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Title: Green function approach to R-matrix theory and applications to light nuclear reactions

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Green function approach to R-matrix theory and applications to light nuclear reactions

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Univ. Notre Dame, Dept. of Physics
Nuclear Physics seminar
2021-04-19

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Outline

1. Introduction & Motivation
2. Theory & Formalism
   - Scattering theory
   - Green functions
   - R-matrix in Green-Bloch formulation
3. Evaluations
   - NN
   - ^{5}Li
   - ^{10}Be
4. Conclusion & Outlook

Introduction

- Who: Light-element nuclear data evaluation "team" @ LANL/Theoretical Div.
  - Gerry Hale & MP
  - LANL collaborators
    - *D. Dodder, K. Witte, A. Sierk*, *R. MacFarlane*, N. Gibson, W. Haeck
  - External collaborators
    - D.Brown(BNL), C.Brune(OU), J.deBoer(ND), R.Capote(IAEA), V.Dimitriou(IAEA), I.Thompson(LLNL) *& many others*
- What: Light-element cross section evaluation for science and applications
- When: 70's → current
- Why...motivations, next slides

Motivation I

<u>Theoretical</u>

Address *open* problem of relativistic, multichannel scattering/reactions of composite strongly interacting (QCD) ***objects*** (*a.k.a.*, ***nuclei***)

1. **Elementary Particle Theory of Composite Particles***

   STEVEN WEINBERG†
   Department of Physics, University of California, Berkeley, California
   (Received 13 November 1962)

   THIS is the first of a series of articles, in which we hope to develop a method for the calculation of strong interaction processes.

2. **Quasiparticles and the Born Series***

   THIS is the second of a series of papers, in which we hope to develop a practicable method of calculating strong interaction processes.

3. **Systematic Solution of Multiparticle Scattering Problems***

   THIS is the third paper in our current series on the quasiparticle method. The first[1] showed how fic-

4. **???** *The 4th paper never appears*

   In the fourth paper we will extend these ideas to the fully relativistic case.[1] Here we shall see that the quasiparticles can provide the force that makes their introduction a necessity.

- ***Phenomenological R-matrix parametrization*** of light-element scattering/reactions (largely non-relativistic) may give clues about the more general problem

Motivation II

Practical Applications

Continuous (and multi-group) representation of scattering/reaction data is important for a variety of applications

- Nuclear astrophysics & cosmology
- Neutrinos and fundamental symmetries
- Energy
- Nuclear criticality & safety
- Nuclear security

LANL light-element program

- All compound systems A<20 (and a few above)
- Recent work in 2020:

Projectile\Target	^{1}H	^{2}H	^{3}H	^{3}He	^{4}He	^{6}Li	^{7}Li
n	2020	VIII.0	VIII.0	VIII.0	VIII.0	2020	VIII.0
p	2020	VIII.0	VIII.0	VIII.0	2020	VIII.0	VIII.0
d		VIII.0	VIII.0	2020	VIII.0[a]	VIII.0	VIII.0
t			VIII.0	VIII.0	2020	VIII.0	TENDL09
$h(^{3}\mathrm{He})$				VIII.0	VIII.0	VIII.0	TENDL09
α					VIII.0	TENDL09	TENDL09

^{11}B (α+^{7}Li, α+^{7}Li*, t+^{8}Be, n+^{10}B); ^{11}C (α+^{7}Be, p+^{10}B)
^{12}C (α+^{8}Be, p+^{11}B)
^{13}C (n+^{12}C, n+^{12}C*)
^{14}C (n+^{13}C)
^{15}N (p+^{14}C, n+^{14}N, α+^{11}B)
^{16}O (g+^{16}O, α+^{12}C)
^{17}O (n+^{16}O, α+^{13}C)
^{18}Ne (p+^{17}F, p+^{17}F*, α+^{14}O)

Theory

Overview of R-matrix approach

I. Solve the Schrodinger equation for the scattering problem

(by imposition of scattering *Boundary Conditions* – see next slide)

II. But rather than match the data at macroscopically large distances from the scatterer

(*as is usually done*)

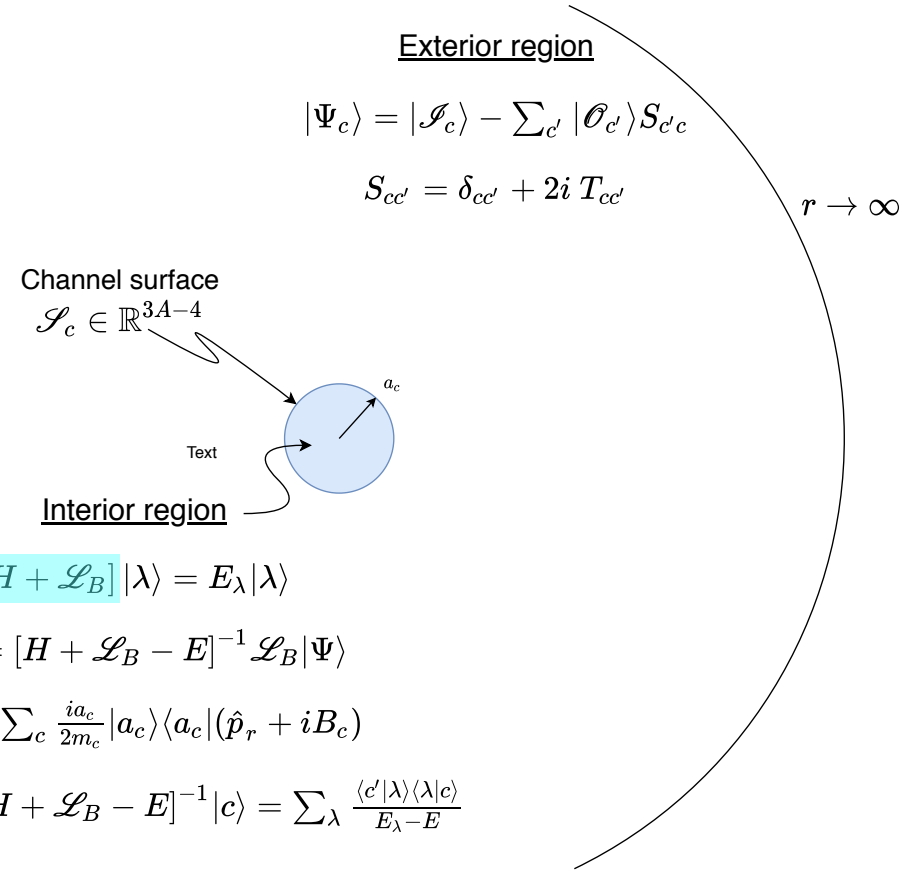
III. We assume that the asymptotic wave function is known down to microscopic scales

(*Coulomb* or *free*)

IV. Match at a finite radius – the *channel radius*: r_c or a_c

V. Why?

The finite channel surface boundary between *Interior* & *Exterior* regions allows the definition of a *compact, Hermitian* operator



$$[H + \mathscr{L}_B]\,|\lambda\rangle = E_\lambda |\lambda\rangle$$

$$|\Psi\rangle = [H + \mathscr{L}_B - E]^{-1}\,\mathscr{L}_B |\Psi\rangle$$

$$\mathscr{L}_B = \sum_c \frac{i a_c}{2 m_c} |a_c\rangle\langle a_c| (\hat{p}_r + i B_c)$$

$$R_{B,c'c} = \langle c'|[H + \mathscr{L}_B - E]^{-1}|c\rangle = \sum_\lambda \frac{\langle c'|\lambda\rangle\langle\lambda|c\rangle}{E_\lambda - E}$$

<u>Compound system & channels</u>

- ^{5}Li – interior region
- p+^{4}He, d+^{3}He, ... – exterior, asymptotic region

Theory
Scattering: Boundary condition

- ***Solve*** the Schrodinger equation for E>0, *in the continuum*

$$\left\{-\frac{\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r})\right\}\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

- ***Boundary condition***
  - Suppose

$$\Psi(\mathbf{r}) = \int \frac{d^3k'}{(2\pi)^{3/2}}\, e^{i\mathbf{k}'\cdot\mathbf{r}}\Psi(\mathbf{k}') \implies \lim_{|\mathbf{r}|\to\infty} \Psi(\mathbf{r}) \to 0 \text{ (by Riemann-Lebesgue)}$$

  - ***Correct BC*** for incoming plane wave with ***k***

$$\Psi(\mathbf{r}) = \int \frac{d^3k'}{(2\pi)^{3/2}}\, e^{i\mathbf{k}'\cdot\mathbf{r}}\Psi(\mathbf{k}') + e^{i\mathbf{k}\cdot\mathbf{r}}$$

only remaining term as $|\mathbf{r}| \to \infty$

  - ***Energy conservation*** [assume ℓ=0, elastic only]

$$\lim_{|\mathbf{r}|\to\infty} \Psi(\mathbf{r}) \to \underbrace{\frac{e^{-ikr}}{r}}_{\text{Incoming wave}} - \underbrace{\frac{e^{+ikr}}{r}}_{\text{Outgoing wave}} S_{\ell=0}(k)$$

Scattering "matrix"

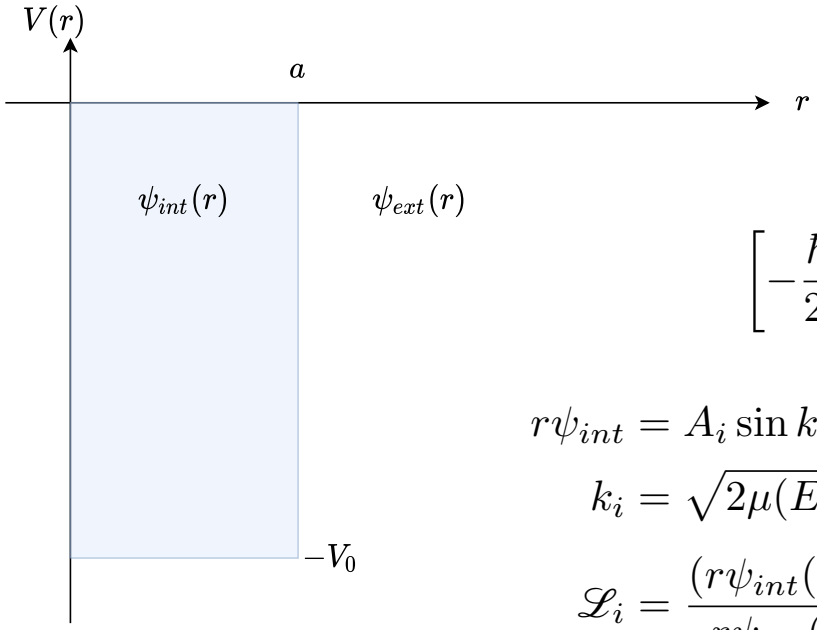
$$S_{\ell=0}(k) = e^{2i\delta_0(k)}$$

Phase shift

Theory

Scattering: Matching example [finite square well; ℓ=0]

- Finite square well



$$\left[-\frac{\hbar^2}{2\mu}(r\psi(r))'' + V(r)\right](r\psi(r)) = E(r\psi(r))$$

$$r\psi_{int} = A_i \sin k_i r \qquad r\psi_{ext} = A_e \sin(k_e r + \delta_0(E))$$

$$k_i = \sqrt{2\mu(E+V_0)} \qquad k_e = \sqrt{2\mu E}$$

$$\mathscr{L}_i = \left.\frac{(r\psi_{int}(r))'}{r\psi_{int}(r)}\right|_{r=a} \qquad \mathscr{L}_e = \left.\frac{(r\psi_{ext}(r))'}{r\psi_{ext}(r)}\right|_{r=a}$$

Matching condition at r=a: $\mathscr{L}_i = \mathscr{L}_e$

- Logarithmic derivative continuity

$$k_i^{-1}\tan k_i a = k_e^{-1}\tan(k_e a + \delta_0)$$

Caveat: unlike here, R-matrix matching occurs anywhere outside the range of the strong interaction

Theory
Green functions

- Usual application to inhomogeneous differential equations
  - Such as the Poisson equation EM
  - The Green function (or operator) is the *inverse* of the differential operator:

$$-\nabla^2\phi(\mathbf{r}) = 4\pi\rho(\mathbf{r})$$
$$\phi(\mathbf{r}) = \int d^3r' \frac{1}{|\mathbf{r}-\mathbf{r}'|}\rho(\mathbf{r}')$$

$$\boxed{\text{“}G = -(\nabla^2)^{-1}\text{”} \longleftrightarrow -\nabla'^2 G(\mathbf{r}') = 4\pi\delta(\mathbf{r}')}$$

- R-matrix approach requires *generalized* Green function
  - Incorporate *boundary condition* information directly into Green function

$$\left(H + \hat{\mathscr{L}}_a^{(0)} - E\right)|\Psi\rangle = |F\rangle$$
$$|F\rangle = |f\rangle + A|a\rangle$$
$$\hat{\mathscr{L}}_a^{(0)} = \frac{i\hbar}{2\mu}|a\rangle\langle a|\hat{p}_r$$
$$\langle r|\hat{p}_r = \frac{-i}{r}\frac{\partial}{\partial r}r\langle r|$$

$$\boxed{\left(H(r) + \hat{\mathscr{L}}_a^{(0)}(r) - E\right)\Psi(r) = F(r)}$$
$$F(r) = f(r) + A\frac{\delta(r-a)}{r^2}$$
$$\hat{\mathscr{L}}_a^{(0)}(r) = \frac{\hbar^2}{2ma}\frac{\delta(r-a)}{r^2}\frac{d}{r}r$$

$$\int_{a-\epsilon}^{a+\epsilon} dr$$

$$\boxed{\begin{aligned} &(H(r) - E)\,\Psi(r) = f(r) && \forall r \\ &\frac{\hbar^2}{2\mu a}\frac{d}{dr}\left(r\Psi(r)\right)\Big|_{r=a} = A && r = a \end{aligned}}$$

Theory

R-matrix: Exterior & Interior region wave functions

<u>Exterior region</u>

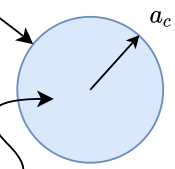
$$[H_E - E]\,|\mathscr{E}_c\rangle = 0$$

$$\mathscr{E}_c = \mathscr{O}_c \text{ or } \mathscr{I}_c$$

$$|\Psi_c\rangle = |\mathscr{I}_c\rangle - \sum_{c'} |\mathscr{O}_{c'}\rangle S_{c'c}$$

Channel surface

$\mathscr{S}_c \in \mathbb{R}^{3A-4}$



<u>Interior region</u>

$$\mathscr{H}_I(a_c, b_c)|\lambda(a_c, b_c)\rangle = E_\lambda(a_c, b_c)|\lambda(a_c, b_c)\rangle$$

$$\mathscr{H}_I(a_c, b_c) = H_I + \mathscr{L}_b(a_c)$$

$$\mathscr{L}_b(a_c) = \sum_c |a_c; c\rangle\langle a_c; c| \frac{i a_c^2}{2\mu_c}(\hat{p}_r + i b_c)$$

$r \to \infty$

Theory

Bloch-Green formalism

Algebraic mnemonic
Operators ~ Matrices

- Solve the multichannel, scattering (Schrodinger) equation

$$(H - E)\,|\Psi_c\rangle = 0$$

$$\left(H + \hat{\mathscr{L}}_b - E\right)|\Psi_c\rangle = \hat{\mathscr{L}}_b|\Psi_c\rangle$$

$$G_b = \left(H + \hat{\mathscr{L}}_b - E\right)^{-1}$$

$$|\Psi_c\rangle = G_b\hat{\mathscr{L}}_b|\Psi_c\rangle$$

$$\mathscr{H}_I(a_c, b_c)|\lambda(a_c, b_c)\rangle = E_\lambda(a_c, b_c)|\lambda(a_c, b_c)\rangle$$

$$\mathscr{H}_I(a_c, b_c) = H_I + \hat{\mathscr{L}}_b(a_c)$$

$$\hat{\mathscr{L}}_b(a_c) = \sum_c |a_c; c\rangle\langle a_c; c|\frac{ia_c^2}{2\mu_c}(\hat{p}_r + ib_c)$$

$$|a_c; c\rangle = |a_c; j_c m_c; \ell_c s_c\rangle\langle a_c; j_c m_c; \ell_c s_c|$$

- Matching @ $r_c = a_c$:

$$|\Psi_c\rangle = G_b\hat{\mathscr{L}}_b|\Psi_c\rangle \qquad |\Psi_c\rangle = |\mathscr{I}\rangle_c - \sum_{c'}|\mathscr{O}\rangle_{c'}S_{c'c}$$

$$|\mathscr{I}\rangle - |\mathscr{O}\rangle S = G_b(a_c)(\mathscr{D} - b)\left\{|\mathscr{I}\rangle - |\mathscr{O}\rangle S\right\} \quad \longleftarrow \text{Matching at } a_c$$

- Definition of R-matrix and S-matrix

$$G_{b;c',c} = \langle c'|\left(H + \hat{\mathscr{L}}_b - E\right)^{-1}|c\rangle$$

$$= \sum_\lambda \langle c'|\left(H + \hat{\mathscr{L}}_b - E\right)^{-1}|\lambda\rangle\langle\lambda|c\rangle$$

$$= \sum \frac{\langle c'|\lambda\rangle\langle\lambda|c\rangle}{E_\lambda - E} \longleftarrow \textit{Spectral} \text{ representation}$$

$$R(a_c, b_c) = \sum_\lambda \frac{\gamma_{\lambda,c'}\gamma_{\lambda,c}}{E_\lambda - E}$$

$$\gamma_{\lambda,c} = \frac{a_c}{\sqrt{2\mu_c}}\langle\lambda|c\rangle \in \mathbb{R}$$

$$S = O^{-1}I + 2iO^{-1}R_L O^{-1}$$

$$R_L = \left[1 + R(B - L)\right]^{-1}R$$

NB : S matrix does not depend on a_c, b_c

$$L \leftrightarrow L_{c'c} = \delta_{c'c}L_c \qquad L_c = \frac{a_c}{O_c}\frac{\partial O_c}{\partial r_c}\Big|_{r_c = a_c}$$

$$B \leftrightarrow B_{c'c} = \delta_{c'c}b_c$$

Theory

Bloch-Green formalism: S-matrix unitarity

$$S = O^{-1} I + 2iO^{-1} R_L O^{-1}$$

$$R_L^{-1} = R^{-1} + B - L$$

$$S^\dagger S = 1 \quad \text{Unitary constraint}$$

$$= 1 + 2iI^{-1} R_L^\dagger \left[(R_L^\dagger)^{-1} - R_L^{-1} - 2iI^{-1} O^{-1} \right] R_L O^{-1}$$

$$= 1 + 4I^{-1} R_L^\dagger \left[\underbrace{\text{Im } B}_{\to 0} - \underbrace{\text{Im } L + I^{-1} O^{-1}}_{\to 0, \implies P = \text{Im } L = (F^2 + G^2)^{-1}} \right] R_L O^{-1}$$

- Unitarity requires B real
- Energy independent level E_λ and reduced width $\gamma_{c\lambda}$ require B constant
- Unitarity is preserved for finite set $\{E_\lambda, \gamma_{c\lambda}\}$

Unitarity implications

$$\left.\begin{aligned} \delta_{fi} &= \textstyle\sum_n S^\dagger_{fn} S_{ni} \\ S_{fi} &= \delta_{fi} + 2i\rho_f\, T_{fi} \\ \rho_n &= \delta(H_0 - E_n) \end{aligned}\right\} \quad \boxed{T_{fi} - T^\dagger_{fi} = 2i \sum_n T^\dagger_{fn} \rho_n T_{ni}}$$

- ***Implications of unitarity constraint on transition matrix***
  1. Doesn't uniquely determine T_{ij}; highly restrictive, however
     Elastic: $\mathrm{Im}\ (T^{-1})_{11} = -\rho_1,\ \ E < E_2$ (assuming T & P invariance)
     Multichannel: $\mathrm{Im}\ \mathbf{T^{-1}} = -\boldsymbol{\rho}$
  2. Unitarity violating transformations
     - Scaling single ampl: $T_{ij} \to \alpha_{ij} T_{ij} \qquad \alpha_{ij} \in \mathbb{R}$
     - Phase x-form: $T_{ij} \to e^{i\theta_{ij}} T_{ij} \qquad \theta_{ij} \in \mathbb{R}$

     ★ consequence of linear 'LHS' $\propto$ quadratic 'RHS'
  3. Unitary parametrizations of data provide constraints that experiment may violate
     ★ *normalization*, in particular → $\boxed{\text{Observable} \propto \text{KF}\ \ |T_{fi}|^2}$
     ★ ^{17}O: Bair & Haas '73 vs. Harissopulos '05
     - ENDF/B-VIII.0 release: *Nucl. Data Sheets 148 (2018) 1–142*

Theory

Unpolarized & polarized scattering/reaction observables

- Wolfenstein trace formalism
  - Spin density matrix

$$\langle O_f \rangle = \frac{\mathrm{Tr}\ \rho_f O_f}{\mathrm{Tr}\ \rho_f}$$

$$\rho_f = M \rho_i M^\dagger \qquad M_{fi} = \frac{4\pi}{k_i} \langle s' m_s' | T | s m_s \rangle$$

$$\rho_i = \frac{1}{\mathrm{Tr}\ \mathbb{1}_i} \sum_i \langle O_i \rangle O_i \qquad \rho_i^{(0)} \equiv \frac{1}{N_s} \mathbb{1}_i$$

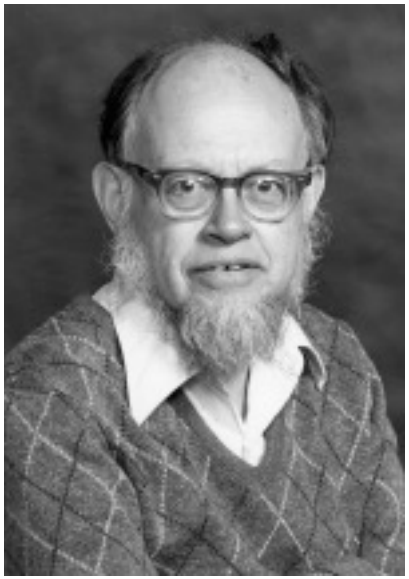
  - Unpolarized

$$\mathrm{Tr}\ \rho_i^{(0)} = \frac{1}{N_s} \mathrm{Tr}\ M M^\dagger$$

$$\sigma^{(0)}(E,\theta) = \frac{4\pi}{k_i^2} \frac{1}{(2s_1+1)(2s_2+1)} \sum_{\{m_s\}} \left| \langle s' m_s' | T(\{E_\lambda, \gamma_{\lambda,c}\}) | s m_s \rangle \right|^2$$

  - General polarization

$$\sigma^{(0)}(E,\theta) \langle O_f \rangle = \frac{1}{\mathrm{Tr}\ \mathbb{1}_i} \sum_i \langle O_i \rangle \mathrm{Tr}\ M O_i M^\dagger O_f \qquad \begin{cases} O_i = O_1 \otimes O_2 \\ O_f = O_3 \otimes O_4 \end{cases}$$



Lincoln Wolfenstein
1923-2015

R-matrix parametrization
Relativistic kinematics

$$R_{c'c}(E_\lambda, \gamma_{\lambda,c}) = \sum_\lambda \frac{\gamma_{\lambda,c'}\gamma_{\lambda,c}}{E_\lambda(s) - E(s)}$$

- Mandelstam s variable
  - Lorentz invariant
  - Channel invariant

$$p^\mu_{c,1} = (m_{c,1} + E_c, \mathbf{p}_{c,1}) \qquad p^\mu_{c,2} = (m_{c,2}, 0)$$

$$s = (p_{c,1} + p_{c,2})^2 = m_c^2 + 2m_{c,2}E_c$$

$$m_c = m_{c,1} + m_{c,2}$$

  - Relativistic parametrization form (reference channel c_0)

$$E(s) = \frac{s - m_{c_0}^2}{2m_{c_0}}$$

R-matrix evaluation for light nuclear systems

Nuclear Data Pipeline

EDA cross section evaluation

Observation
- ***Single*** experiment observations of yield
- Unpolarized: $\sigma_{tot}, \sigma, \sigma(\theta)$
- Polarization: $A_y, C_{xx'}, K_x^{x'}, \Sigma(\gamma), \ldots$

e.g. $\sigma(^4\mathrm{He}(t,n)^6\mathrm{Li})$

→

Compilation
- Combination of single-experiment ***differential*** data (EXFOR/CSISRS)
- ***Compound-system*** data deck

e.g.: $^7\mathrm{Li}$=$^4\mathrm{He}(t,t)^4\mathrm{He}$ $+^4\mathrm{He}(t,n)^6\mathrm{Li}+^6\mathrm{Li}(n,n)^6\mathrm{Li}$ $+\cdots$

RULE: Include ***all*** data

→

Evaluation
- Determination of initial parameters $(E_\lambda, \gamma_{\lambda,c})$ from known/guessed resonance structure (ENSDF, TUNL-NDEP)
- Optimization of $\chi^2 = \sum_{\text{expt's}} \chi^2_{\text{expt}}$

→

Processing
- Continuous-energy (ACE) & multigroup (NDI) formatted cross section libraries (NJOY)

→

Testing & Evaluation
- ***Integral*** benchmark testing (ICSBEP/IRPhEP/etc)
- Other applications codes

Optimize (currently via *email*)

- Cross section evaluation for light-elements (A≦20)
  - Quantum mechanical R-matrix (Wigner)
  - Correlates ***all*** experimental data simultaneously
    - pol/unpol; neutrons/charged-particles
    - Elastic/inel/transfer/reaction/break-up
    - Upper energy-limit restricted (break-up) < 20 MeV

Exterior region

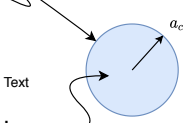
$$|\Psi_c\rangle = |\mathscr{I}_c\rangle - \sum_{c'} |\mathscr{O}_{c'}\rangle S_{c'c}$$

$$S_{cc'} = \delta_{cc'} + 2i\, T_{cc'}$$

$r \to \infty$

Channel surface

$\mathscr{S}_c \in \mathbb{R}^{3A-4}$



Interior region

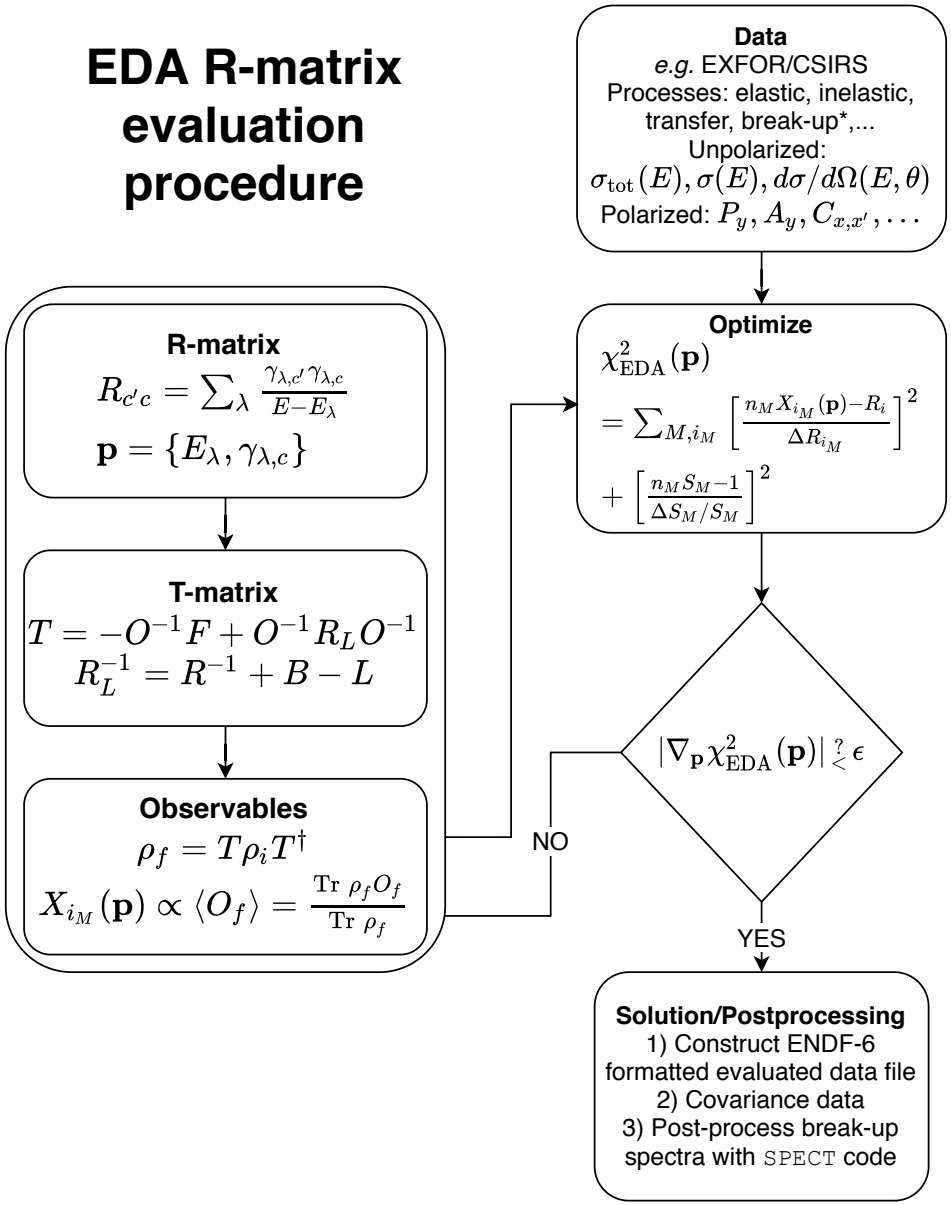
$$[H + \mathscr{L}_B]\,|\lambda\rangle = E_\lambda |\lambda\rangle$$

$$|\Psi\rangle = [H + \mathscr{L}_B - E]^{-1} \mathscr{L}_B |\Psi\rangle$$

$$\mathscr{L}_B = \sum_c \frac{i a_c}{2m_c} |a_c\rangle\langle a_c| (\hat{p}_r + iB_c)$$

$$R_{B,c'c} = \langle c'|[H + \mathscr{L}_B - E]^{-1}|c\rangle = \sum_\lambda \frac{\langle c'|\lambda\rangle\langle\lambda|c\rangle}{E_\lambda - E}$$

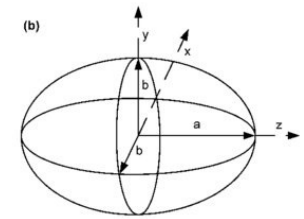
EDA evaluation procedure



Parameter uncertainty from χ^2

The Old Way gives too-small uncertainty

- At a solution: $\left.\frac{\partial \chi^2}{\partial p}\right|_{\hat{p}} \approx 0 \qquad \chi^2(p) \approx \chi^2(\hat{p}) + \sum_{\alpha,\beta=1}^{N_p} \delta p_\alpha (C^{-1})_{\alpha\beta} \delta p_\beta$



- Variations at $\hat{p}$:

$$\delta\chi^2(p) = \chi^2(\hat{p} + \delta p) - \chi^2(\hat{p})$$
$$= \delta p_1 A \delta p_1 + \delta p_1 B \delta p_2 + \delta p_2 B^T \delta p_1 + \delta p_2 D \delta p_2$$

- Change in χ^2 when $\{p_2\}$ change, re-optimize $\delta\chi^2$ w.r.t. $\{p_1\}$

$$\delta\chi^2(p_1 + \delta p_1^{min}, p_2 + \delta p_2) = \sum_{\alpha,\beta=N_1+1}^{N_2} \delta p_{2,\alpha} \tilde{D}^{-1}_{\alpha\beta} \delta p_{2,\beta}$$

- $\tilde{D}$: restriction of C to $\{p_2\}$-subspace

$$\delta\chi^2 = \frac{(\delta p_0)^2}{C_{00}} \implies \delta p_0 = (C_{00})^{1/2} \iff \delta\chi^2 = 1$$

- <u>NB</u>: the $\delta\chi^2 = 1$ hypersurface's average distance shrinks with incr. N_p

Parameter variance

- At a solution $\left.\frac{\partial \chi^2}{\partial p}\right|_{\hat{p}} \approx 0$ $\quad \chi^2(p) \approx \chi^2(\hat{p}) + \sum_{\alpha,\beta=1}^{N_p} \delta p_\alpha (C^{-1})_{\alpha\beta} \delta p_\beta$

- Assuming a normal distribution

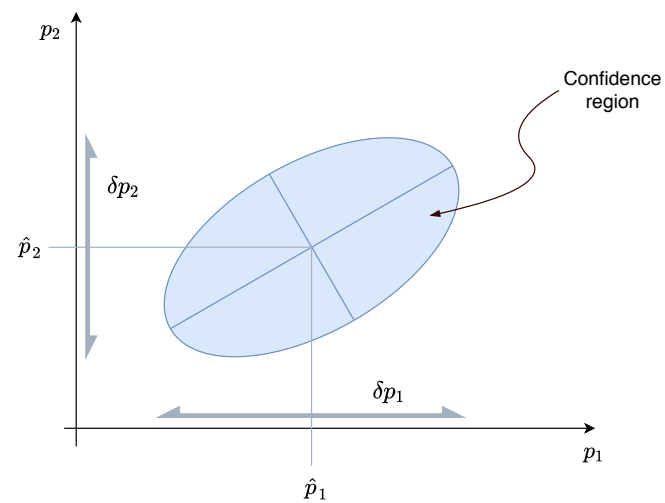
$$P_c(p|y) = \frac{1}{\det C^{1/2} (2\pi)^{N_p/2}} e^{-\frac{1}{2}\left[\chi^2(p) - \chi^2(\hat{p})\right]},$$

$$\langle (\delta p_\alpha)^2 \rangle = \int_{-\infty}^{\infty} dp_1 \cdots \int_{-\infty}^{\infty} dp_{N_p}\, P_c(p|y) (\delta p_\alpha)^2 = C_{\alpha\alpha}$$

- Change in chi-squared $\quad \delta p_\mu = (C_{\alpha\alpha})^{1/2} \delta_{\mu\alpha}$

$$\delta\chi^2(p) = \chi^2(\hat{p} + \delta p) - \chi^2(\hat{p}) = \sum_{\alpha,\beta} \delta p_\alpha (C^{-1})_{\alpha\beta} \delta p_\beta$$

$$\delta\chi^2(\delta p_\mu) = C_{\mu\mu} C^{-1}_{\mu\mu} = 1 - \sum_{\beta \neq \mu} (C_{\mu\beta})^2 < 1$$



- <u>NB</u>: adding redundant params can lower $\quad \delta\chi^2(\delta p_\mu)$

Uncertainties from chi-squared minimization

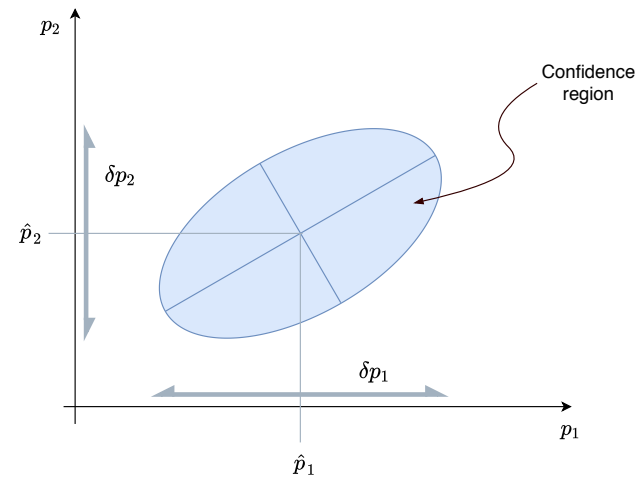
$$\chi^2_{\mathrm{EDA}}(\mathbf{p}) = \sum_{M,i_M} \left[\frac{n_{i_M} X_{i_M}(\mathbf{p}) - R_{i_M}}{\delta R_{i_M}}\right]^2 + \left[\frac{n_M S_M - 1}{\delta S_M / S_M}\right]^2 \left\{ \begin{array}{rl} M & : \text{experimental setup} \\ i & : \text{observable} \\ R_{i_M}, \delta R_{i_M} & : \text{relative measurement, uncert.} \\ X_{i_M} & : \text{calc'd observable} \\ n_M & : \text{normalization} \end{array} \right.$$

<u>Uncertainty determination comparison:</u>

1) previous: $\delta\chi^2 = 1 \implies$ Uncertainties too small; scaling: $\delta p_i = (C^0_{ii})^{1/2} \sim \mathcal{O}(N_p^{-1/2})$
2) improved:

$$P(\delta\chi^2 | k \text{ DOF}) = \frac{1}{2^{k/2}\Gamma(k/2)} \int_0^{\delta\chi^2} dt\, t^{k/2-1} e^{-t/2} = \mathrm{CL}(68\%: 1-\sigma;\ 95\%: 2-\sigma; \ldots)$$

Better scaling: $\delta p_i \sim (N_p C_{ii})^{1/2}$



Observable error propagation

Covariance matrix

The parameter covariance matrix is $\mathbf{C}_0 = 2\mathbf{G}_0^{-1}$, and so first-order error propagation gives for the cross-section covariances

$$\chi^2(\mathbf{p}) = \chi_0^2 + (\mathbf{p}-\mathbf{p}_0)^{\mathrm{T}}\mathbf{g}_0 + \tfrac{1}{2}(\mathbf{p}-\mathbf{p}_0)^{\mathrm{T}}\mathbf{G}_0(\mathbf{p}-\mathbf{p}_0)$$
$$= \chi_0^2 + \Delta\chi^2.$$

$$\begin{cases} \chi_0^2 = \chi^2(\mathbf{p}_0) \\ \mathbf{g}_0 = \nabla_{\mathbf{p}}\chi^2(\mathbf{p})\big|_{\mathbf{p}=\mathbf{p}_0} \approx 0 \\ \mathbf{G}_0 = \nabla_{\mathbf{p}}\mathbf{g}(\mathbf{p})\big|_{\mathbf{p}=\mathbf{p}_0} \end{cases}$$

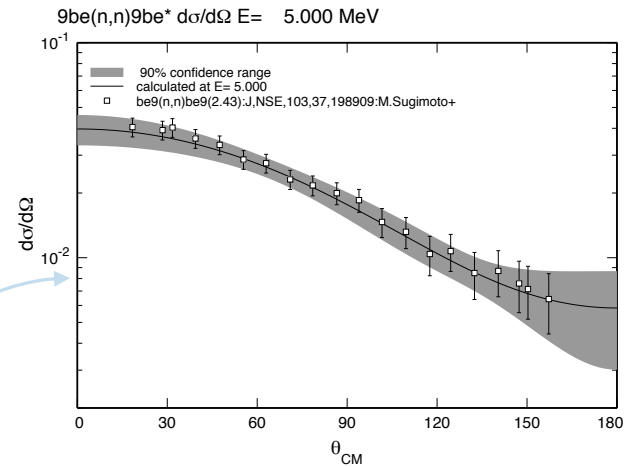
$$\boxed{\begin{aligned} \mathrm{cov}[\sigma_{\mathrm{i}}(E)\sigma_j(E')] &= \left[\nabla_{\mathbf{p}}\sigma_{\mathrm{i}}(E)\right]^{\mathrm{T}}\mathbf{C}_0\left[\nabla_{\mathbf{p}}\sigma_{\mathrm{j}}(E')\right]\Big|_{\mathbf{p}=\mathbf{p}_0} \\ &= \Delta\sigma_{\mathrm{i}}(E)\Delta\sigma_{\mathrm{j}}(E')\rho_{ij}(E,E'). \end{aligned}}$$

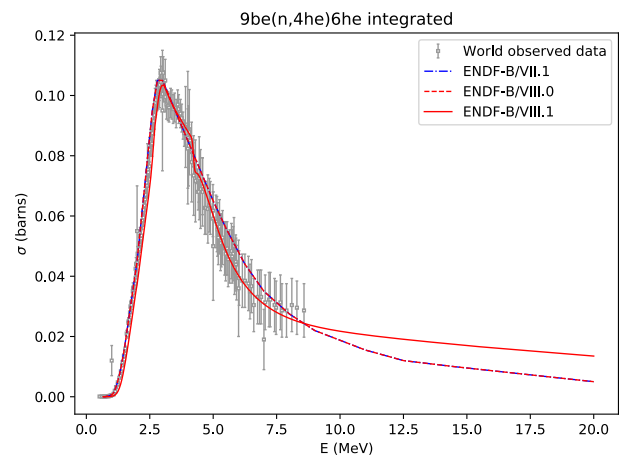
observable uncertainties

correlation coefficient

New code implementation

- Previous version **EDA5**
  - Versatile, numerically stable; legacy [F66 remnants] → difficult to modify/debug
- Current version **EDAf90**
  - **ModernFORTRAN(F90)** implementation
  - Identical numerically to **EDA5**
  - Interfaces with **NJOY2016/NJOY21**
  - Backend interface with **ENDFtk**
  - Frontend (observed data) interface with EXFOR/CSISRS (**c5** format)





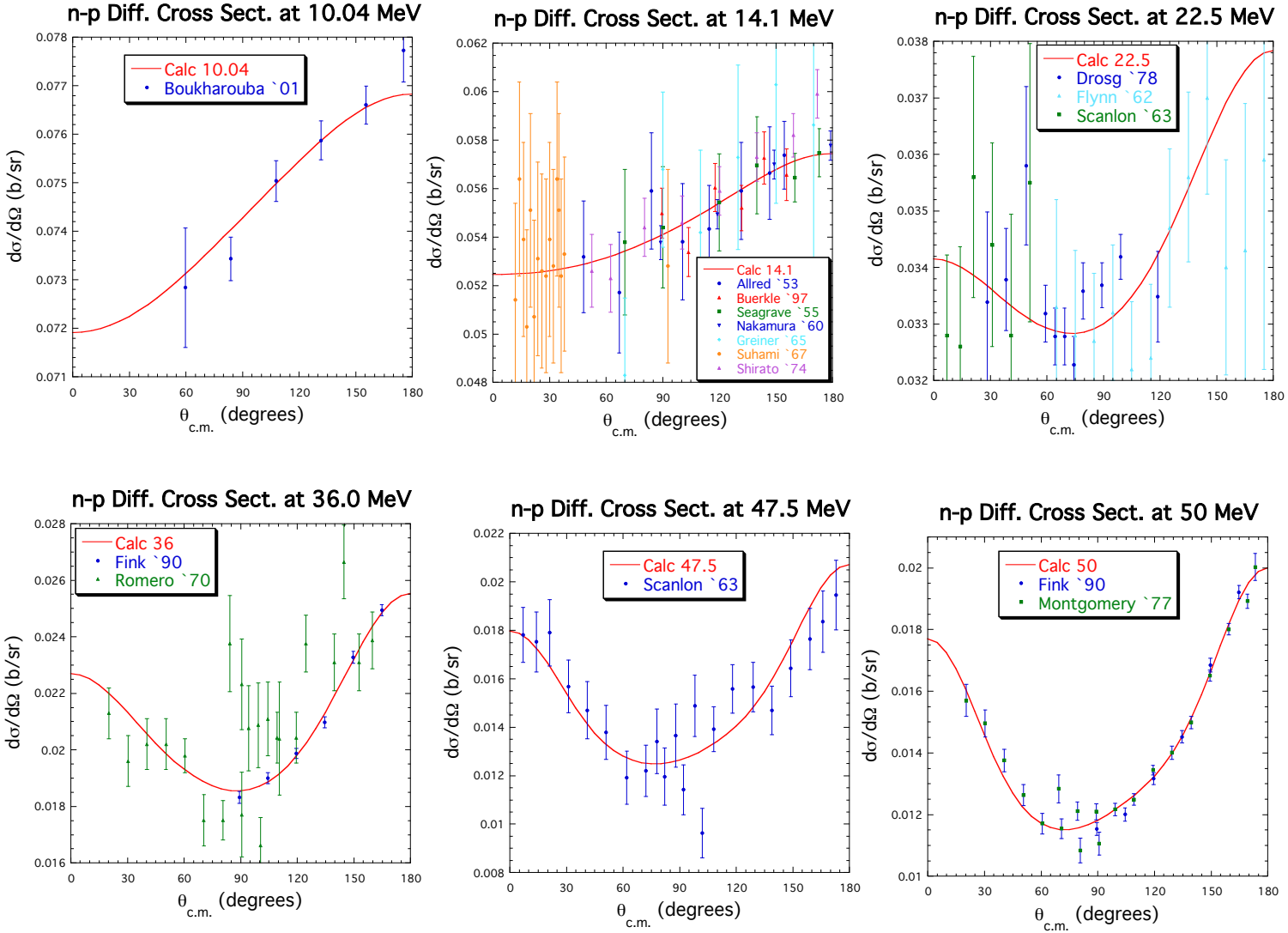
Charge-Independent Analysis of N-N Scattering up to 50 MeV

Channel	a_c (fm)	l_{max}
p+p	3.26	3
n+p	3.26	3
γ+d	40	1
n+n	3.26	3

Reaction	# Pts.	χ^2	Observable Types
p(p,p)p	675	950	$\sigma(\theta)$, $A_y(p)$, $C_{x,x}$, $C_{y,y}$, $K_x^{x'}$, $K_y^{y'}$, $K_z^{x'}$
p(n,n)p	4815	3764	σ_T, $\sigma(\theta)$, $A_y(n)$, $C_{y,y}$, $K_y^{y'}$
p(n,γ)d	86	179	σ_{int}, $\sigma(\theta)$, $A_y(n)$
d(γ,n)p	88	77	σ_{int}, $\sigma(\theta)$, $\Sigma(\gamma)$, $P_y(n)$
n(n,n)n	1	0	a_0
Norms.	183	86	
Total	5848	5056	20

free parameters = 43+183 $\Rightarrow$ χ^2/degree of freedom = 0.899

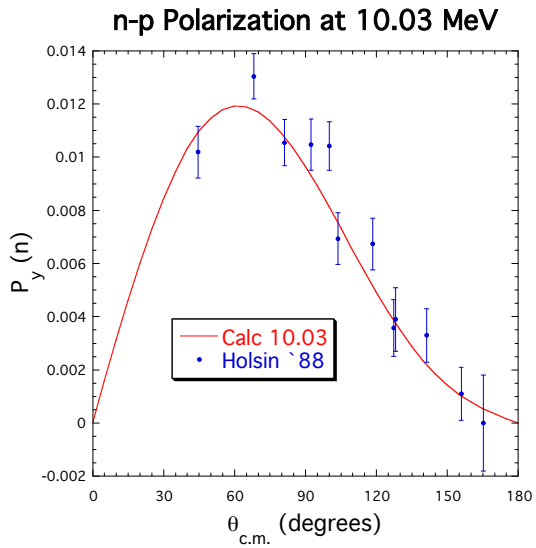
n-p Elastic Scattering Differential Cross Sections

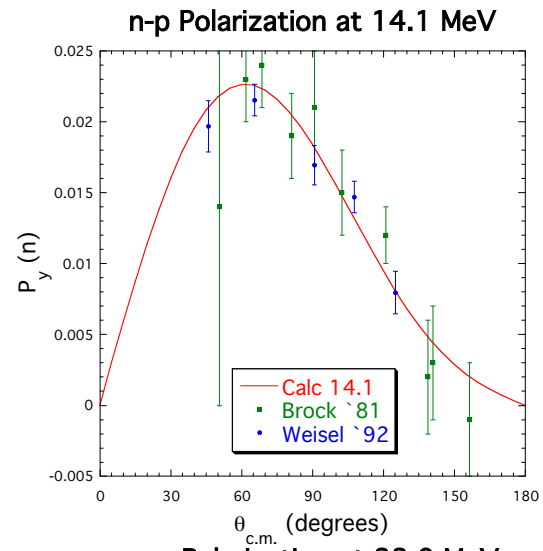


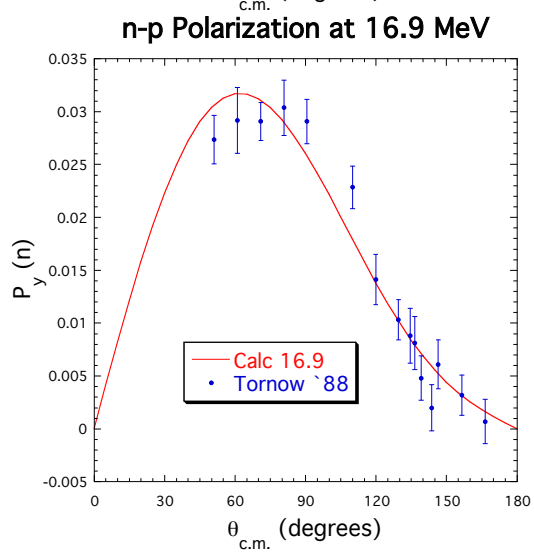
n-p Elastic Scattering Polarizations

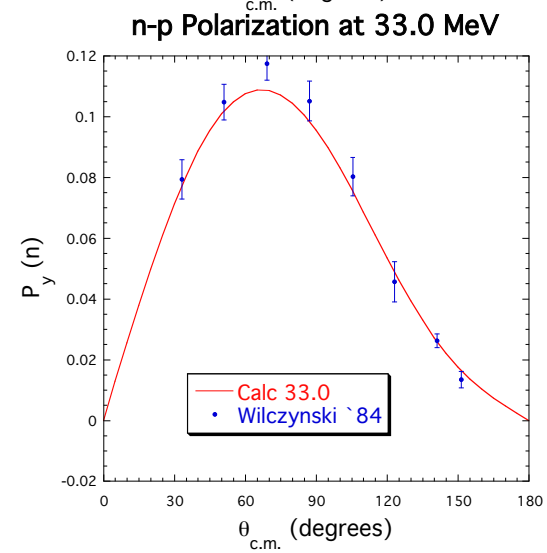
- Why include polarizations?

- Further constrain the scattering amplitudes and possibly find a unique solution (χ^2 minimum).

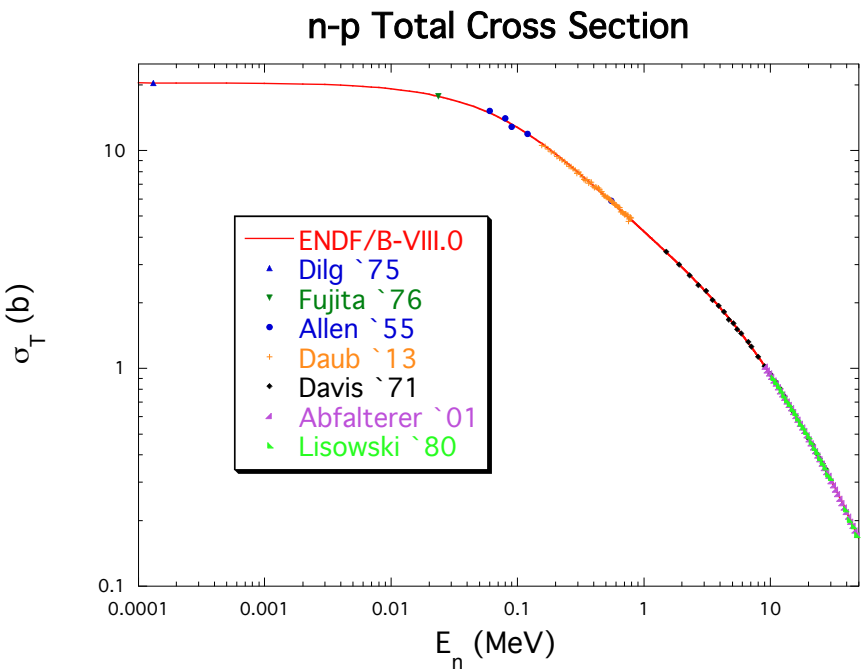


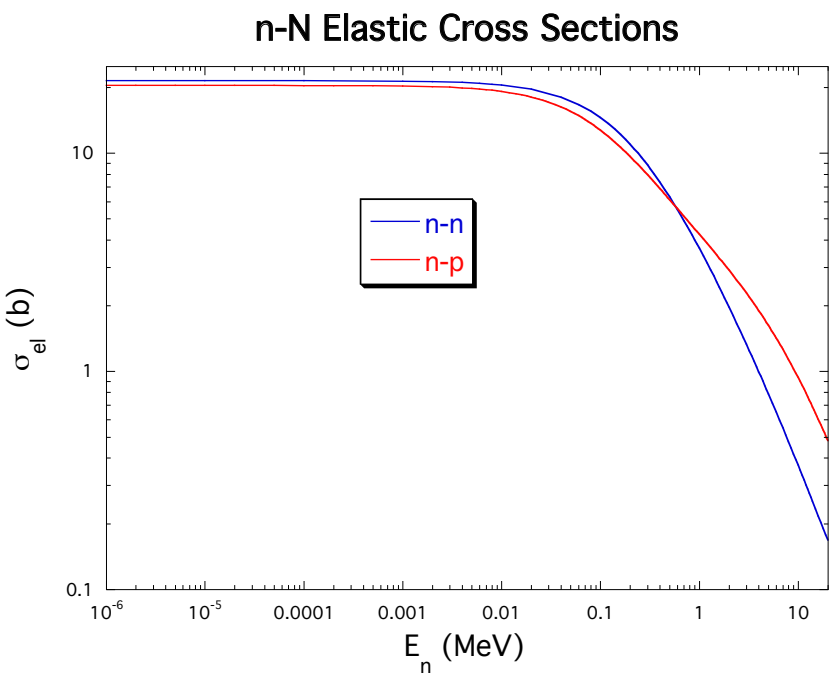




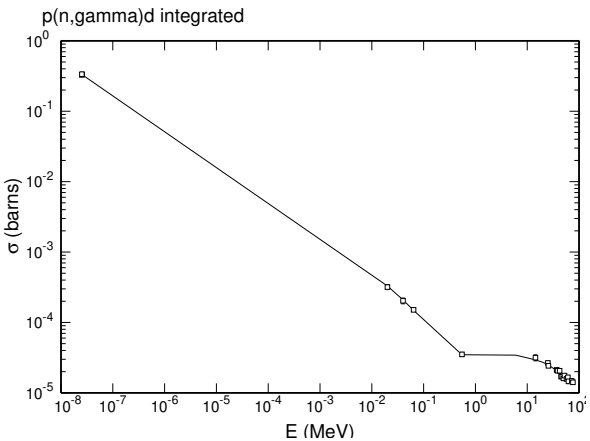


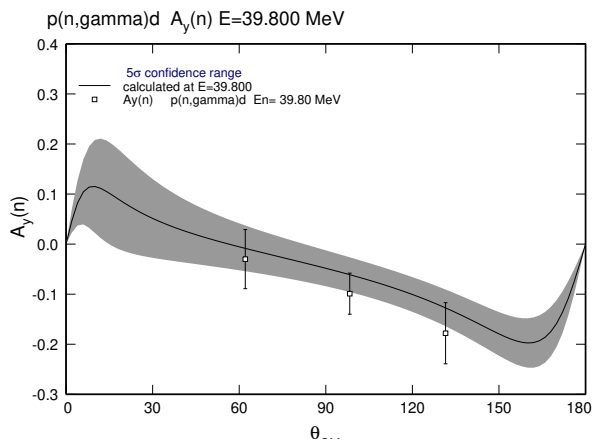
Integrated Cross Sections for n-p and n-n Scattering

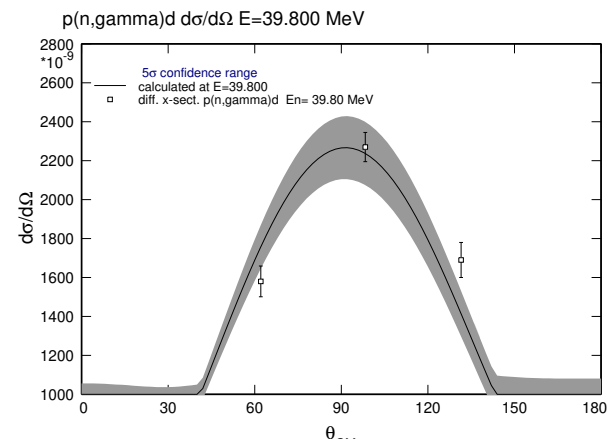


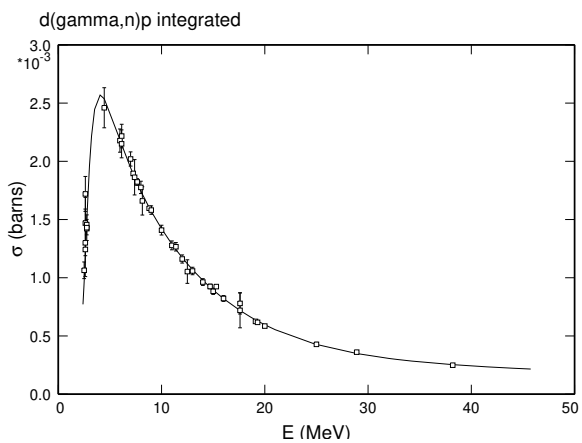


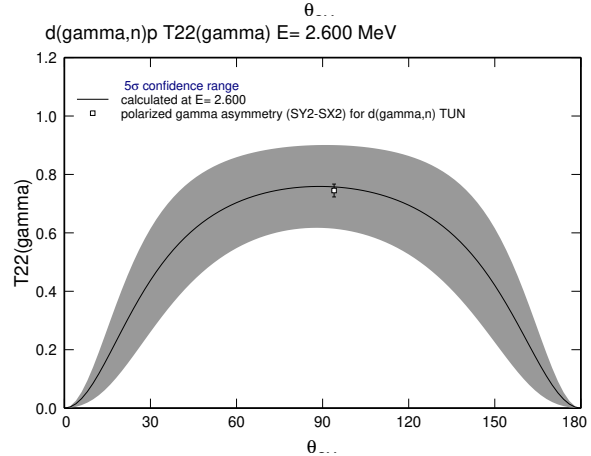
n+p Capture and g+d Photodisintegration Data

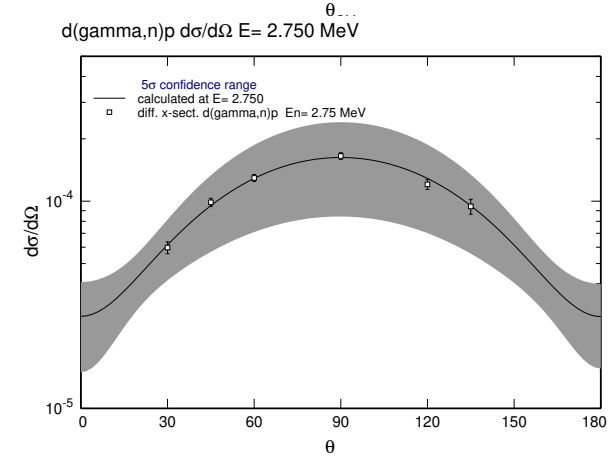




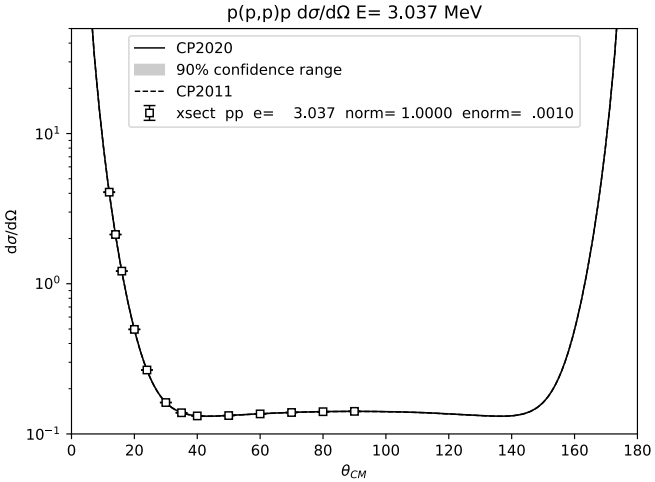


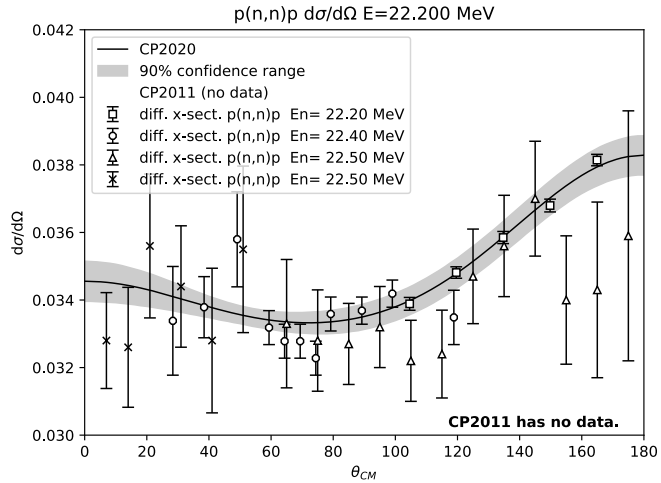


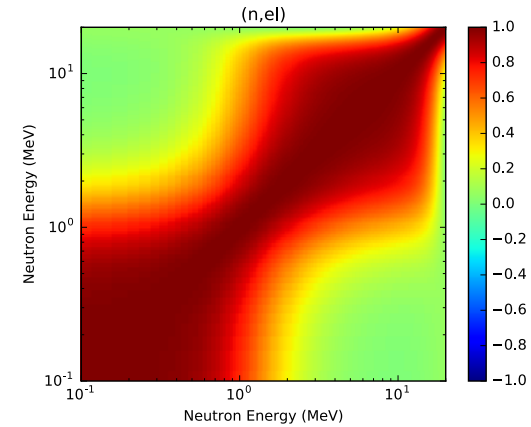




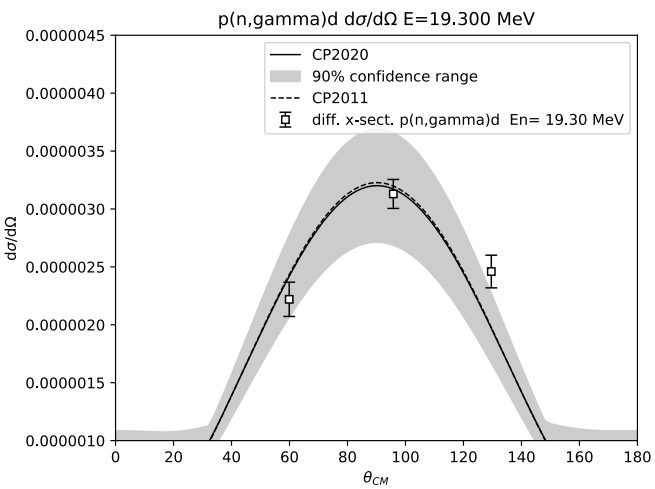
NN system covariance data

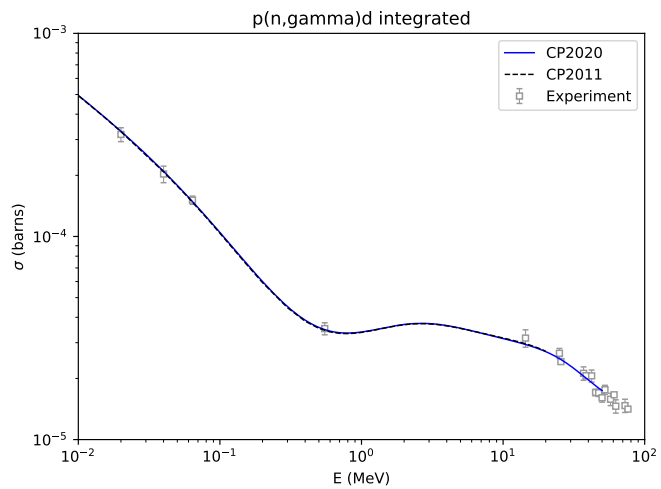






Covariance matrix





Partitions:

$$pp(\ell \leq 3); np(\ell \leq 3);$$
$$\gamma d(\ell \leq 1); nn(\ell \leq 3)$$

36 channels $(J^\pi LS)$

$$\chi^2/\mathrm{dof} \simeq 0.9$$

R-matrix evaluation

^{5}Li system

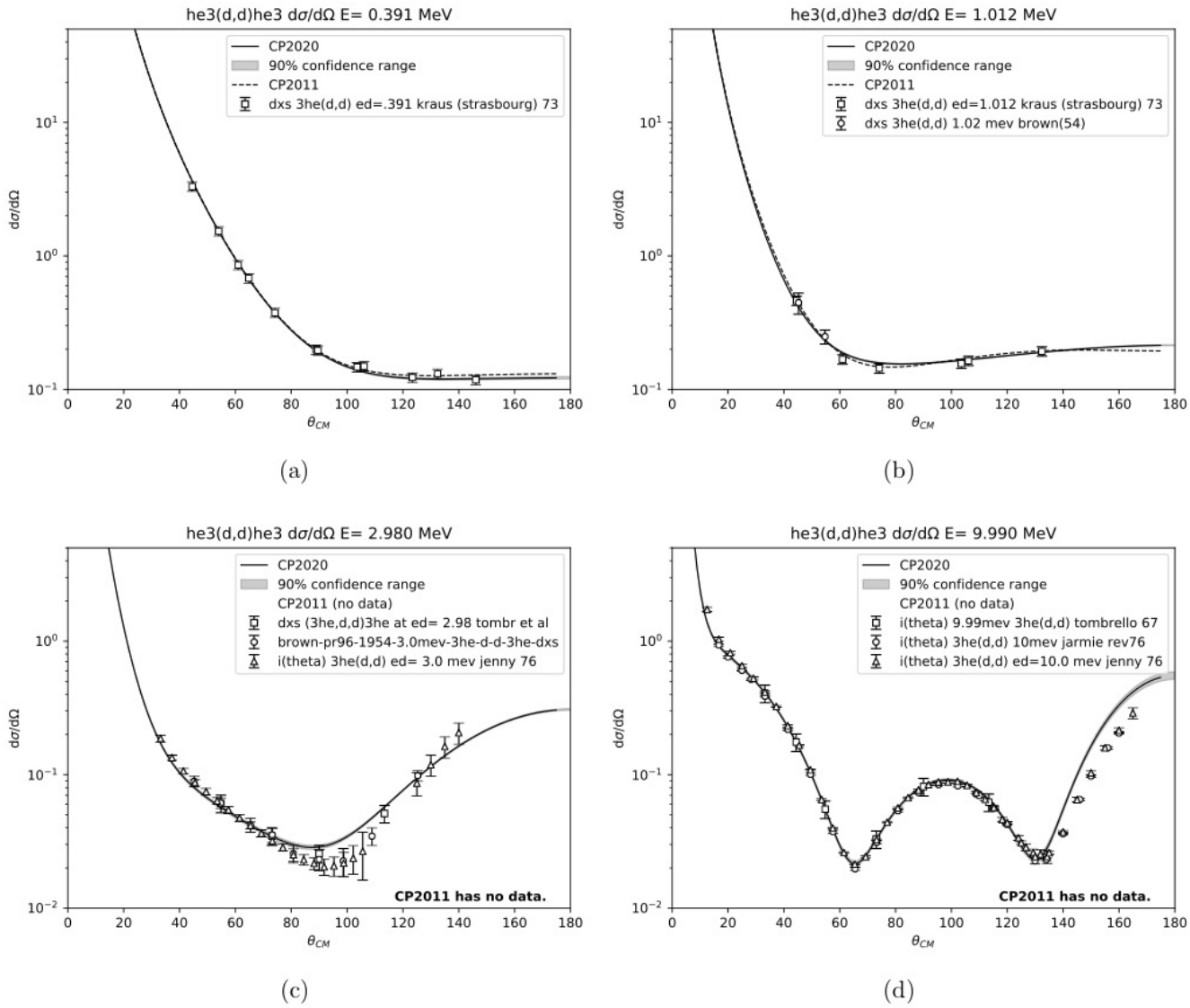
Channel	a_c (fm)	l_{max}
$d + {}^3\mathrm{He}(\frac{1}{2}^+)$	4.8	4
$p + {}^4\mathrm{He}(0^+)$	2.9	4
$p + {}^4\mathrm{He}^*(0^+;\ 20.2\ \mathrm{MeV})$	3.4	2
$d_0 + {}^3\mathrm{He}(\frac{1}{2}^+)$	5.1	0

Reaction	Energy Range (MeV)	# Data Points	Observables
${}^3\mathrm{He}(d,d){}^3\mathrm{He}$	$E_d = 0.32 - 10.0$	2,229	$\sigma(\theta), A_i, A_{ii}, C_{i,j}, C_{ij,k}, K_{i,j'k'}, K_{ij,k'l'}$
${}^3\mathrm{He}(d,p){}^4\mathrm{He}$	$E_d = 0.13 - 10.0$	3,839	$\sigma(E), \sigma(\theta), A_i, A_{ii}, C_{i,j}, K_{ij,k'}$
${}^3\mathrm{He}(d,p){}^4\mathrm{He}^*$	$E_d = 3.70 - 6.70$	28	$\sigma(\theta)$
${}^4\mathrm{He}(p,p){}^4\mathrm{He}$	$E_p = 0.92 - 34.3$	867	$\sigma(E), \sigma(\theta), A_y, P_y$
	Total:	6963	

Table 1: Channel configuration (top) and data summary (bottom) for the ^{5}Li system analysis. The column labeled "Observables" indicates the following data types: $\sigma(E)$, integrated cross section; $\sigma(\theta)$, unpolarized angular distributions (energy-dependence suppressed); A initial-state analyzing power; P final-state polarization; C spin correlation coefficients; K polarization transfer coefficients. (We have suppressed the indices $i, j, \ldots$ which take on values x, y, z for spins/polarization directions in configuration space.) All polarization and spin distributions are angular distributions, which depend on the angle of the outgoing particle. Chi-squared per degree of freedom for the analysis is $\chi^2/\mathrm{dof} \simeq 2.7$ over 7,178 data points, 215 of which were discarded by eliminating individual data points which contribute to $\chi^2 > 40$.

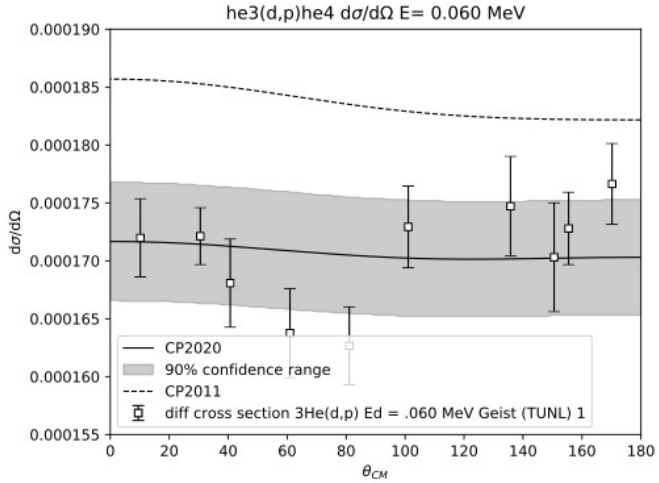
^{5}Li system evaluation

^{3}He(d,d)^{3}He

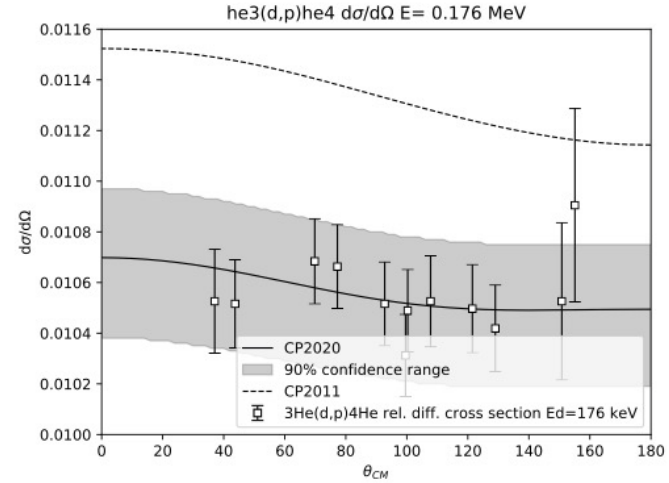


^{5}Li system evaluation

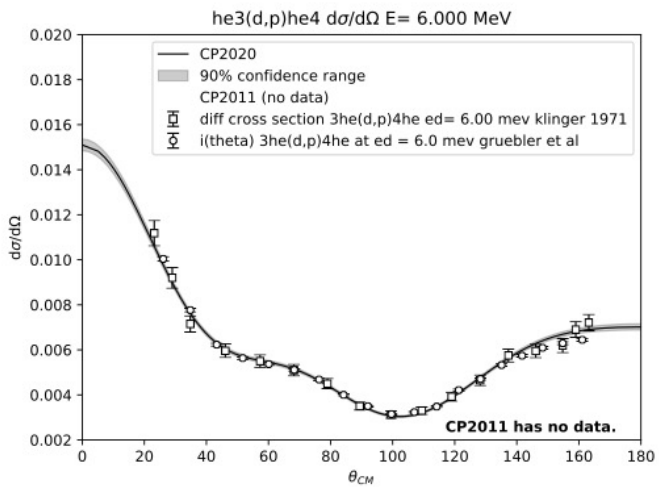
^{3}He(d,p)^{4}He



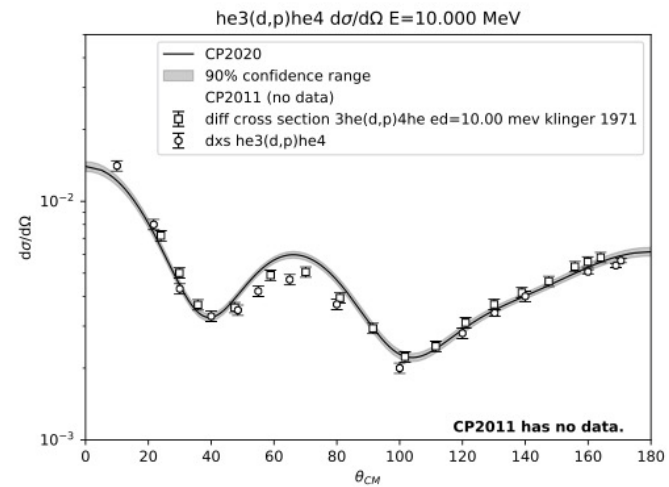
(a)



(b)



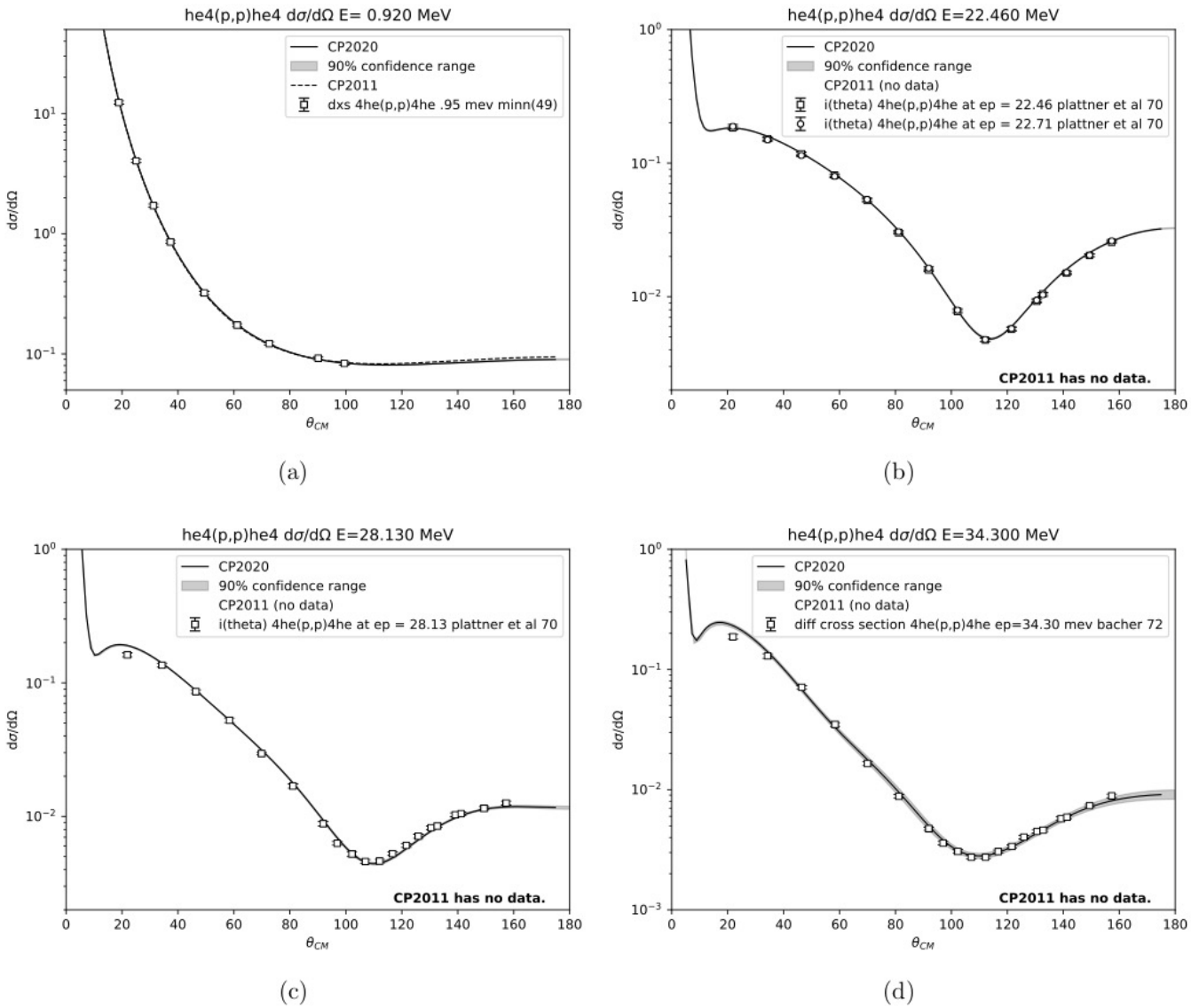
(c)



(d)

^{5}Li system evaluation

^{4}He(p,p)^{4}He



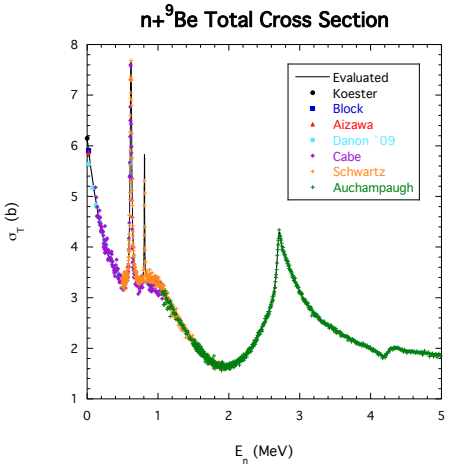
n+^{9}Be
New evaluation

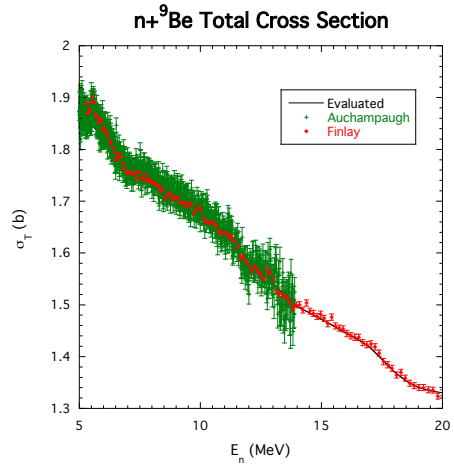
- Added data: elastic, (n,α), (n,n$_1$)

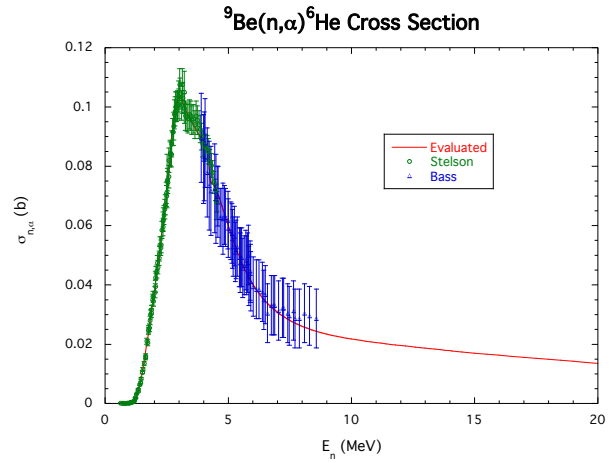
Channel	a_c(fm)	$\ell_{\max}$
$n+^9\mathrm{Be}(\frac{3}{2}^-)$	4.67	3
$^4\mathrm{He}+^6\mathrm{He}(0^+)$	5.00	4
$(nn)_0+^8\mathrm{Be}(2^+)$	5.20	3
$n+^9\mathrm{Be}^*(\frac{5}{2}^-)$	5.20	1

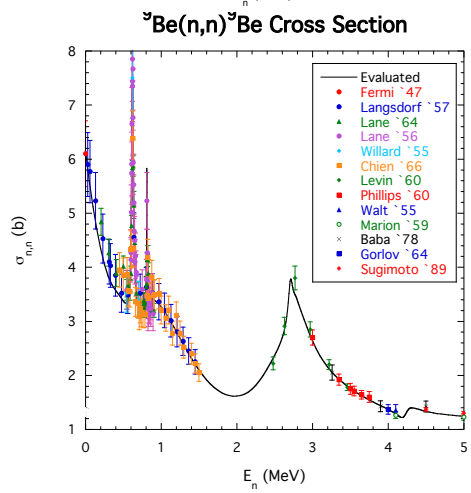
Process	E_n range	Observables	N_{dat}	χ^2/N_{dat}
$^9\mathrm{Be}(n,n_0)^9\mathrm{Be}$	(1.25 eV, 15.4 MeV)	$\sigma_{\mathrm{tot}}, \sigma, \sigma(\theta), A_y(\theta)$	5782	1.65
$^9\mathrm{Be}(n,{}^4\mathrm{He})^6\mathrm{He}$	(0.63, 8.5) MeV	$\sigma, \sigma(\theta)$	178	1.40
$^9\mathrm{Be}(n,2n)^8\mathrm{Be}$	(1.8, 14.7) MeV	σ	40	NA
$^9\mathrm{Be}(n,n_1)^9\mathrm{Be}^*$	(2.7, 5.0) MeV	$\sigma(\theta)$	83	1.65
Total			6083	1.75

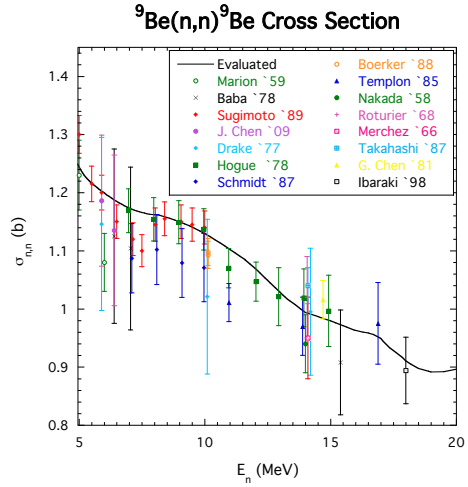
n+^{9}Be Integrated Cross Sections

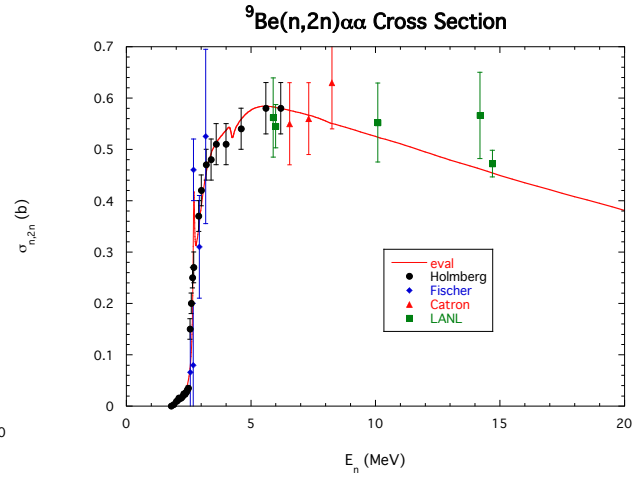




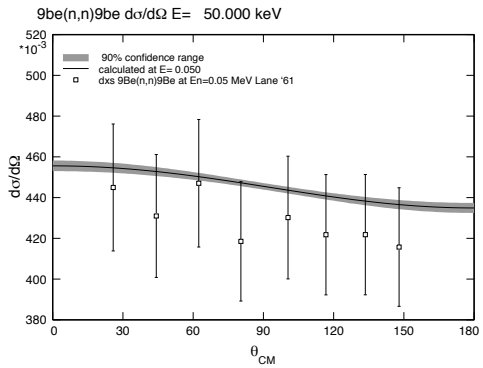


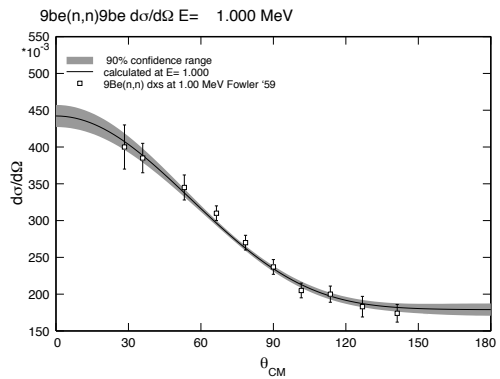


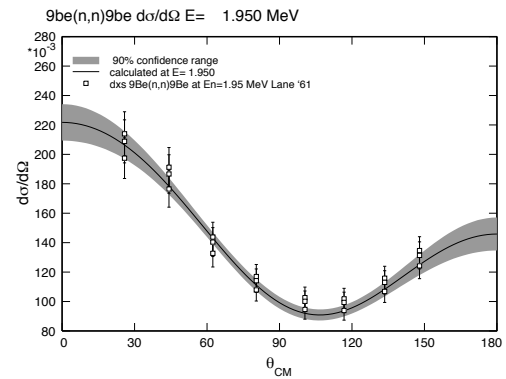


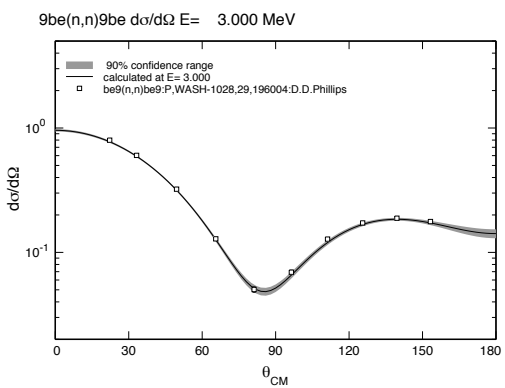


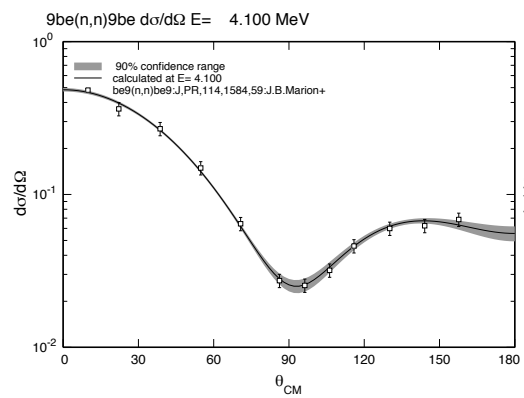
^{9}Be(n,n)^{9}Be Differential Cross Sections

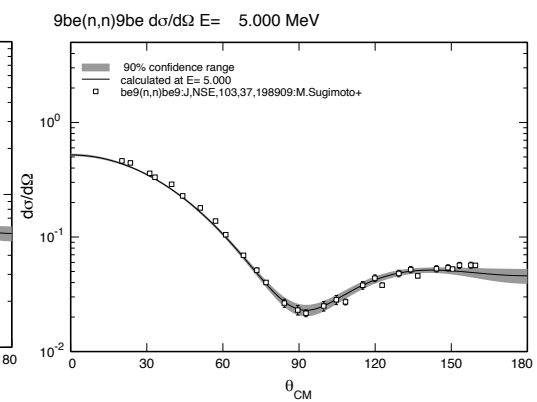




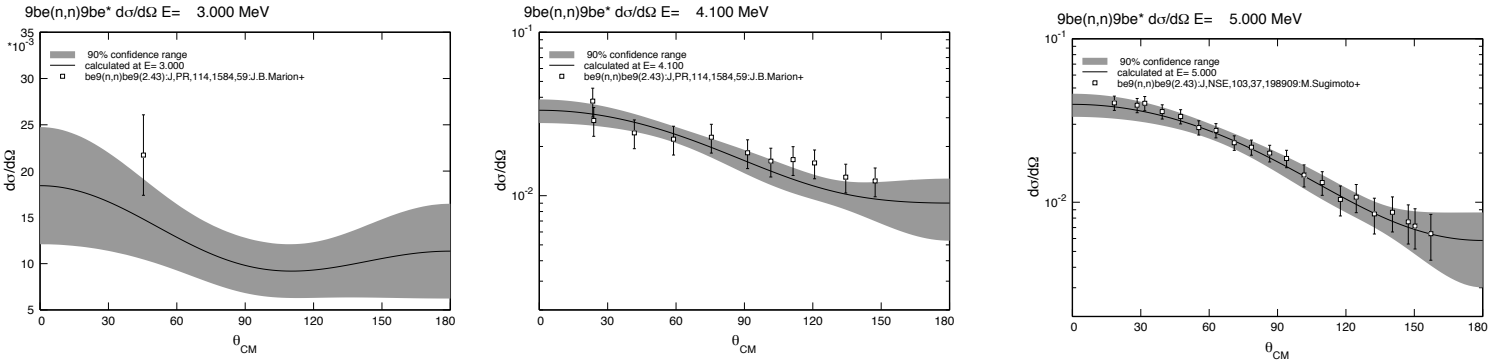








$^{9}Be(n,n_2)^{9}Be^{*}$ Differential Cross Sections

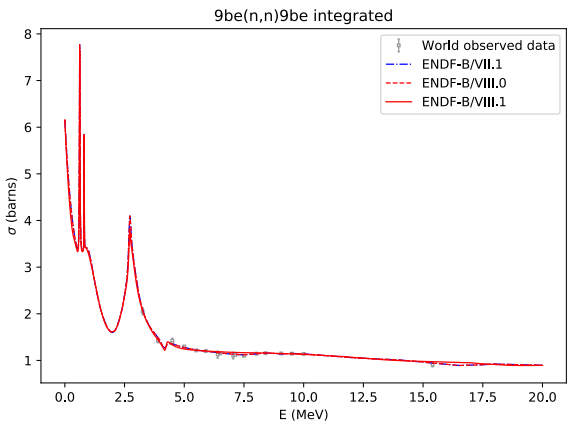


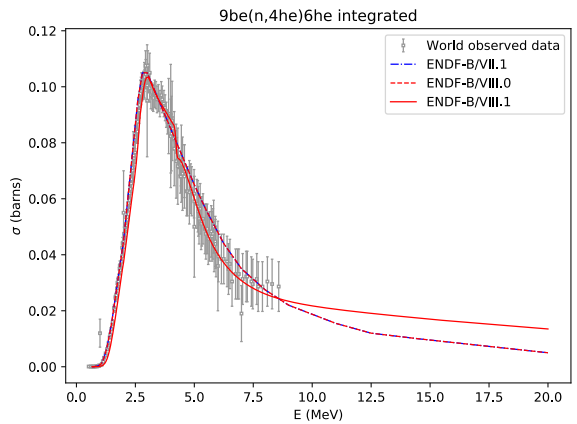
Summary of new evaluation:

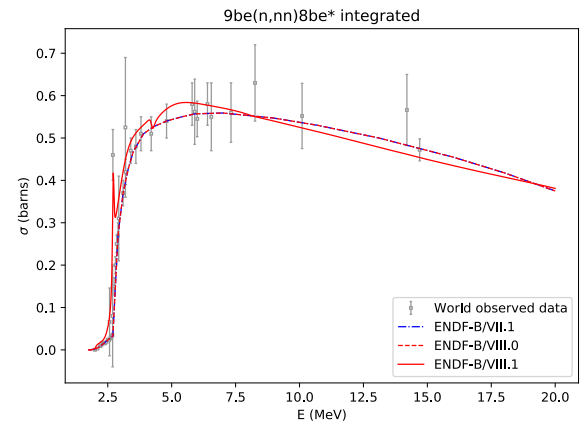
- ^{10}Be analysis has produced a consistent set of cross sections and angular distributions that are in agreement with most of the experimental data at energies up to 5 MeV. Extensions above that energy were based on the experimental data alone.
- Level assignments for the overlapping resonances near E_n=2.7 MeV have the opposite parity ($4^-,3^+ \rightarrow 4^+,3^-$).
- Excited states of ^{9}Be make important contributions to the (n,2n) cross section (MT=16 → 24 in the new evaluation).
- Testing/benchmarking: (M. Herman, LANL) and thick-target angular neutron yields (Y. Danon, RPI) on the following slides

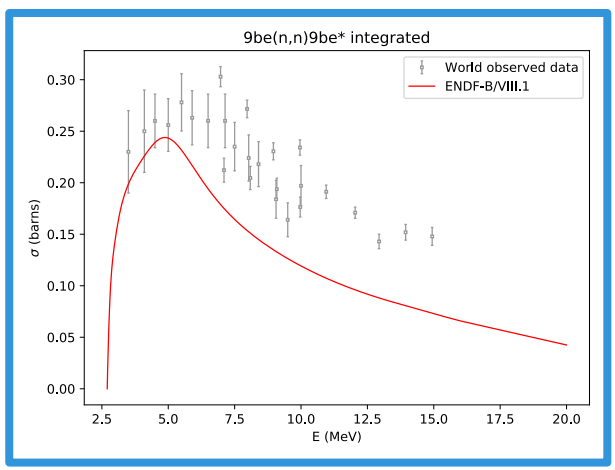
Comparison to previous ENDF/B

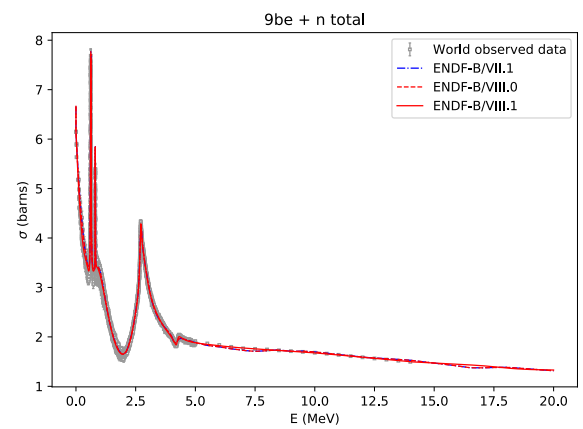
Integrated cross sections











Conclusions

- R-matrix
  - Correlates all processes associated with a given compound system
  - Enforces
    - Unitarity, relating the *magnitudes* and *phases* of amplitudes of different processes (total, elastic, inelastic, reaction, etc.)
    - Causality; proper complex-analytic properties
- Systematically improvable
  - More data
    - Polarized observables
    - Higher-energy data

Outlook

- Continued code modernization & improvement
  - Higher energies → break-up reactions
    - Currently post-processed by auxiliary codes
    - Immediate objective: *(z,z'n)*, *(z,z'γ)*, etc.
- Uncertainty quantification
  - Currently
    - χ^2 minimization with per-experimental setup normalization
    - Appears sufficient for 2⟼2 body scattering/reactions, single compound system
  - Planned
    - Bayesian statistical methods
      - Data covariances
      - Several compound systems concurrently
- Ongoing/planned evaluation
  - ^{9}Be, ^{17}O
  - Neutrons on H,C,N,O

Thank you for your patience and attention.