Uncertainty quantification in R-matrix calculations

Uncertainties in Calculations of Nuclear Reactions of Astrophysical Interest

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Mainz Institute for Theoretical Physics, Johannes Gutenberg University

Mark Paris & Gerry Hale

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Outline

- Overview
- Bloch-Green formalism
- Application to ^{7}Li compound system
- Uncertainty quantification

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

Bloch-Green formalism
Reaction theory

- Wigner PR72 29 1947
- Lane&Thomas RMP30 257 1953
- Bloch NP4 503 1957

- Solve Schrodinger given external solution ('a' chan. rad.)

$$[H-E]\Psi=0, \qquad [H-E+\mathscr{L}]\Psi=\mathscr{L}\Psi, \qquad \Psi=r^{-1}\Big[I-OS\Big]_{r\geq a}$$

$$\Psi=G\mathscr{L}\Psi, \qquad G=[H-E+\mathscr{L}]^{-1}, \qquad \mathscr{L}=a^{-1}\left(\rho\frac{\partial}{\partial\rho}-B\right)$$

$$I-OS=R\left(\rho\frac{\partial}{\partial\rho}-B\right)[I-OS], \qquad R\equiv G\Big|_{\mathscr{S}}, \qquad \rho\frac{\partial}{\partial\rho}O=LO$$

$$S=O^{-1}I+2i\rho O^{-1}R_LO^{-1}, \qquad R_L=\Big[1+R(B-L)\Big]^{-1}R, \qquad \rho\frac{\partial}{\partial\rho}I=LI-2i\rho O^{-1}$$

- External (Coulomb) wave function relations

$$O=I^*=G+iF, \qquad 1=GF'-G'F,$$

$$L=\rho O^{-1}\frac{\partial}{\partial\rho}O\equiv\mathcal{S}+iP, \qquad \mathcal{S}=\rho\frac{GG'+FF'}{G^2+F^2}, \qquad P=\rho\frac{1}{G^2+F^2}$$

Bloch-Green formalism

S-matrix unitarity

$$S = O^{-1}I + 2i\rho O^{-1}R_L O^{-1}$$

$$S^\dagger = OI^{-1} - 2i\rho I^{-1}R_L^\dagger I^{-1}$$

$$S^\dagger S = 1 + 2i\rho I^{-1}R_L^\dagger\left[(R_L^{-1})^\dagger - R_L^{-1} + 2i\rho I^{-1}O^{-1}\right]R_L O^{-1}$$

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

$$B = B^* \implies L - L^* = 2i\rho I^{-1}O^{-1} \text{ or } P = \rho\frac{1}{G^2 + F^2}$$

$$R_{c'c} = (c'|\left[H + \mathscr{L} - E\right]^{-1}|c) = \sum_\lambda \frac{\gamma_{c'\lambda}\gamma_{c\lambda}}{E_\lambda - E}$$

- 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

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

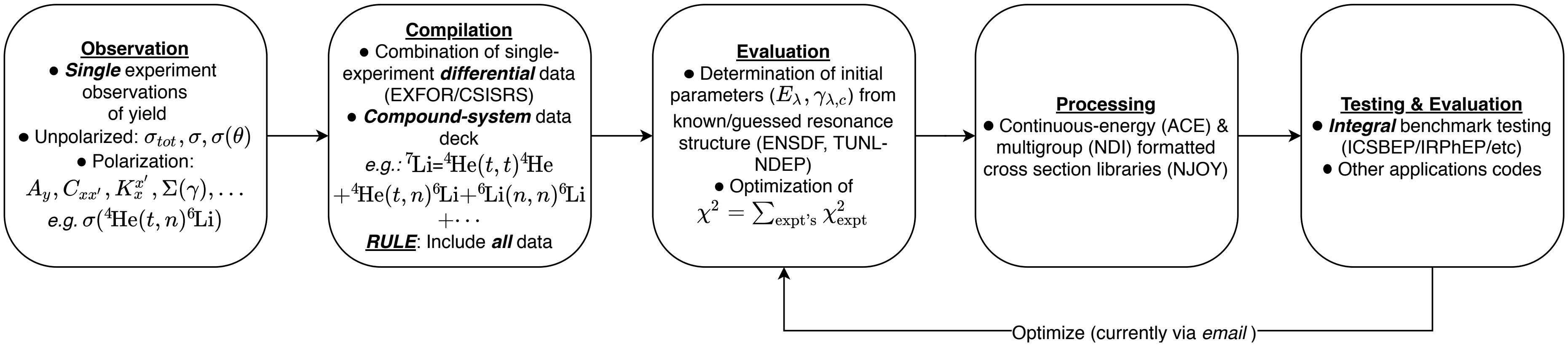
- **Implications of unitarity constraint on transition matrix**
  1. Doesn't uniquely determine T_{ij}; highly restrictive, however
     Elastic: $\mathrm{Im}\, T_{11} = -\rho_1,\ E < E_2$ (assuming T & P invariance)
     Multichannel: $\mathrm{Im}\,\mathbf{T} = -\boldsymbol{\rho}$
  2. Unitarity violating 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 → $\boxed{\text{Observable} \propto \text{KF}\ \left|T_{fi}\right|^2}$

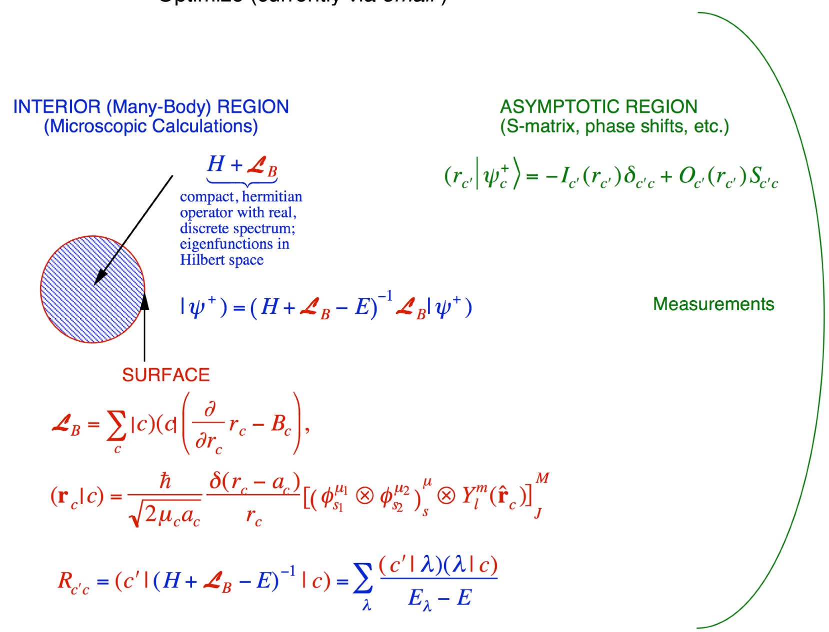
R-matrix evaluation for light nuclear systems

Nuclear Data Pipeline

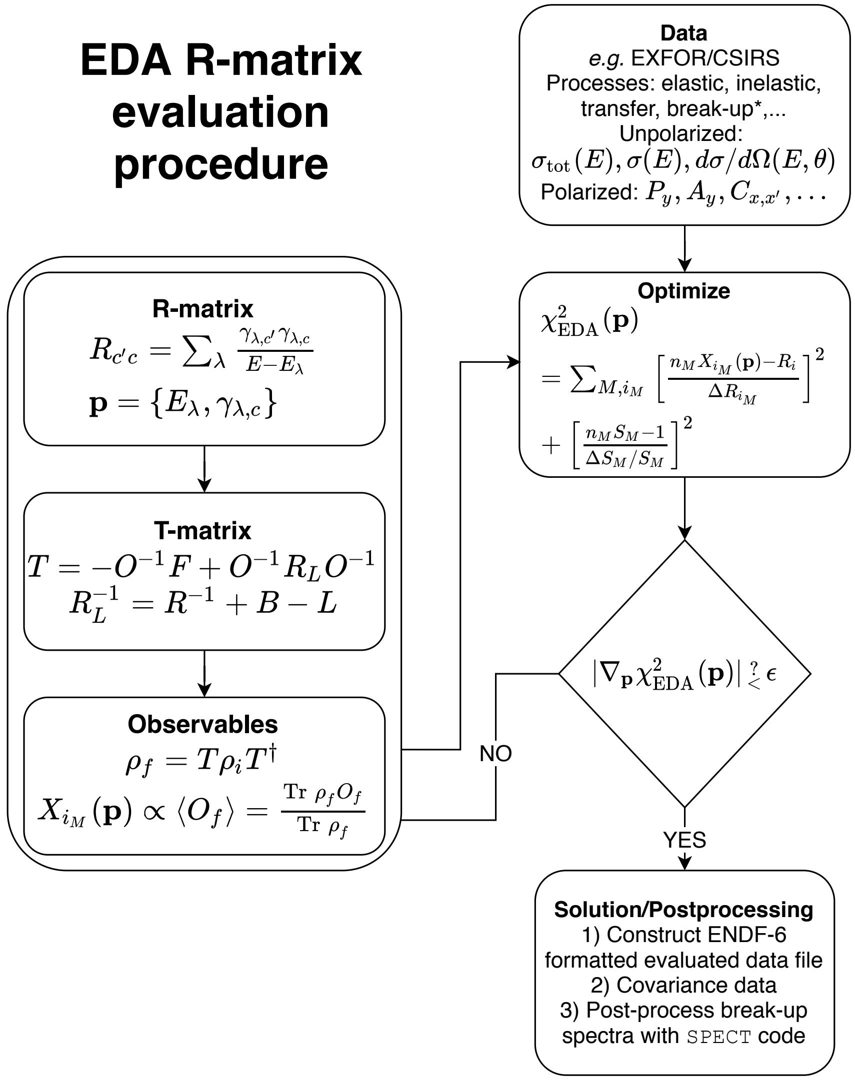
EDA **cross section evaluation**



- 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



EDA evaluation procedure



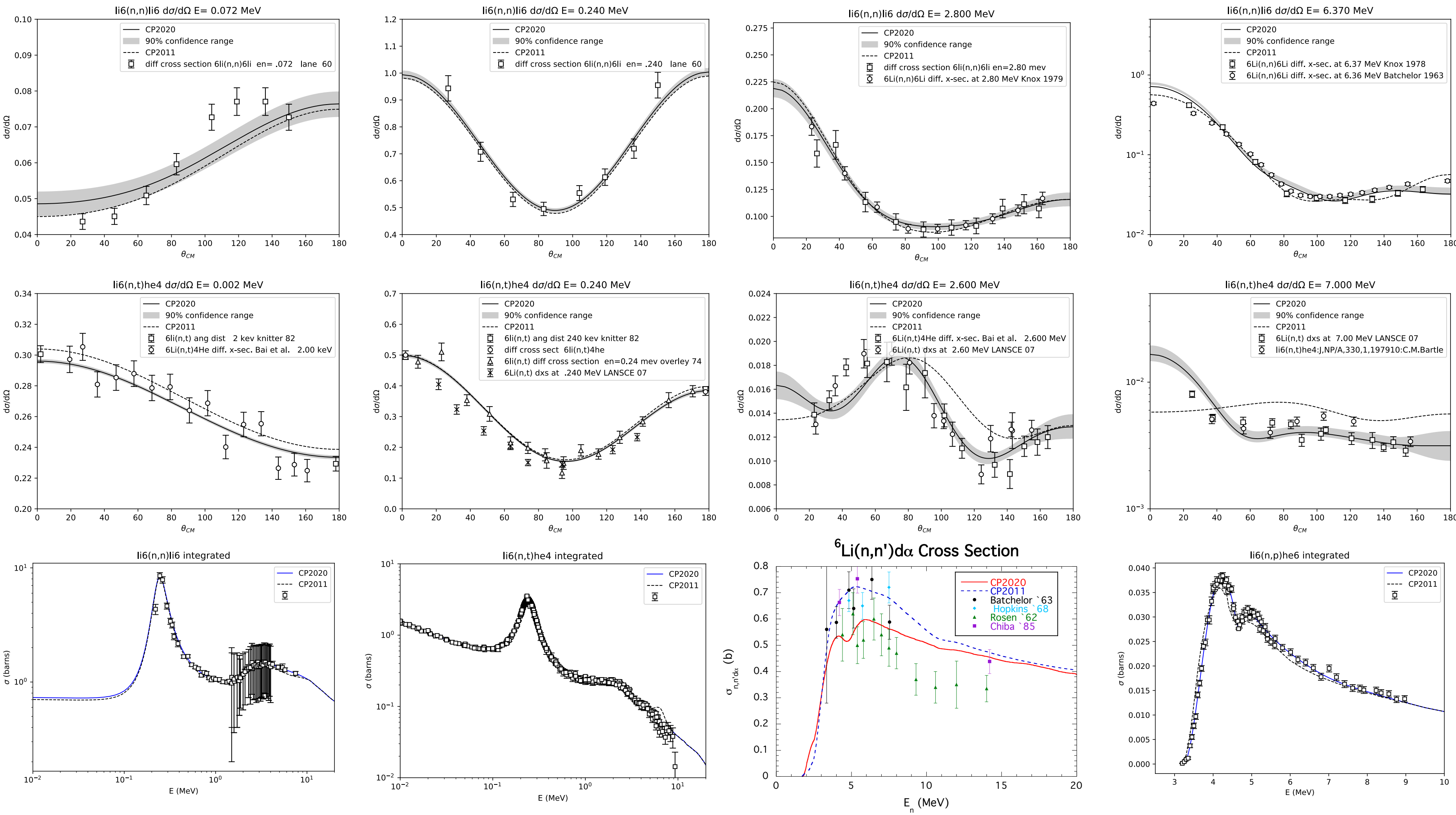
Summary of ^{7}Li R-matrix Analysis

Channel	l_{max}	a_c (fm)
$t+^{4}He$	5	4.0
$n+^{6}Li$	3	5.0
$d+^{5}He$	1	7.5
$n+^{6}Li^{*}$	1	5.0
$p+^{6}He$	1	5.0
$n+^{6}Li^{**}$	1	5.5

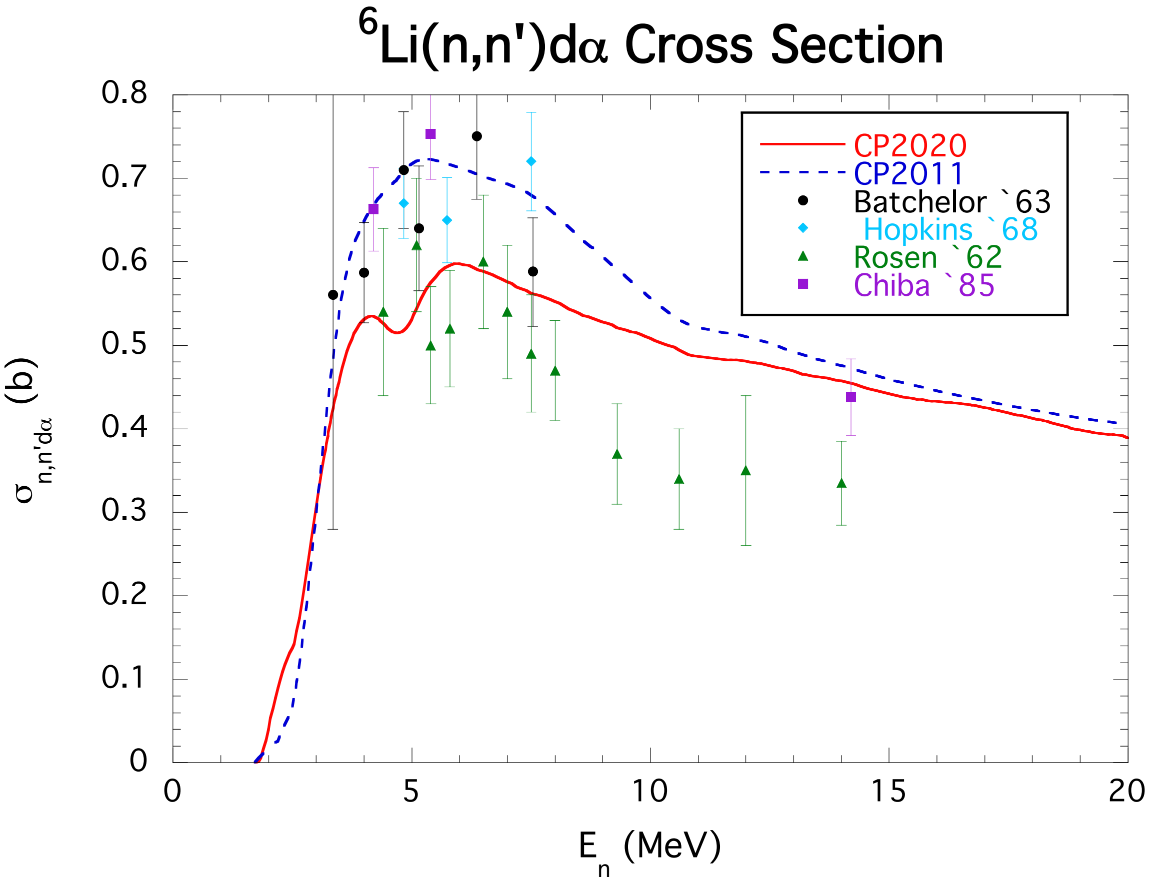
Reaction	Energy range	Observables	# data points	χ^2/point
$^{4}He(t,t)^{4}He$	E_t = 3-17 MeV	$\sigma(\theta)$, $A_y(\theta)$	1689	1.03
$^{4}He(t,n)^{6}Li$	E_t = 8.75-14.4 MeV	$\sigma(\theta)$	39	1.14
$^{4}He(t,n)^{6}Li^{*}$	E_t = 8.75-14.4 MeV	$\sigma(\theta)$	3	0.42
$^{6}Li(n,t)^{4}He$	E_n = 0-8 MeV	σ_{int} , $\sigma(\theta)$	2840	1.44
$^{6}Li(n,n_0)\,^{6}Li$	E_n = 0-8 MeV	σ_{int} , $\sigma_{T,}$ $\sigma(\theta)$, $P_y(\theta)$	1451	1.36
$^{6}Li(n,d)\,^{6}Li$	E_n = 0-8 MeV	σ_{int} , $\sigma(\theta)$	28	11.9
$^{6}Li(n,n_1)\,^{6}Li^{*}$	E_n = 0-8 MeV	σ_{int} , $\sigma(\theta)$	175	2.11
$^{6}Li(n,p)\,^{6}He$	E_n = 0-8 MeV	σ_{int} , $\sigma(\theta)$	92	1.58
$^{6}Li(n,n_2)\,^{6}Li^{**}$	E_n = 0-8 MeV	σ_{int}	41	0.30
Totals		17	6358	1.39*

*For ***170*** free parameters, χ^2/ν = 1.43

Cross Sections for the n+^{6}Li Reactions



^{6}Li(n,n')dα



$$\sigma_{n,n'd\alpha} = \sigma_{n,T} - (\sigma_{n,t} + \sigma_{n,\gamma} + \sigma_{n,n_0} + \sigma_{n,n_2} + \sigma_{n,p} + \sigma_{n,2n})$$

It is somewhat lower in the peak than the previous evaluation because the total cross section is lower for $E_n > 5$ MeV (Abfalterer data), and the elastic cross section is higher.

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

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

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

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

observable uncertainties

correlation coefficient

Parameter variance

• Arndt&MacGregor UCRL-14627-T

- Consider variations near solution $\{p_{1,i}\}_{i=1}^{N_1}$ $\{p_{2,i}\}_{i=1}^{N_2}$

$$\Delta\chi^2(p) = \delta p_1 A \delta p_1 + \delta p_1 B \delta p_2 + \delta p_2 B^T \delta p_1 + \delta p_2 D \delta p_2 \qquad C_0^{-1} = \begin{pmatrix} A & B \\ B^T & D \end{pmatrix}$$

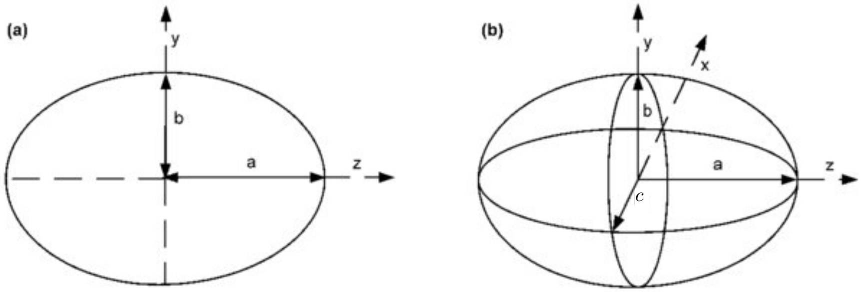
- How does χ^2 change when $\{p_2\}$ move and re-optimize $\Delta\chi^2$ via $\{p_1\}$?

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

- $\tilde{D}^{-1}$ is the restriction of the inverse of C_0 to p_2 subspace; let N_2=1

$$(\delta p_{2,\alpha})^2 = \Delta\chi^2 C_{0,\alpha\alpha} \qquad \Delta\chi^2 = 1 \implies \delta p_{2,\alpha} = \sqrt{C_{0,\alpha\alpha}}$$

- **NB:** larger dimensional parameter spaces give smaller $\delta p_{2,\alpha}$



Uncertainties from chi-squared minimization

$$\chi^2_{\mathrm{EDA}} = \sum_i \left[\frac{nX_i(\mathbf{p}) - R_i}{\Delta R_i}\right]^2 + \left[\frac{nS-1}{\Delta S / S}\right]^2$$

$$\begin{cases} R_i,\ \Delta R_i = \text{relative measurement, uncertainty} \\ S,\ \Delta S = \text{experimental scale, uncertainty} \\ X_i(\mathbf{p}) = \text{observable calc. from res. pars. } \mathbf{p} \\ n = \text{normalization parameter} \end{cases}$$

Near a minimum of the chi-squared function at **p** = **p**$_0$:

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

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

Conventions:

1) previous: $\Delta\chi^2 = 1 \implies$ Very small uncertainties $\delta p_i = (C^0_{ii})^{1/2} \sim \mathcal{O}(N_p^{-1/2})$

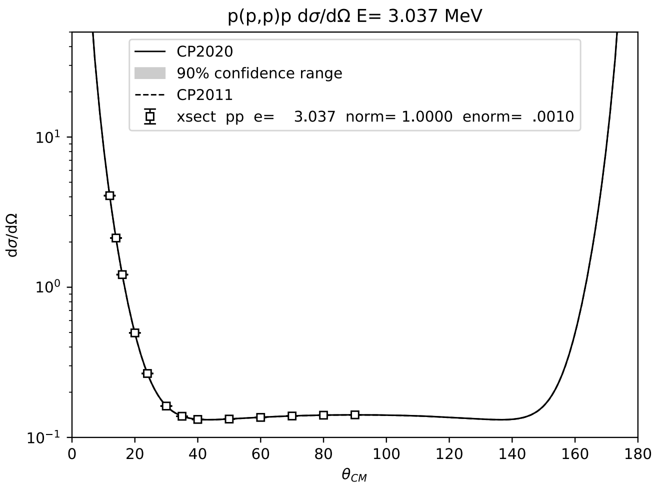
2) improved: $\Delta\chi^2 = \tfrac{1}{2}\Delta\mathbf{p}^{\mathrm{T}}\mathbf{G}_0\Delta\mathbf{p} \le \Delta\chi^2_{\max}$,

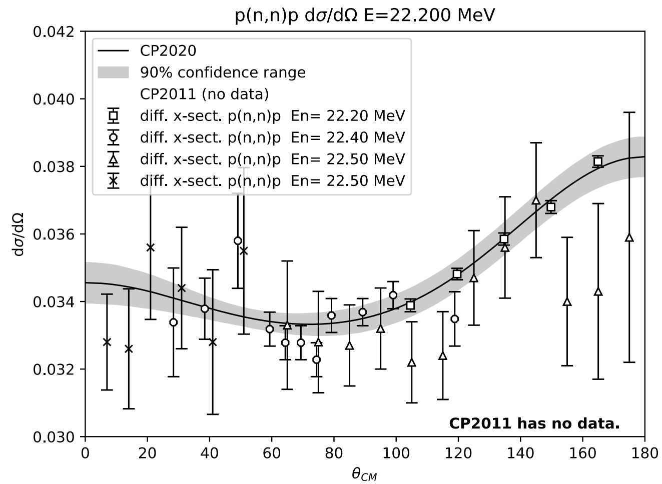
$$P(\Delta\chi^2|k) = \left[2^{\frac{k}{2}}\Gamma(\tfrac{k}{2})\right]^{-1}\int_0^{\Delta\chi^2_{\max}} t^{\frac{k}{2}-1}e^{-\frac{t}{2}}dt = \text{CL (e.g.} \sim 0.68 \text{ for 1-}\sigma\text{), 0.95 for 2-}\sigma\text{, etc.}$$

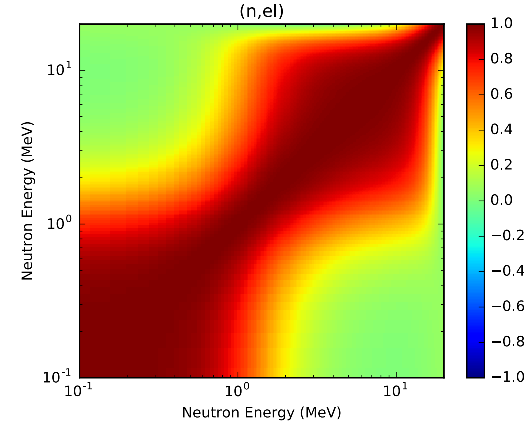
$$\Delta\chi^2_{\max} \approx k = \langle\Delta\chi^2\rangle.$$

$$\delta p_i \sim (N_p C^0_{ii})^{1/2}$$

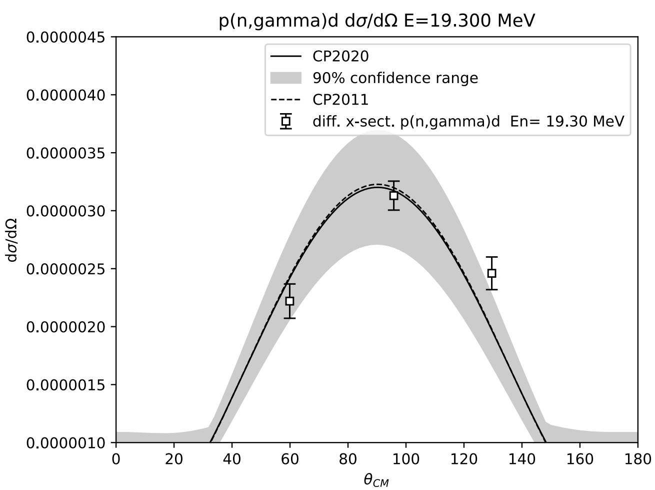
Application to NN system

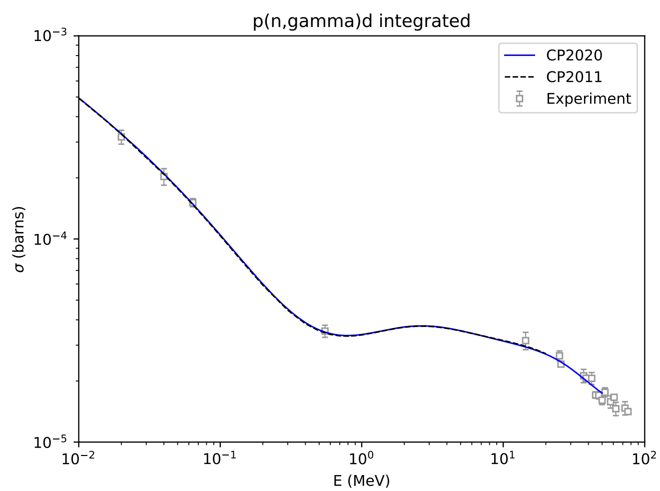






Covariance matrix





Partitions:

$pp(\ell \leq 3); np(\ell \leq 3);$

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

36 channels $(J^\pi LS)$

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

Conclusions & Outlook

- R-matrix
  - Correlates all processes associated with a given compound system
  - Enforces
    - Causality; proper complex-analytic properties; multichannel/multiprocess unitarity
  - Single-observable fits? *Caveat Emptor*.
- Systematic improvement
  - More data
    - Polarized observables
    - Higher-energy data
- 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