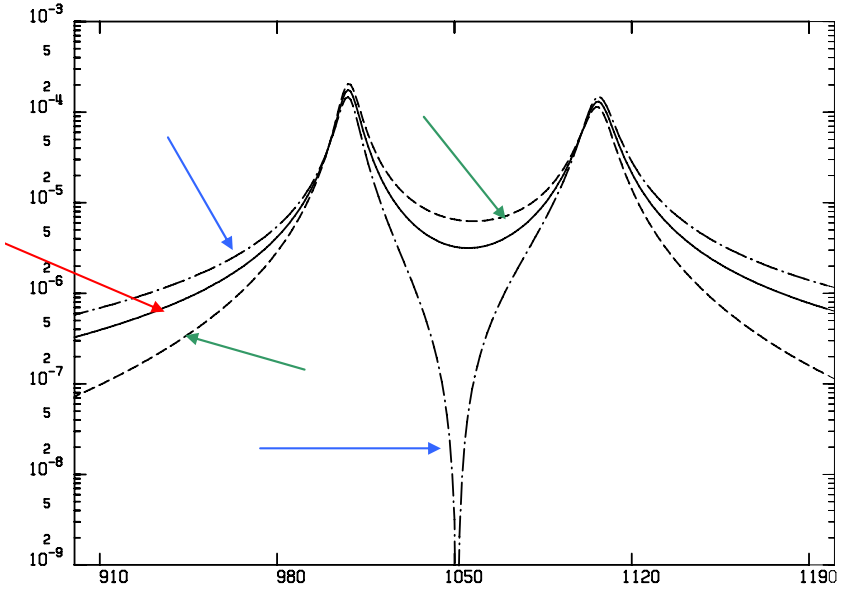


Figure II B2.1. Reich-Moore approximation vs. full R-matrix for artificial example of test case tr110.

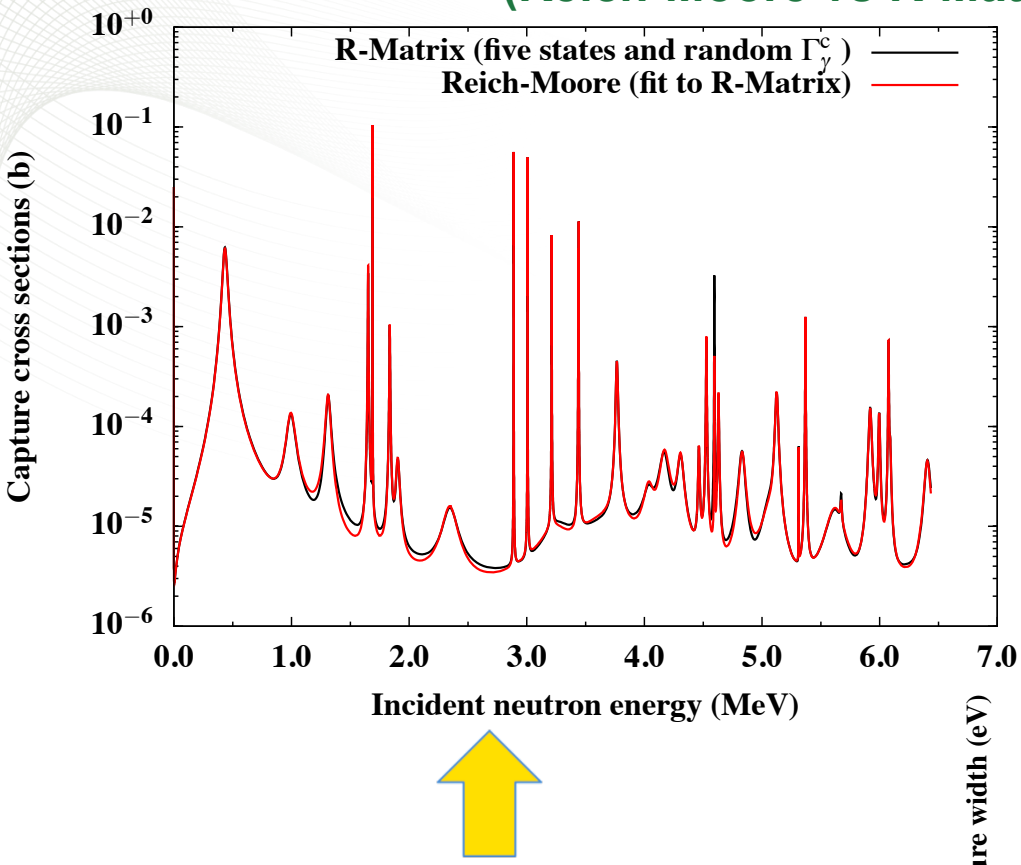
Solid line = Reich Moore

Dot-dash = full R-matrix # 1

Dash = full R-matrix # 2

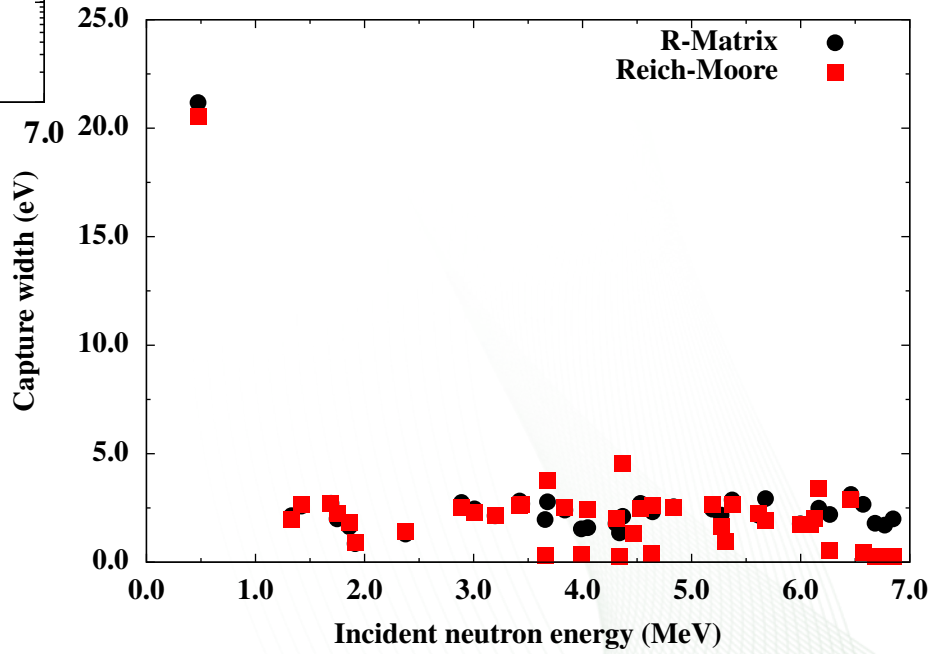
^{16}O Full R-matrix vs. conventional RM toy case

(Reich-Moore vs R-Matrix calculations)



Good agreement between Reich-Moore and R-Matrix capture widths

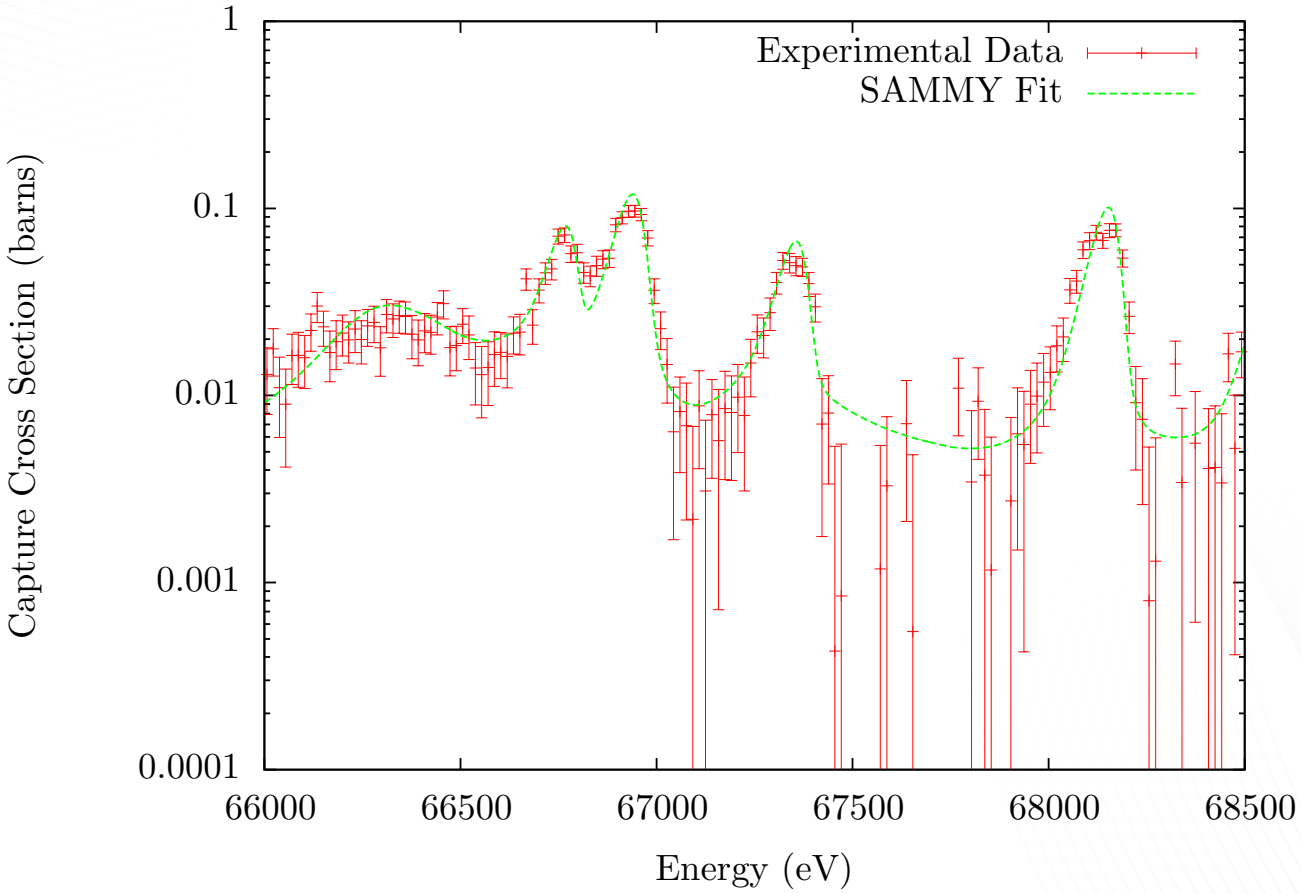
$$\Gamma_{\mu\mu} = 2\sum_c \gamma_{\mu c}\gamma_{\mu c}$$



- R-matrix case (five states for ^{17}O) generated by randomly sampling capture widths (in black)
- The R-matrix capture cross sections were used to obtain capture widths in Reich-Moore approximation and related capture cross sections (in red)
- The fit of the capture cross sections did not impact other reaction channels

Cu(n,γ) evaluation

- Note: other ways to improve the fit besides resorting to gRMA
  - ^{63,65}Cu evaluation by V. Sobes (ORNL)



Tungsten ^{183}W evaluation

- By M. Pigni (ORNL)
- Slight room for improvement:

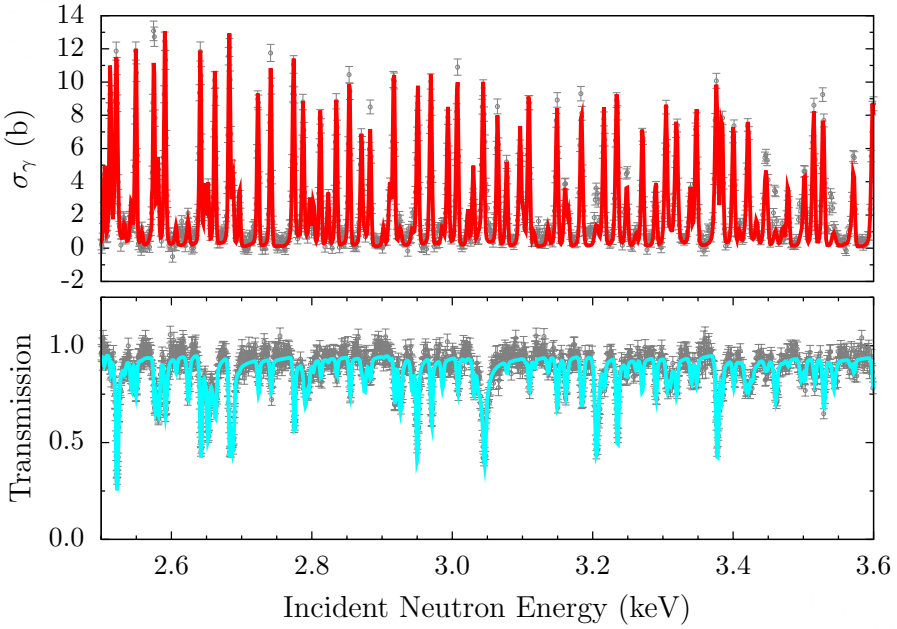


FIG. 1. Neutron capture cross sections (top) and transmission data (bottom) of ^{183}W in the energy range of 2.5-3.6 keV. The solid red lines calculated by the resonance parameters are compared with the experimental data.

Implications: Unitarity

- Generalized RM *R*-matrix is manifestly unitary
  - its *R*-matrix is real, its resonance energies are real
  - A reduced number (N_λ) of "resonant" γ-ray channels is retained
  - *R*-matrix particle-channel sub-matrix alone is not unitary
- Insight: γ-ray channels retained in gRMA make *R*-matrix unitary
- Consequently, conventional RMA is unitary
- gRMA thus provides foundation for Froehner's prescription
  - Total cross section is computed assuming a unitary S- or U-matrix
  - Capture cross section is then a deviation of particle R-matrix from unitarity
  - Total capture computed as difference between total and particle channels
  - Implemented in SAMMY

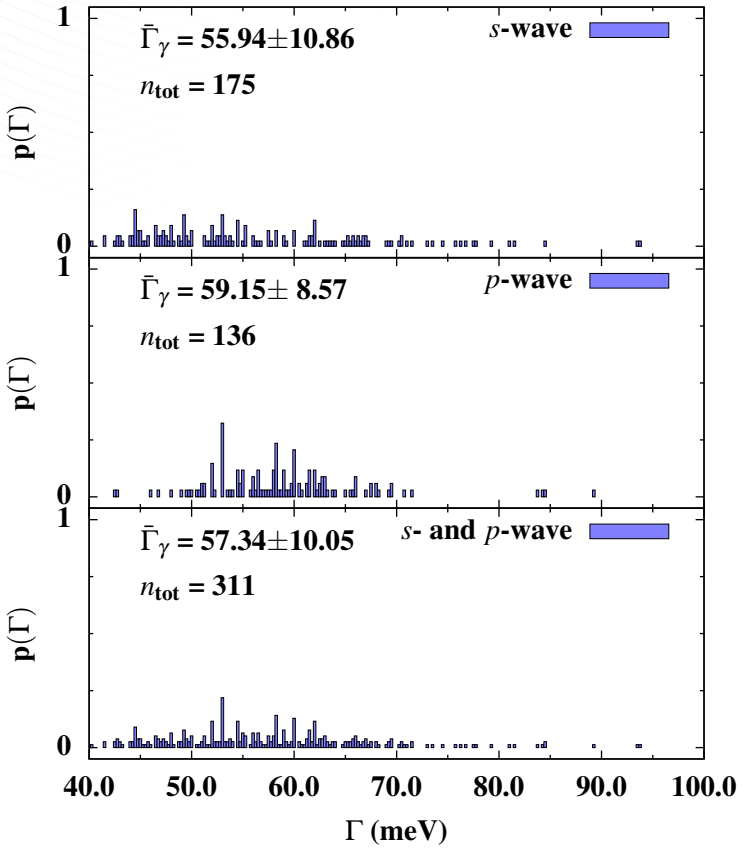
Implications: Statistics

- Related to Wishart matrices
  - Marginal distribution of diagonal and off-diagonal elements
  - Correlations may affect marginal distrib.'s
- Diagonal elements
  - Related to conventional RM capture widths
  - Approximately χ^2-distribution with N_γ degrees of freedom (DOF)
    - Dominant γ-rays may reduce the effective number of DOF
    - P. Koehler finds DOF is smaller than expected in data
- Off-diagonal elements
  - "XY" distribution with mean 0 and variance ½ that of the diagonal
- → Variance of RM widths estimates neglected off-diagonal
  - May be useful to estimate isotopes to re-evaluate.

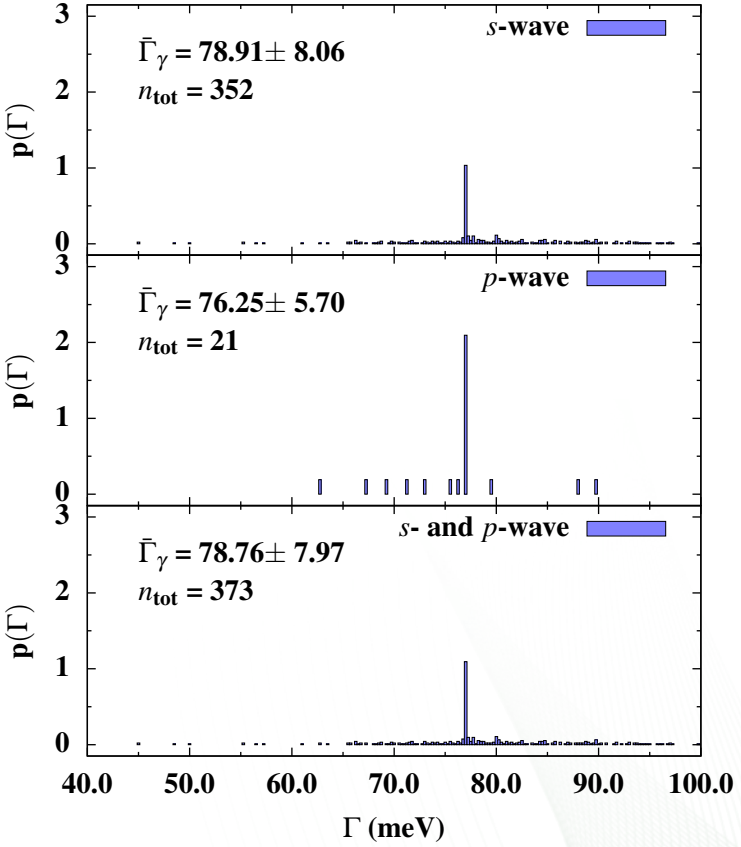
Statistics of conventional RM widths on ^{182,183}W

- Their variance is approx. twice that of (neglected) off-diagonal:

^{182}W (Leal)



^{183}W (Pigni)



Implications: Brune's alternative R-matrix

- Brune alternative R-matrix parameterization:
  - Independent of boundary conditions thanks to
  - $S_c(E)-B_c=0$ energy-dependent boundary conditions
    - The real part of Kapur-Peierls $L_c(E)-B_c=S_c(E)+iP_c(E)-B_c=0$
  - Alternative resonance energies aligned with resonant peaks
    - Intuitive parameterization
  - C. Brune Phys. Rev. **C66** 044611 (2002)
- Generalized RM capture widths
  - Brune transformation matrices not affected by γ-channels, if $S_\gamma(E)=B_\gamma=0$
  - Unambiguous transformation to/from Brune alternative capture widths
  - Also true for conventional RM widths (diagonal only)
    - But these will not remain diagonal when transformed

Alternative R-matrix parameterization

- C. Brune transform C. R. BRUNE PHYSICAL REVIEW C **66**, 044611 (2002)

$$U_{c'c} = \Omega_{c'}\Omega_c[\,\delta_{c'c} + 2\mathrm{i}(P_{c'}P_c)^{1/2}\boldsymbol{\gamma}_{c'}^T \boldsymbol{A}\,\boldsymbol{\gamma}_c]$$

$$\boldsymbol{A}^{-1} = \boldsymbol{e} - E\boldsymbol{1} - \boldsymbol{\gamma}(\boldsymbol{L}-\boldsymbol{B})\,\boldsymbol{\gamma}^T \qquad e_{\lambda\mu} = E_\lambda \delta_{\lambda\mu}$$

  - Transform from Formal to alternative parameters:
    - a non-linear eigenvalue problem:

$$\boldsymbol{\mathcal{E}} = \boldsymbol{e} - \sum_c \boldsymbol{\gamma}_c \boldsymbol{\gamma}_c^T (S_c - B_c)$$

$$\boldsymbol{\mathcal{E}}\boldsymbol{a}_i = \tilde{E}_i \boldsymbol{a}_i$$

  - All widths in generalized Reich-Moore approximation transform as:

$$\tilde{\gamma}_{ic} = \boldsymbol{a}_i^T \boldsymbol{\gamma}_c$$

  - This shows that exact Brune transform is possible in gRM, not in RM
  - Alternative *A*- and *R*-matrix derived by C. Brune (2002)

Generalized RM (gRM): Conclusions and Outlook

- gRM provides a better way to fit *total* capture cross sections
  - It is analytically equivalent to full R-matrix when $S_\gamma - B_\gamma = 0$
  - It will likely improve fitting of total and other partial cross sections too
- gRM is manifestly unitary because its R-matrix is *real*
  - Justifies Froehner's prescription for unitary conventional RM in SAMMY
- gRM alternative resonance parameters are unambiguous
  - Carl Brune (2002) transform can be applied exactly when $S_\gamma - B_\gamma = 0$
- gRM yields insight on distributions of capture matrix elements
  - Deviations from statistics of Wishart matrices may reveal doorways
  - Variance of gRM capture matrix diagonal is 2x that of off-diagonal el.'s
  - Elements near the diagonal (e.g. tri-diagonal) may be sufficient for fitting
- Identify evaluations that may benefit from gRMA
  - Implement it and apply it in a future publication

SAMMY 8.1 coming soon to RSICC.ornl.gov

- Includes SAMINT program designed to adjust nuclear data parameters based on integral data: http://www.osti.gov/scitech/biblio/1185560/
  - In multi-group or continuous-energy framework
  - Informs the evaluation of resolved resonance parameters
  - Leverages ORNL expertise in sensitivity studies of IBE's and applications
    - SCALE modules TSUNAMI and TSURFER
- New detector resolution functions based on MCNP simulations
  - In collaboration with Y. Danon (RPI)
- SAMMY CI and SQA
  - Cmake/ctest build and test on Linux/Mac/Windows, gfortran/ifort
  - Helped identify and resolve several minor problems
- SAMMY code modernization on the way:
  - SAMRML already rewritten into C++
- Many thanks for feedback and inquires from SAMMY users!

Backup SAMMY slides

History

- Developed by Dr. Nancy Larson since 1970's through 2008
- Includes SAMMY + 25 auxiliary codes
  - e.g. SAMRML
- Architecture
  - Large Fortran (77) container array for memory management
- 185 multi-step test cases + 10 tutorial examples
- Comprehensive Documentation:
  - http://info.ornl.gov/sites/publications/files/Pub13056.pdf
- Employed for resolved resonance evaluations in ENDF
- Distributed via RSICC https://rsicc.ornl.gov/
  - SAMMY 8.1 is forthcoming

Capabilities

- Multi-level Multi-channel R-matrix code
- Bayesian fitting of R-matrix resonance parameters (RP)
  - a.k.a. Generalized Least Squares
  - yields covariance matrix of RP
- Data reduction:
  - Experimental Facility Resolution functions: ORELA, RPI, GELINA
  - Normalization, background
- Detector resolution functions
  - Configurable for variety of detectors
- Doppler broadening
  - Solbrig's kernel, Leal-Hwang method
- Multiple scattering effects, and other target effects
- Charged projectiles (p, α)
- Unresolved Resonance Range (FITACS by F. Froehner)

Capabilities: R-matrix *and* Reich-Moore Approx.

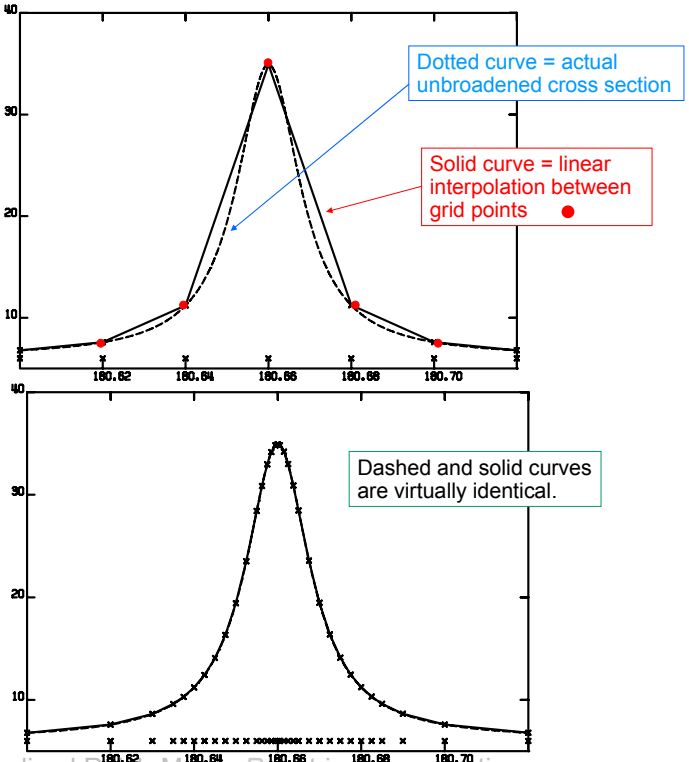
- Reich-Moore approximation (RMA)
  - For channels approximated statistically via Random Phase Hypothesis
  - Applied mostly for capture channels
    - penetrability *P=1* for capture in RMA (and in exact R-matrix below)
- R-matrix w/o RMA
  - Make capture channels as reaction channels in SAMMY input files
  - Marco Pigni's talk:
    - Quantify accuracy of RMA relative to R-matrix on ^{16}O using 5 γ-rays/level

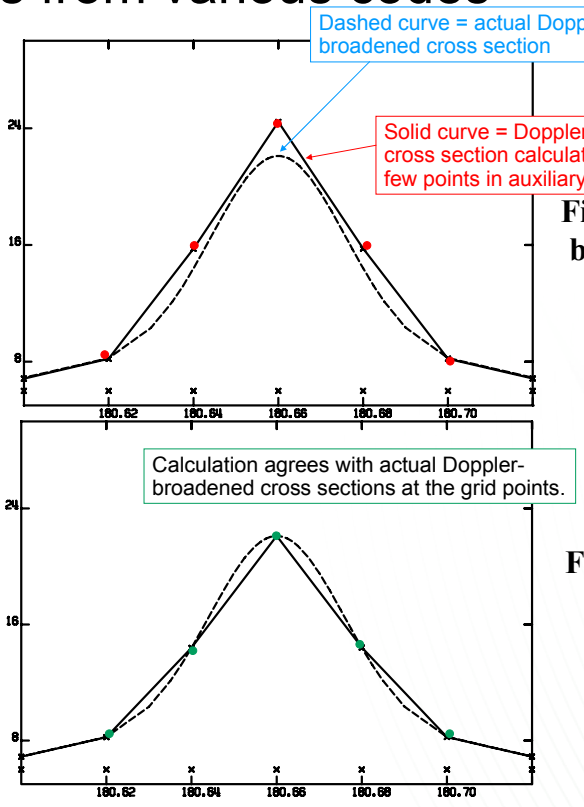
Capabilities: Resolution broadening

- Experimental Resolution broadening
  - Convolution of 4 components:
    - The electron burst
      - a square function of time
    - Neutron sources:
      - tantalum target
      - water moderator
    - Neutron detectors
      - model NE-110 recoil proton detector
      - lithium glass detector
    - Time-of-flight channel width
      - a square function of time
- Doppler broadening (DB)
  - numerical convolution of cross sections by Solbrig kernel over *E*
  - Double-differential c.s. DB-ed approximately by SAMMY now
    - our group developed and published an exact method
  - Leal-Hwang: efficient, used by SCALE

Capabilities: configurable energy mesh

- Auxiliary energy mesh for computations
  - Includes data energy points and additional points
    - especially at and near resonance peaks to trace their shapes completely
    - Needed because resonance are narrower at T=0 K before Doppler broadening to room temperature for data
  - Useful for comparing results from various codes





Figures from SAMMY Users' Guide:

Figure III A1.2. Incorrect Doppler-broadened cross section calculated with too few points in the auxiliary grid.

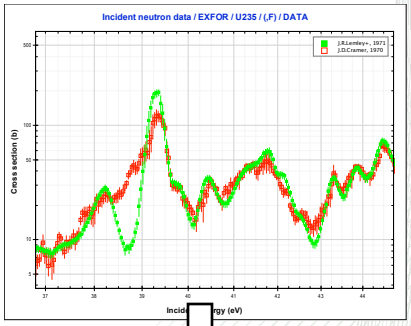
Figure III A1.4. Doppler-broadened cross section calculated with an adequate number of points in the auxiliary grid.

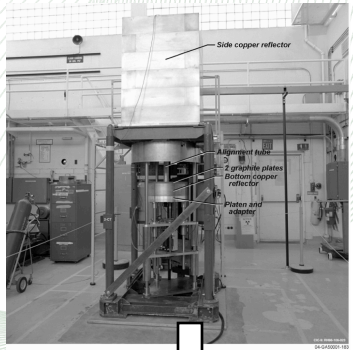
SAMINT: Nuclear Data Adjustment Based on Integral Benchmark Experiments (IBE)

- SAMINT is an auxiliary program designed to allow SAMMY to adjust nuclear data parameters based on integral data.
- Enables coupling of differential and integral data evaluation in a continuous-energy framework
- Informs the evaluation of resolved resonance parameters
  - Based on performance in simulations of IBE's
- Leverages RNSD (ORNL) expertise in sensitivity studies of nuclear IBE's and applications
  - SCALE modules TSUNAMI and TSURFER

Integral Experiments to Aid Nuclear Data Evaluation

- SAMINT can be used to extract information from integral benchmarks to aid the nuclear data evaluation process.
- Near the end of the evaluation based on differential experimental data, integral data can be used to:
  - Resolve remaining ambiguity between differential data sets
  - Guide the evaluator to troublesome energy regions
  - Inform the evaluator of the most important nuclear data parameters to integral benchmark calculations
  - Improve the nuclear data covariance matrix evaluation





SAMMY

ENDF

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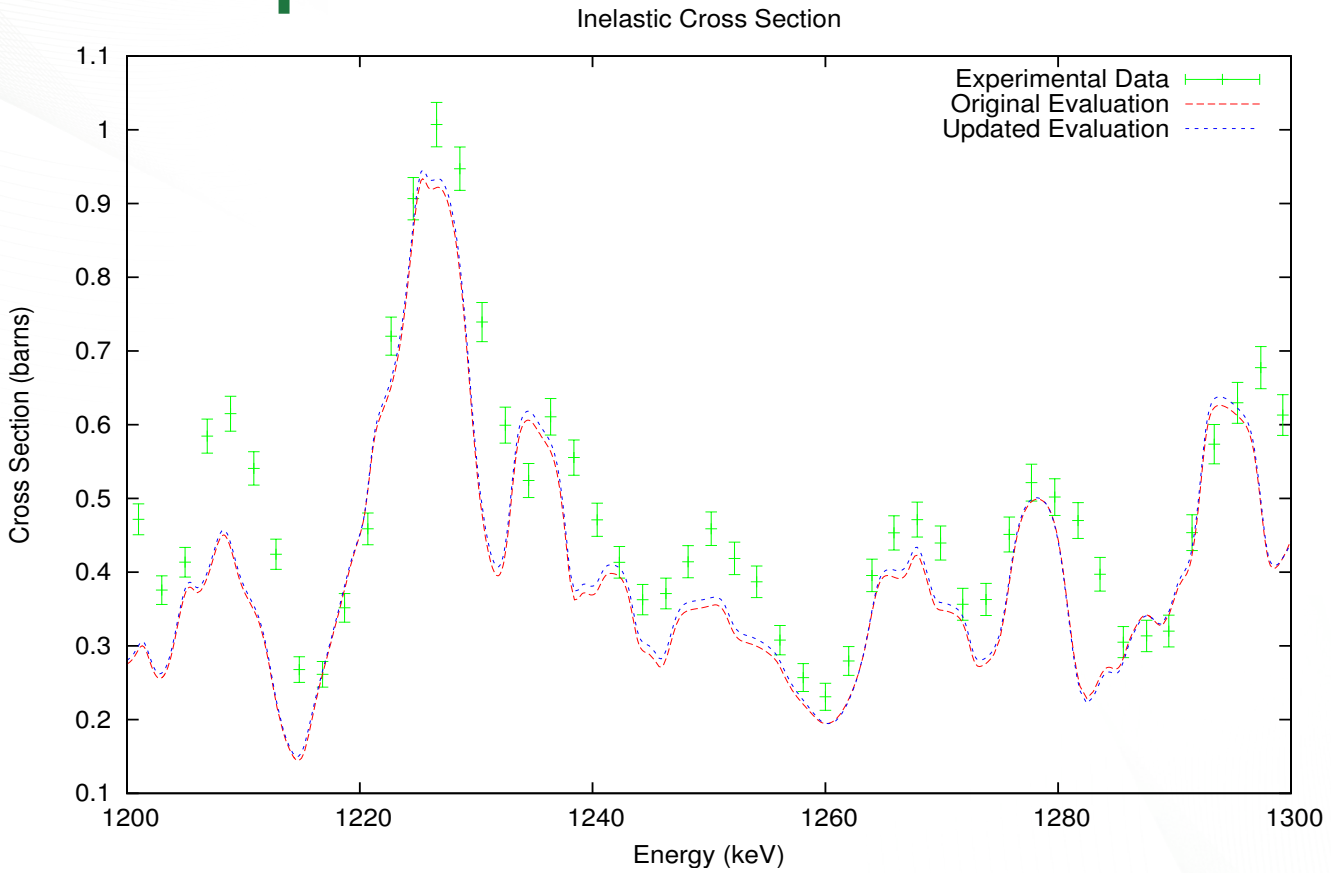
Cross Section Changes: Finer Scale than Differential Experimental Data



Inelastic cross section of ^{56}Fe before (χ^2 = 23.6023) and after (χ^2 = 22.9036) the adjustment based on integral experimental data plotted on top of differential experimental data of Perey, presented with one standard deviation error bars.

Connections to AMPX and SCALE

- AMPX: data processing suite for SCALE data libraries
  - Dorothea Wiarda, Andrew Holcomb, Michael Dunn (ORNL)
  - Shipped with SCALE 6.2 via https://rsicc.ornl.gov
- SCALE: nuclear modeling suite for design, safety, licensing
  - http://scale.ornl.gov Brad Rearden (ORNL) Manager
- SAMMY modernization follows AMPX and SCALE
  - Mercurial version control system
  - Cmake automated build and ctest automated testing
  - Fogbugz Bug tracking system
- SAMMY Module SAMRML “shared” with AMPX:
  - Stripped-down SAMMY for computing resonant cross sections
    - no parameter fitting, no Doppler or resolution broadening
  - also used in data processing codes: AMPX, NJOY, PREPRO
  - Modernized into C++ by Andrew Holcomb
    - Provides a framework for modernizing SAMMY

Modernization: SQA

- Version control of source code and test cases using Mercurial
- Bug tracking and workflow
- Cmake: auto configuration build (make –j)
- 25 executables built automatically on several platforms
- Ctest: auto testing tool
  - Test whether result are within a prescribed tolerance (1E-4)
    - SAMMY files tested: LST, PAR, LPT…
    - Makes it much easier to notice discrepancies.
  - 178 test cases from SAMMY 8.0.0 and
  - 4 new test cases for SAMINT
  - 1 new test case for RPI Lithium Glass detector resolution function
  - (All test cases include subcases.)

Supported Platforms and Compilers

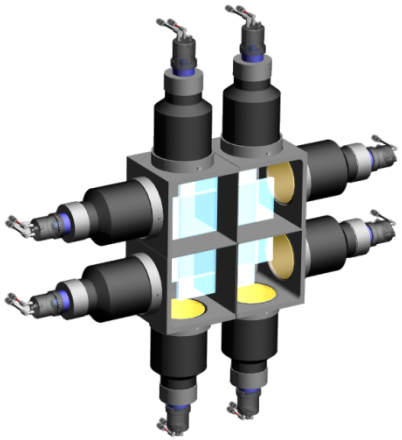
- Mac: gfortran
- Linux: gfortran, ifort
- Windows: ifort
  - Revealed few remaining issues that were corrected

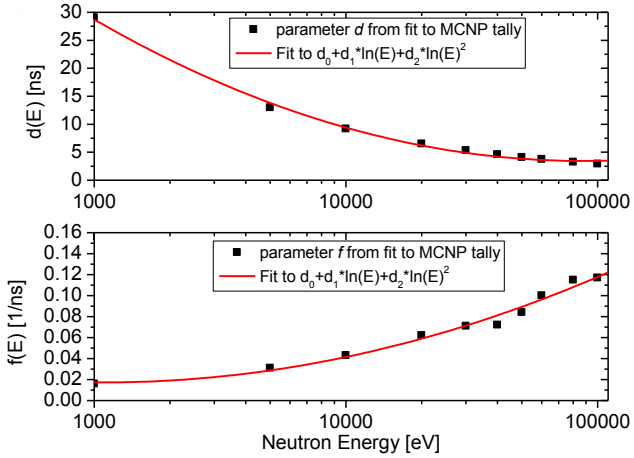
Modernization cont.'d

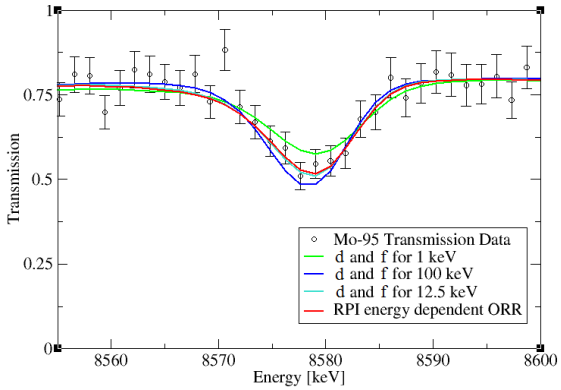
- Proposed SAMMY re-organization
  - Delineate modules that compute cross sections from those that fit resonance parameters to the data
  - i.e. keep SAMRML a standalone module called by a fitting program
  - Fitting method could remain Bayesian or Generalized Least Squares

^{6}Li-glass Neutron Detector Array MELINDA

- Improved parameterization
  - Based on MCNP simulations by Amanda Youmans (RPI)







Comparing the original SAMMY detector resolution function to the modified function with Mo-95 data

Before:

$$I(l) = \begin{cases} Dg & for\ 0 < t < d \\ De^{-f(t-d)} & for\ d < t \end{cases}$$

After:

$$d(E) = d_0 + \ln(E) * (d_1 + d_2 * \ln(E))$$

$$f(E) = f_0 + \ln(E) * (f_1 + f_2 * \ln(E))$$

Liquid Scintillator Detector liquid $CH_{1.212}$

- Based on MCNP simulations by Amanda Youmans (RPI)

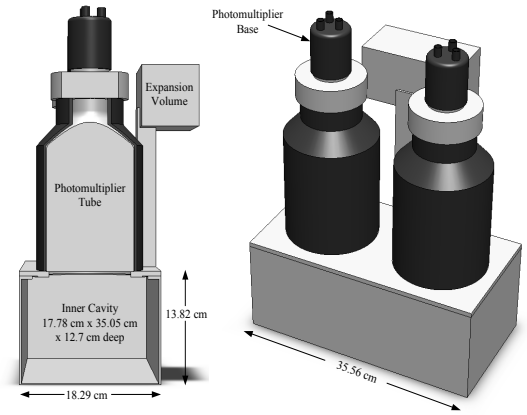
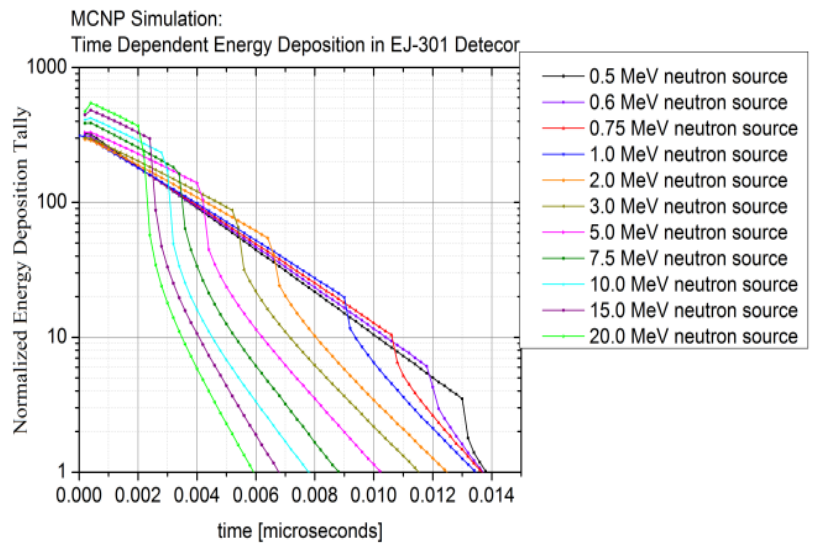
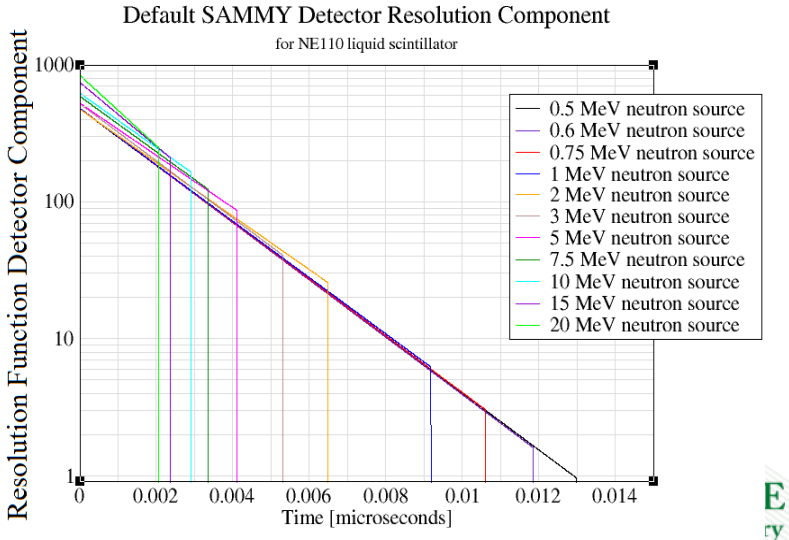


Table IV: Cross Sections for EJ-301 SAMMY Input	
Energy [eV]	Cross section [b]
500,000	7.967348
600,000	6.963397
750,000	5.958675
1,000,000	4.953201
2,000,000	3.101132
3,000,000	2.329274
5,000,000	1.683733
7,500,000	1.554593
10,000,000	1.172541
15,000,000	0.877705
20,000,000	0.663136





Minor improvements in SAMMY 8.1

- Updated physical constants
  - Consistent with SAMRML
  - SAMMY and SAMRML yield identical results now
- Corrected a misplaced index causing incorrect matrix multiplication for non-diagonal data covariance matrix
  - (uncovered and corrected by Vlad Sobes)
- Several other minor bug fixes
  - Revealed by compiler or platform idiosyncrasies

Recent Developments

- Convert SAMMY resonance parameters to formal R-matrix
  - SAMMY evaluations set $S_c(E)-B_c=0$ boundary condition (b.c.)
    - Advantage: resonance energies coincide with resonance peaks
    - Disadvantage: slight deviations from formal R-matrix
    - SAMMY does support formal R-matrix $B_c=-1$ b.c.
  - Andrew Holcomb programmed conversion to/from formal R-matrix
    - Converted ^{16}O $S_c(E)-B_c=0$ into formal parameters for Marco Pigni's talk
    - and is extending it to $L_c(E)-B_c=0$ in complex plane
- S-matrix pole representation of R-matrix
  - via e.g. Brune transform of R-matrix param.'s for $L_c(E)-B_c=0$ b.c.
  - Useful for on-the-fly Doppler broadening in neutron transport app.'s
    - Developed by Hwang (ANL) and Fritz Froehner (INR, Karlsruhe)
    - Ongoing collaboration Vlad Sobes and N.E. at M.I.T. (Pablo Ducru)
      - Talk by Vlad Sobes this Friday
  - Use Nicolas Michel's complex Coulomb w.f. library (CPC, 176 (2007) 232)

Conclusions and outlook

- ORNL has enlarged SAMMY user and developer expertise
  - various RRR evaluations ongoing and upcoming
    - Marco Pigni, Vlad Sobes, Luiz Leal
    - Klaus Guber collecting data at GELINA
  - SAMMY modernization continuing in a modern SQA framework
  - code sharing with AMPX modules
    - e.g. SAMRML modernized into C++ by Andrew Holcomb
  - Interaction with other R-matrix and data evaluation codes is encouraged.