CHALLENGES IN NUCLEAR DATA EVALUATION OF LIGHT NUCLEAR SYSTEMS

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This work has been carried out within the Euratom Project SANDA (Supplying Accurate Nuclear Data for energy and non-energy Applications) under grant agreement No 847552. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

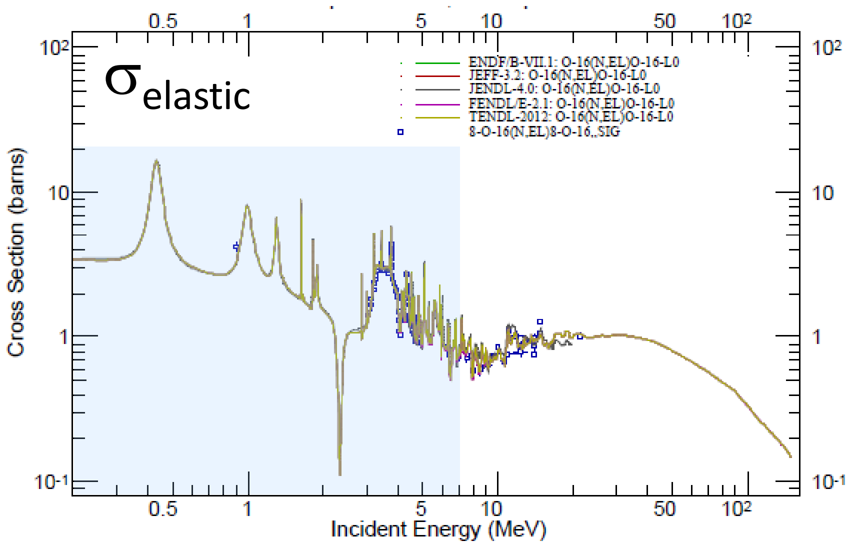
Importance of Light Nuclear Systems

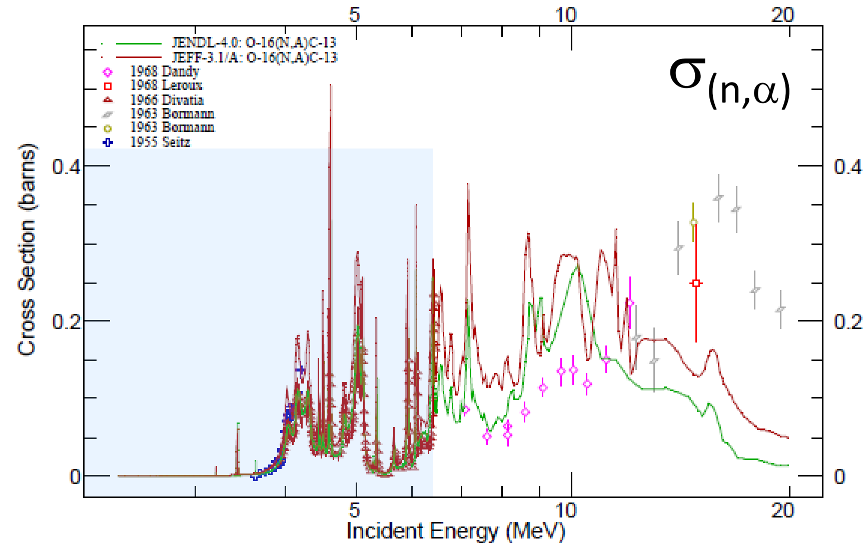
Reactions of light nuclear systems are of importance in several fields of of technology and science → a good knowledge of the cross sections is required

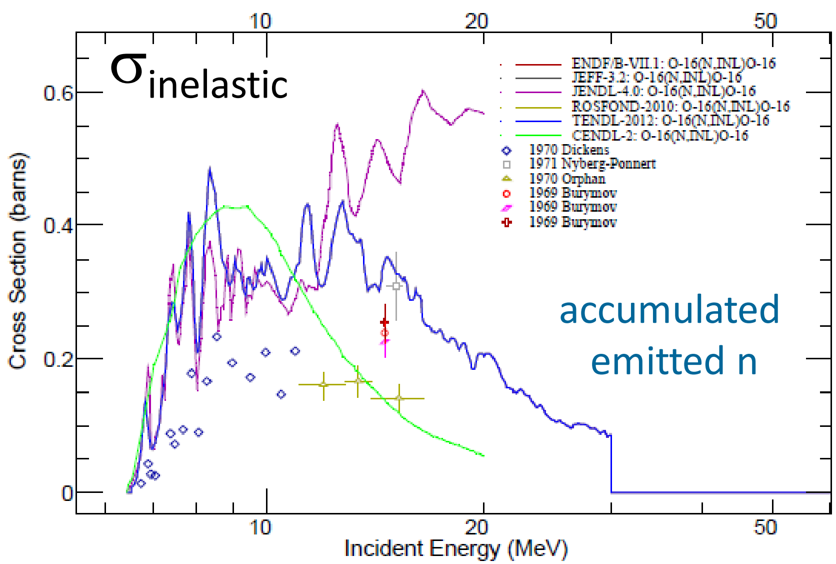
Some Examples:

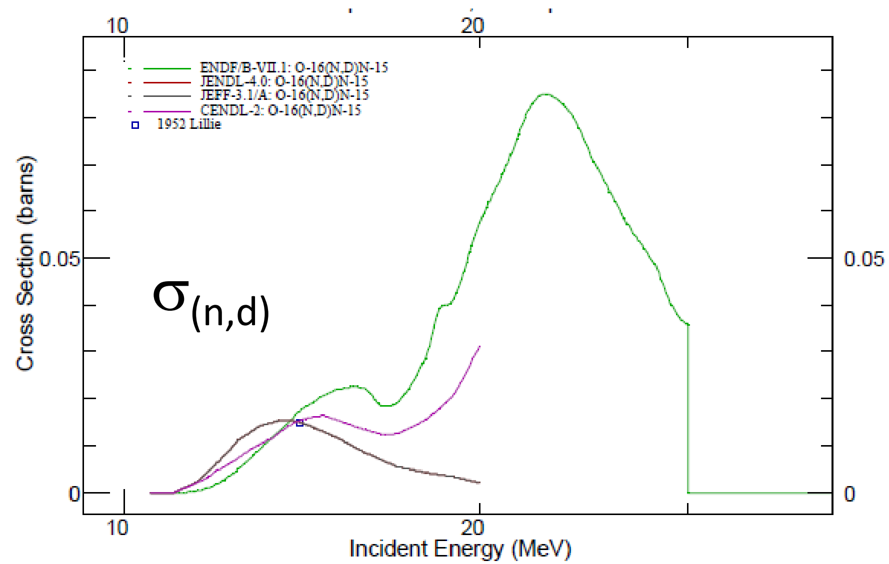
$n+{}^{9}Be \rightarrow \alpha+\alpha+n+n$	neutron source in fusion devices
$n+{}^{6}Li \rightarrow t+\alpha$	tritium generation in fusion devices
$n+{}^{16}O \rightarrow {}^{13}C+\alpha$	radiation aging of structure materials (steel)
$\alpha+{}^{13}C \rightarrow n+{}^{16}O$	neutron source for s-process nucleosynthesis
$\alpha+{}^{12}C \rightarrow {}^{16}O+\gamma$	astrophysics – ratio of carbon/oxigen abundance
$n+{}^{12}C \rightarrow \alpha+X$	radiation aging of structure materials
$n+{}^{12}C \rightarrow p+X$	radiation aging of structure materials

Example: Evaluated Files for n+^{16}O Reactions









1. Introduction

Pecularities of Light Nuclear Systems

Properties of Light Nuclear Systems

- in light nuclear systems the number of nucleons is small (*A*< 25)
- at low excitation energy of the compound nucleus the number of levels is small
- statistical considerations not applicable

Problems:

- the statistical nuclear model is not applicable except for higher excitation energies
- applicability of mean field concepts is questionable
- (semi-)microscopic calculations are very involved and limited with regard to quantitative reliability (Cluster models, shell model extensions, Faddeev-Yakubowski equations, ab-initio shell model calculations, Multi-channel algebraic approach,…)
  [Uncertainty of the nucleon-nucleon interaction, the actual nuclear structure of the collsion partners and the unclear impact of 3-nucleon forces]

Available Methods used for Quantitative Description:

R-matrix analyses of experimental data providing resonance parameters

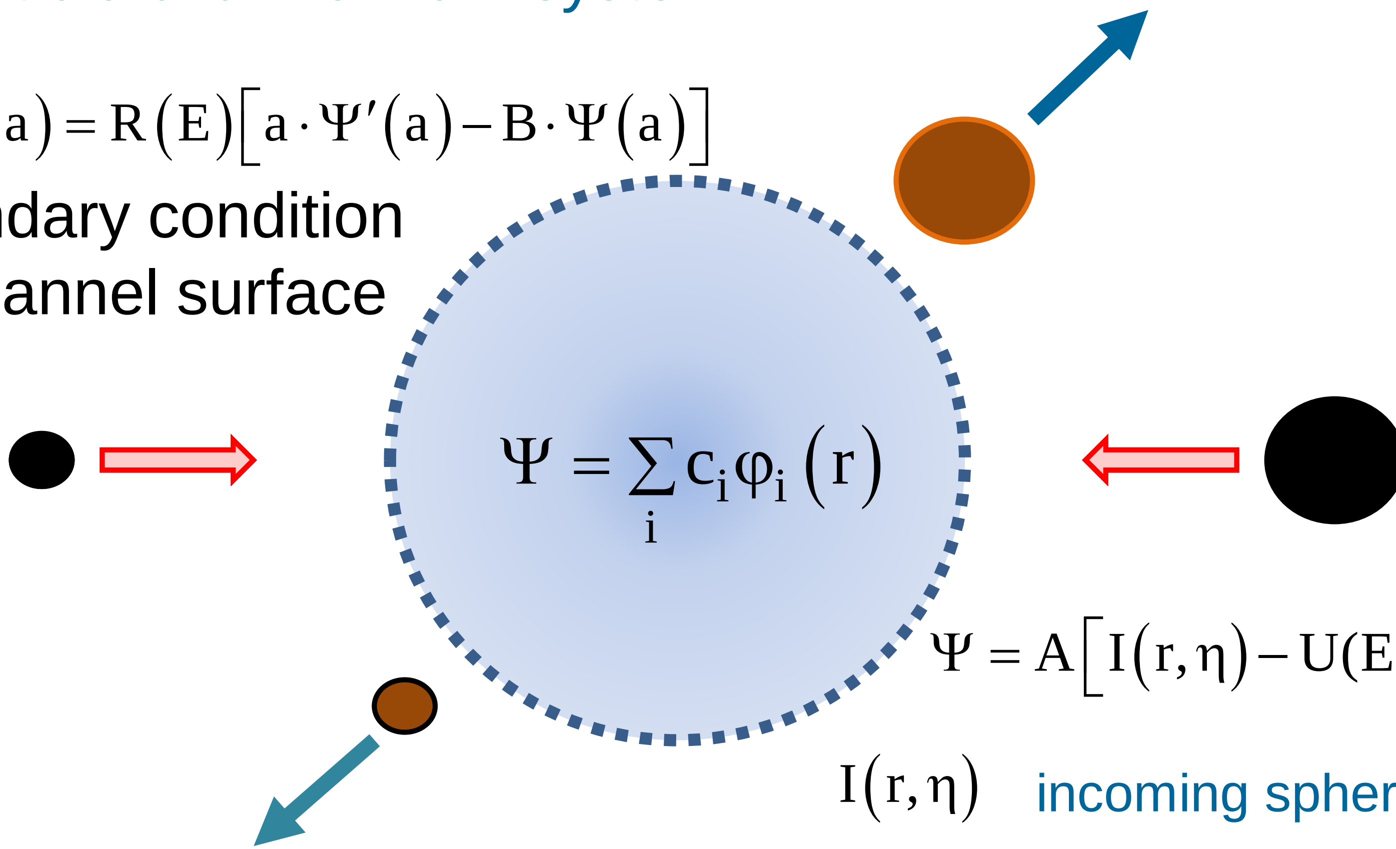
- *Standard R-matrix codes: SAMMY, REFIT, CONRAD, AZUR, AMUR, …*
- *Unitary R-matrix codes* (EDA, RAC,….,FRESCO and GECCCOS modules)

Standard R-Matrix Formalism: wave function

2-particle channel: cm-system

$$\Psi(r=a) = R(E)\left[a \cdot \Psi'(a) - B \cdot \Psi(a)\right]$$

boundary condition
at channel surface



$$\Psi = \sum_i c_i \varphi_i(r)$$

$$\Psi = A\left[I(r,\eta) - U(E) \cdot O(r,\eta)\right]$$

$I(r,\eta)$ incoming spherical wave

$O(r,\eta)$ outgoing spherical wave

$U(E)$ collision matrix, S-matrix

$\varphi_i(r)$ basis functions i=1,2,…

c_i coefficients i=1,2,…

Concept of Standard *R*-matrix

2. R-Matrix Developments

Idea: Separation of unknown internal and known external region
E.P.Wigner, L. Eisenbud, P.L. Kapur, R.E. Peierls, A.M. Lane, R.G. Thomas …

$$u_c^{\text{int}}(a) = u_c^{\text{ext}}(a)$$ matching condition 1

$$\left.\frac{\partial}{\partial r} u_c^{\text{int}}(r)\right|_{r=a} = \left.\frac{\partial}{\partial r} u_c^{\text{ext}}(r)\right|_{r=a}$$ matching condition 2

$$u_c^{\text{int}}(r) = \sum_{j=1}^{N} g_{cj}\, \varphi_j(r) \qquad u_{cc_0}^{ext}(r) = v_c^{-1/2}\left[I_c(k_c r)\delta_{cc_0} - U_{cc_0} O_c(k_c r)\right] \quad \text{for } E > E_c$$ wave function

0 r=a r

- R-matrix at Energy E maps the derivative u'_c onto the wave function u_c at the matching radius a:

$$u_c(a) = \sum_{c'} \left(\frac{\mu_c}{\mu_{c'}}\right)^{1/2} R_{cc'}\left[a \cdot u'_{c'}(a) - B_{c'} u_{c'}(a)\right]$$

B_c … boundary param. in channel c
μ_c… reduced mass in channel c

- R-matrix can be represented as a sum of pole terms

$$R_{cc'} = \sum_n \frac{\gamma_{nc}\gamma_{nc'}}{E_n - E}$$

γ_{nc} … n-th reduced width . in channel c
E_n … n-th pole energy in channel c

- which is directly related with the collision matrix U

$$Z_{Occ'} = (k_{c'}a)^{-1/2}\left[O_c(k_c a)\delta_{cc'} - k_{c'} a R_{cc'} O'_{c'}(k_{c'} a)\right]$$

$$Z_{Icc'} = (k_{c'}a)^{-1/2}\left[I_c(k_c a)\delta_{cc'} - k_{c'} a R_{cc'} I'_{c'}(k_{c'} a)\right]$$

$$U_{cc'} = Z_{Occ'}^{-1} \cdot Z_{Icc'}$$

R-Matrix: Strengths and Limitations

Strengths:

- R-matrix analyses provide **excellent descriptions of the resonance** cross sections
- R-matrix analyses **satisfiy conservation rules** – yields consistent cross section values

Limitations:

- R-matrix theory is **not a microscopic model** → predictive power is limited
- In general the available data are incomplete – unitarity is not satisfied
- R-matrix theory is **limited to binary channels** A(a,b)B, usually capture and breakup channels are treated in approximations
- The applicability of R-matrix analyses is **practically limited in energy** – the number of open parameters is drastically increasing with energy

R-Matrix Analyses of Reaction Data of Light Nuclear Systems

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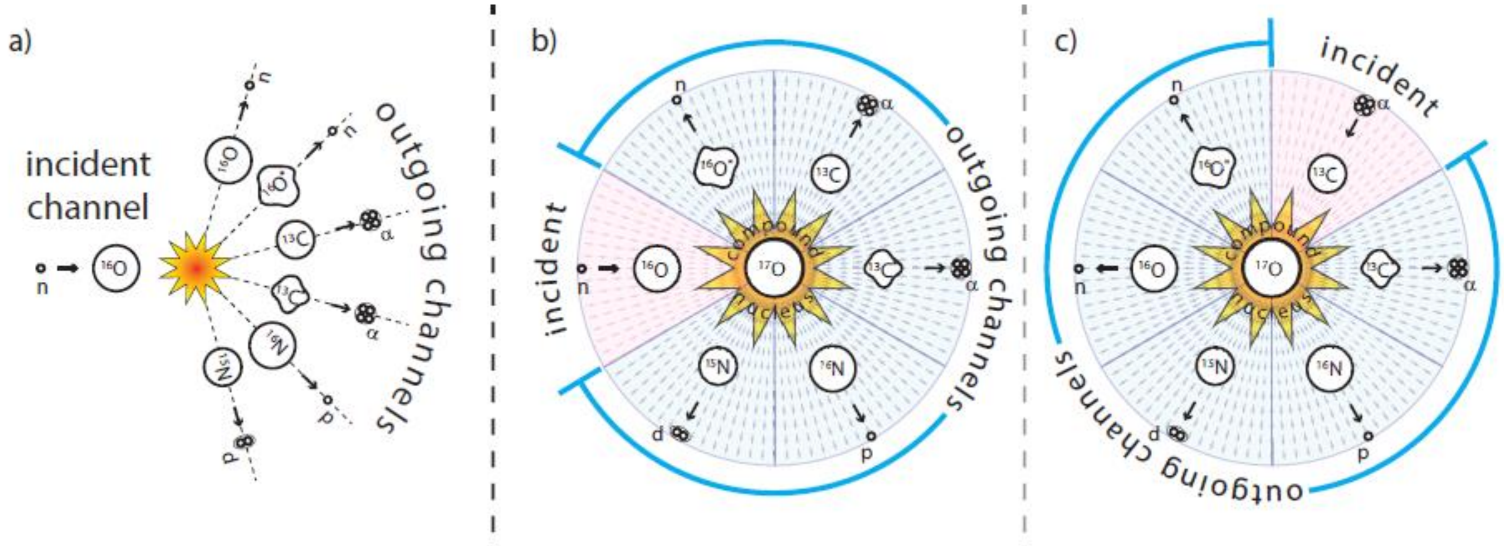
2. R-Matrix Developments

For light nuclear systems a simultaneous treatment of reaction data of all incident channels leading to the same compound nucleus is preferable – use of excitation energy E_x of compound nucleus as reference energy scale.



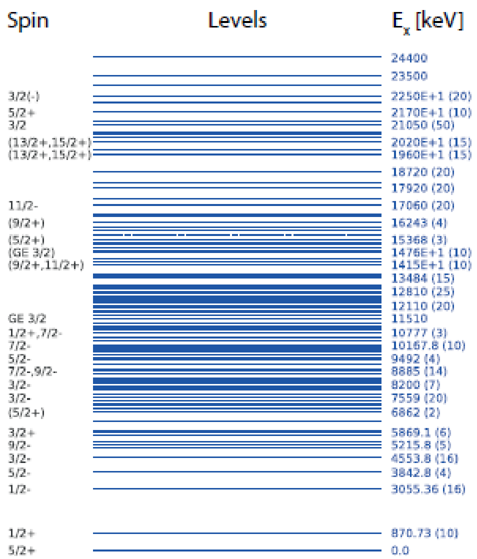
Optimization capabilities for following experimental observables should be included:

- angle integrated data
- angle differential data in cm- and lab-frame
- excitation functions in cm- and lab-frame
- analyzing power and vector polarizations in cm- and lab-frame
- 3-body R-matrix on Faddeev basis under development.

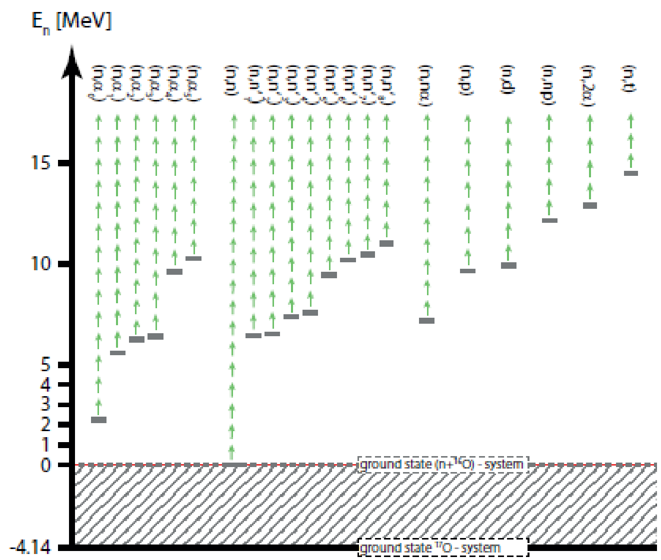
R-Matrix Analysis: Extending the Energy Range

The number of levels increases with energy – thus also the number of parameters.

Consequently R-matrix analyses require fits of an enourmous number of widths parameters. Finally one reaches the limit of feasibility.



compound nucleus ^{17}O



possible decompositions up to 13 MeV

^{17}O, n+^{16}O, α+^{13}C, p+^{16}N, d+^{15}N

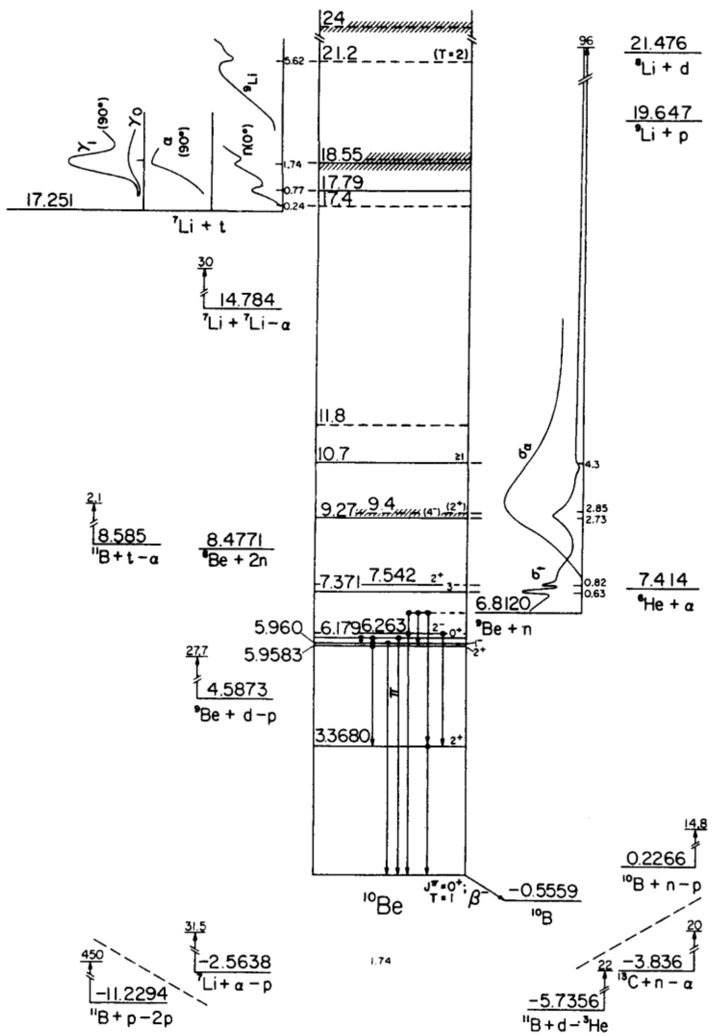
Challenge for the evaluation of light nuclear systems:

extension of energy range of R-matrix analyses in the unresolved resonance range

Recently some attempts were started, but there is no viable solution of the problem at present.

Example: Neutron-induced Reactions of ^{9}Be

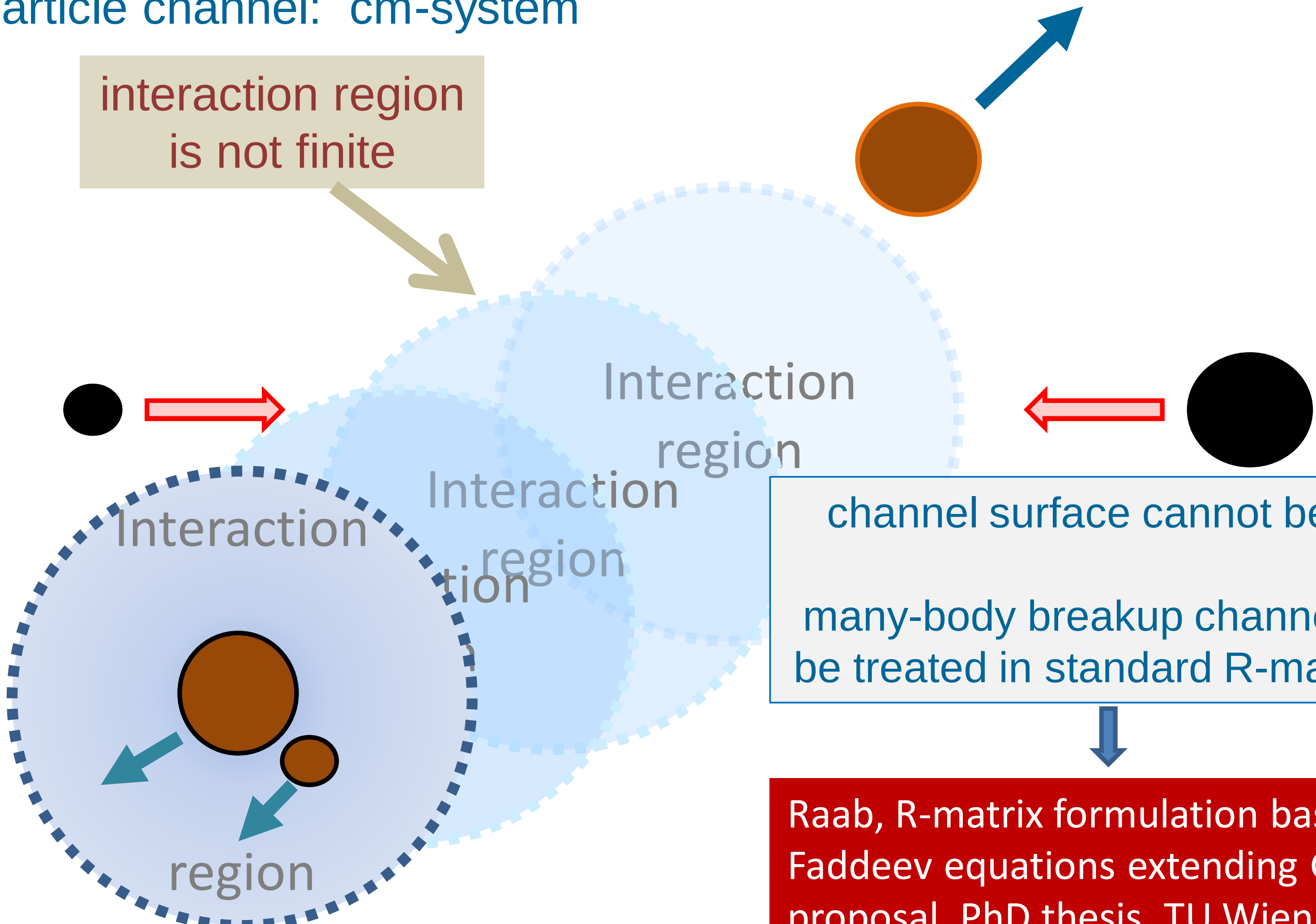
level scheme of ^{10}Be



^{9}Be(n,n)^{9}Be	Q= 0.0000 MeV
^{9}Be(n,α)^{6}He	Q= -0.5971 MeV
^{9}Be(n,2nα)^{4}He	Q= -1.6636 MeV ←
^{9}Be(n,nα)(^{5}He)	Q= -2.3073 MeV ⇠
^{9}Be(n,n')^{9}Be*	various Q-values
^{9}Be(n,t)^{7}Li	Q=-10.4373 MeV
^{9}Be(n,p)^{9}Li	Q=-12.8248 MeV
^{9}Be(n,tα)t	Q=-12.9049 MeV ←
^{9}Be(n,d)^{8}Li	Q=-14.6615 MeV
^{9}Be(n,t)^{7}Li	Q=-14.6615 MeV
^{9}Be(n,nd)^{7}Li	Q=-16.6932 MeV ←
^{9}Be(n,np)^{8}Li	Q=-16.8861 MeV ←
^{9}Be(n,nt)^{6}Li	Q=-17.6871 MeV ←
^{9}Be(n,α)^{6}Li	Q=-19.2874 MeV
^{9}Be(n,pt)^{6}He	Q=-20.4108 MeV ←
^{9}Be(n,^{3}He)(^{7}He)	Q=-21.5845 MeV ⇠
^{9}Be(n,pα)(^{5}H)	Q=-23.1857 MeV ←

Reaction with Three-Body Exit Channel

3-particle channel: cm-system



channel surface cannot be defined

many-body breakup channels cannot be treated in standard R-matrix theory

Raab, R-matrix formulation based on the Faddeev equations extending Glöckles proposal, PhD thesis, TU Wien (2023)

Lane and Thomas, Rev. Modern Physics 30, 257 (1958)

Reduced R-Matrix Analysis

2. R-Matrix Developments

the complete R-matrix

the $\mathbf{R}_{rr}$-submatrix

$$\mathbf{R} = \begin{pmatrix} R_{11} & R_{12} & \ldots\ldots & R_{15} & .. & R_{1n} \\ R_{21} & R_{22} & \ldots\ldots & R_{25} & .. & R_{2n} \\ R_{31} & R_{32} & \ldots\ldots & R_{35} & .. & R_{3n} \\ R_{41} & R_{42} & \ldots\ldots & R_{45} & .. & R_{4n} \\ R_{51} & R_{52} & \ldots\ldots & R_{55} & .. & R_{5n} \\ \ldots & \ldots & \ldots\ldots & \ldots & .. & \ldots \\ R_{n1} & R_{n2} & \ldots\ldots & R_{n5} & .. & R_{nn} \end{pmatrix}$$

Maintaining the S-matrix elements of S_{rr} equivalent leads to the following relationship

Lane and Thomas, Rev. Modern Physics 30, 257 (1958)

$$\tilde{R}_{rr} = R_{rr} + R_{re} L_e^O \left[1 - R_{ee} L_e^O\right]^{-1} R_{er}$$

$$\tilde{R}_{er} = \left[1 - R_{ee} L_e^O\right]^{-1} R_{er}$$

$\mathbf{R}_{ee}$ eliminated channels

Simplified parametrisation for reduced R-matrix analyses: valid for for well separated poles

$$R_{cd} = \sum_{\lambda=1}^{N_\lambda} \frac{\gamma_\lambda^c \gamma_\lambda^d}{E_\lambda - E} \quad \Rightarrow \quad \tilde{R}_{c,d} = \sum_{\lambda=1}^{N_\lambda} \frac{\gamma_\lambda^c \gamma_\lambda^d}{E_\lambda - E - \sum_{m=M_r+1}^{M_r+M_e} \left(\gamma_\lambda^m\right)^2 L_m\left(k_m a\right)}$$

$c,d = 1,2,\ldots, M_r$

$$L_m\left(k_m \cdot a\right) = k_m \cdot a \frac{O'\left(k_m \cdot a\right)}{O\left(k_m \cdot a\right)}$$

Property of $L(k_m a)$:

$L(k_m a)$ guarantees the correct threshold behaviour

$L(k_m a)$ is real valued below threshold

$L(k_m a)$ is complex above threshold

Reduced R-Matrix Analysis
Cross Section associated with ignored channels

Although not explicitly considered in *Reduced R-Matrix Analyses* one is able to determine the total cross section associated with the sum of ignored channels.

Basic idea: Unitarity defect of the collision matrix associated with the *Reduced R-Matrix*

Nichtelastischer Wirkungsquerschnitt

$$\sigma_{c\to c'} = \frac{\pi}{k_c^2}\frac{1}{(2I_1+1)\cdot(2I_1+1)}\sum_{J\pi}(2J+1)\sum_{I,\ell}\sum_{I',\ell'}\left|U^{J\pi}_{c'I'\ell',cI\ell}(E)\right|^2$$

Reduced R-Matrix formalism: Interest in the fraction of the cross sections ignored

$$\sigma^{\mathrm{redRMat}}_{\mathrm{excluded}}(E) = \sum_{c'\mathrm{excluded}}\sigma_{c\to c'} = \frac{\pi}{k_c^2}\frac{1}{(2I_1+1))\cdot(2I_2+1))}\sum_{J\pi}(2J+1)\sum_{I\ell}\Delta^{J\pi}_{cI\ell}$$

with

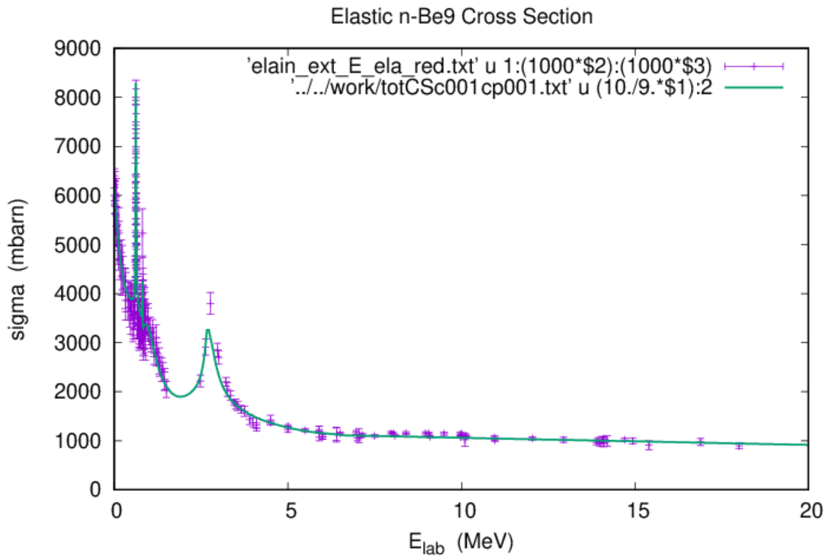
$$\Delta^{J\pi}_{cI\ell} = 1 - \sum_{c'I'\ell'}^{\mathrm{included}}\left|\widetilde{U}^{J\pi}_{c'I'\ell',cI\ell}(E)\right|^2$$

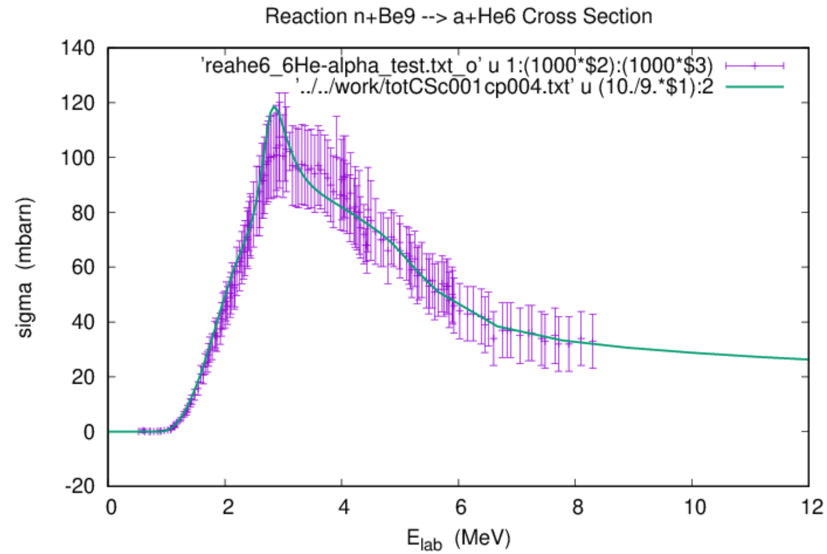
The total reaction cross section can be additionally used in reduced R-matrix analyses

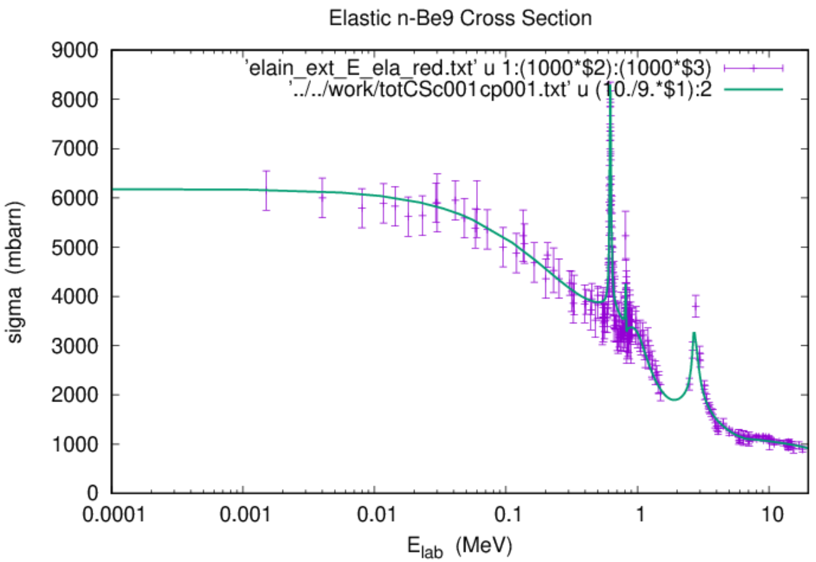
2. R-Matrix Developments

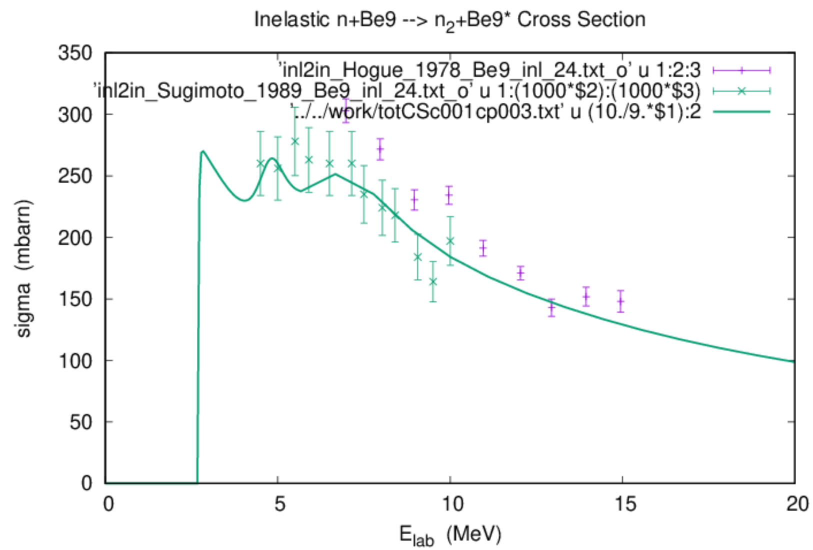
R-Matrix Analysis of n+^{9}Be

2. R-Matrix Developments





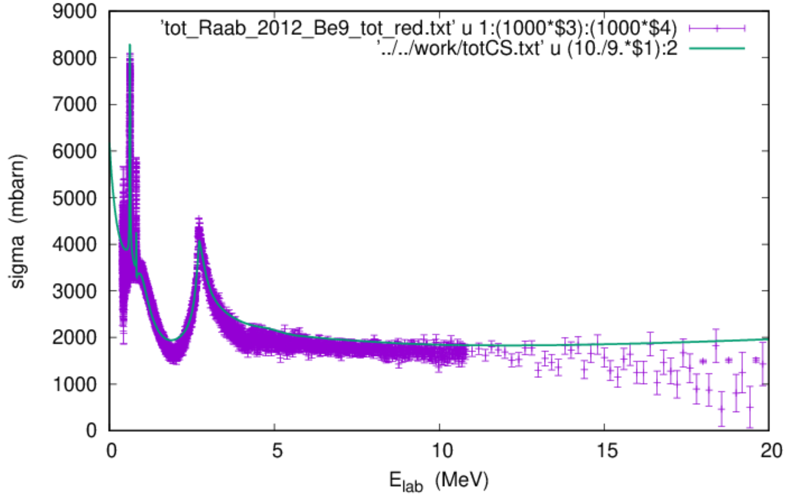




R-Matrix Analysis of n+^{9}Be

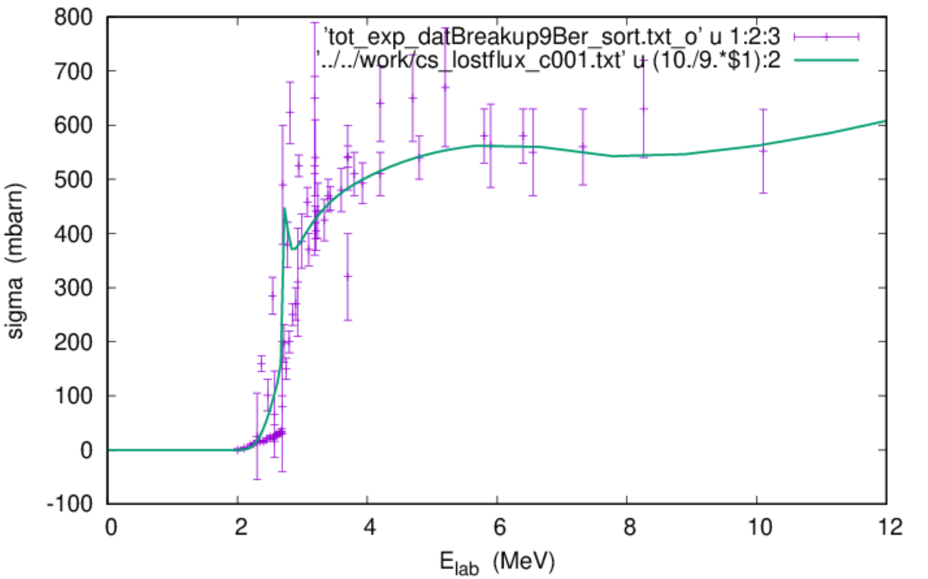
2. R-Matrix Developments

total n+^{9}Be cross section



Reduced R-matrix analysis of Neutron-induced reactions of ^{10}Be performed within the framework of the EUROfusion grant 2022

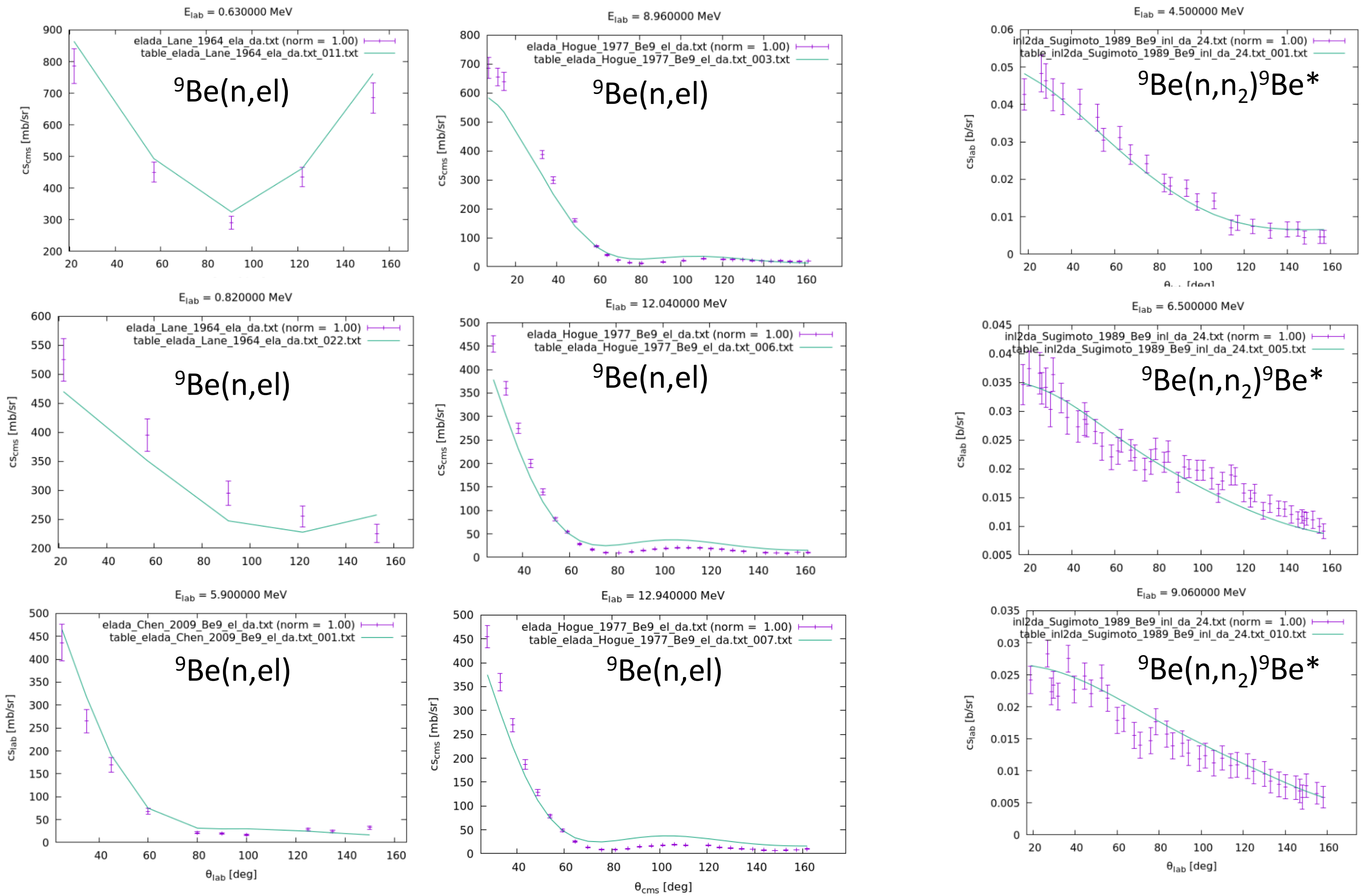
total n+^{9}Be(n,α2n)^{4}He breakup cross section



R-Matrix Analysis n+^{9}Be

elastic and inelastic differential cross sections

2. R-Matrix Developments



Generating evaluated files:
Nuclear reaction data of light nuclear systems

Coarse Overview:
The available evaluated files of nuclear data for light nuclear systems are generated by one of the following methods

1) **Evaluation generated exclusively from available experimental data**
   - limitation to channels with experimental data, consistency not guaranteed, prior of complete ignorance should be used.

2) **Evaluation generated by combining an R-matrix analyses at low energy with a fit of available experimental data at high energies**
   - same problems as in 1) for the fit of experimental data.

Problem: Uncertainties generated from the Hessian of the χ^2-fit either of the experimental data, or the resonance parameters. Frequently too small uncertainties are obtained

In general: No Bayesian evalation procedure is usually performed.

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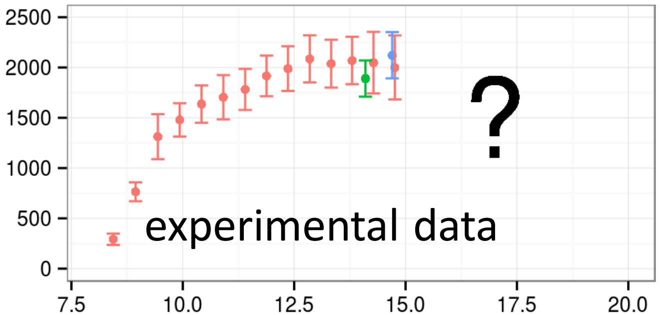
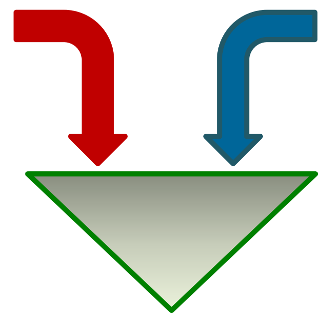
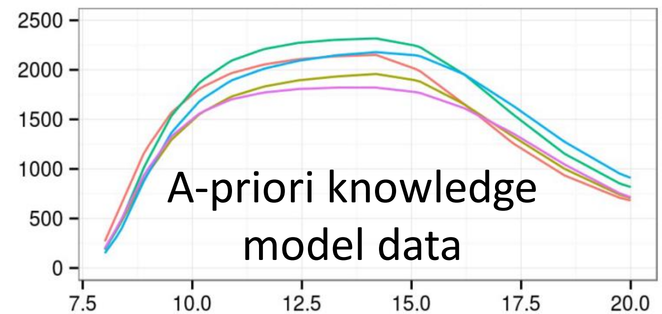
Nuclear Data Evaluation aims to combine experimental data and theory information to determine the best knowledge of reaction processes







Bayesian Evaluation Process

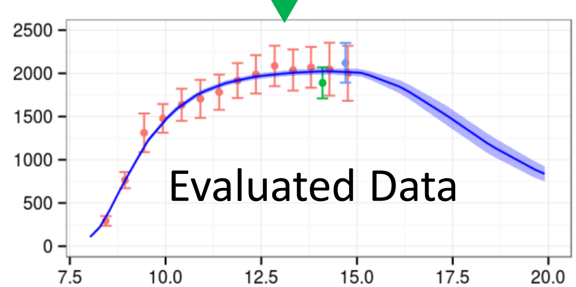
Bayes Theorem (1761):

$$\pi\left(\vec{p}\,|\,\vec{\sigma}_{\text{exp}}\right) = \frac{1}{\int d^d p\; \ell\left(\vec{\sigma}_{\text{exp}}\,|\,\vec{p}\right)\pi\left(\vec{p}\right)}\; \ell\left(\vec{\sigma}_{\text{exp}}\,|\,\vec{p}\right)\;\; \pi\left(\vec{p}\right)$$

aposteriori distribution
distribution of para-meters taking a-priori and experimental info

apriori distribution
provides the apriori knowledge, e.g. the nuclear model

likelihood
Experimental information



Linearized Bayesian Update

normal distributions assumed for

experimental uncertainties, $\vec{\varepsilon}_{\text{exp}} \sim N(0, \mathbf{B})$

likelihood and $\ell(\vec{\sigma}_{\text{exp}} \mid \vec{p}) \sim N(M(\vec{p}), \mathbf{B})$

model parameters $\pi(\vec{p}) \sim N(\vec{p}_0, \mathbf{A}_0)$,

GENERALISED LEAST SQUARE (GLS): Using multi-variate normal distributions allows linearization of Bayesian Theorem for update:

$$\vec{\sigma}_1 = \vec{\sigma}_0 + \mathbf{A}_0 \mathbf{S}^T \left(\mathbf{S}\mathbf{A}_0\mathbf{S}^T + \mathbf{B}\right)^{-1} \left(\vec{\sigma}_{\text{exp}} - \mathbf{S}\vec{\sigma}_0\right)$$

$$\mathbf{A}_1 = \mathbf{A}_0 - \mathbf{A}_0 \mathbf{S}^T \left(\mathbf{S}\mathbf{A}_0\mathbf{S}^T + \mathbf{B}\right)^{-1} \mathbf{S}\mathbf{A}_0$$

Sensitivity Matrix: $\vec{\sigma}_{\text{int}} = M_{\text{surr}}\left(\vec{\sigma}_{\text{mod}}\right) = \mathbf{S}\vec{\sigma}_{\text{mod}}$

Bayesian Evaluation of Reaction Data of Light Nuclear Systems

Question:
Is the concept of Bayesian statistics applicable in light nuclear systems?

Bayesian Evaluation Process

$$\pi(\vec{p}\mid\vec{\sigma}_{\exp}) = \frac{1}{\int d^d p\, \ell(\vec{\sigma}_{\exp}\mid\vec{p})\pi(\vec{p})}\, \ell(\vec{\sigma}_{\exp}\mid\vec{p})\, \pi(\vec{p})$$

What is the apriori knowledge ?

Problem:
Parameters of R-matrix are determined from experimental data
What is the a-priori knowledge????

Proposal for generating a prior for the R-matrix analyses

Available a-priori information

level scheme of the compound nucleus (E_{lv} , J^{π})
partitions, thresholds E_{th}

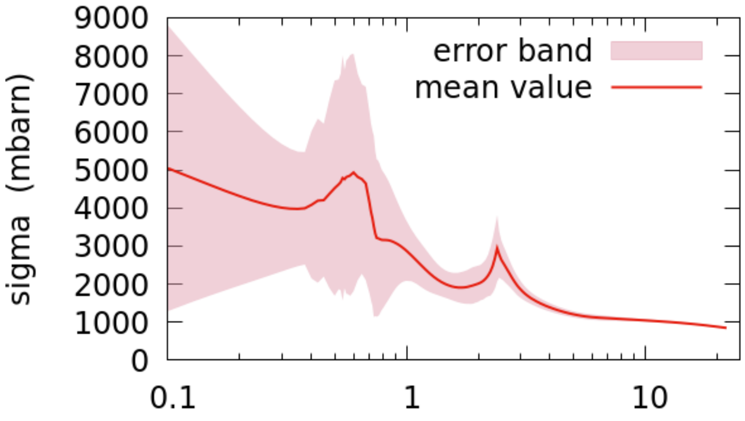
R-matrix parameters: resonance energy E_r form of resonance reduced widths γ_i

Generate Monte Carlo sweeps of cross sections with R-matrix code
variation of E_r within 0.5 MeV, matching radius 0.2 fm,
γ-widths of previous R-matrix analysis varied within Turchin/0,25

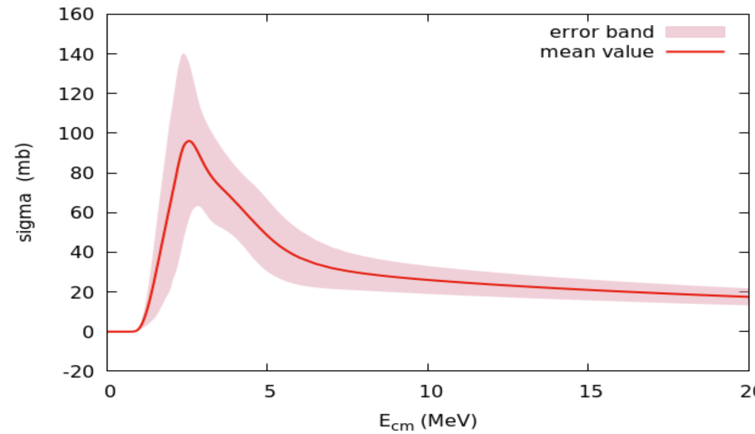
Quasi a-priori covariance matrix extracted:
limited knowledge on the position of resonances
knowledge of J^{π} included and thus features of the resonance
high energy behaviour determined variation of matching radius a

Generated Prior for n+^{9}Be Evaluation in the R-matrix regime

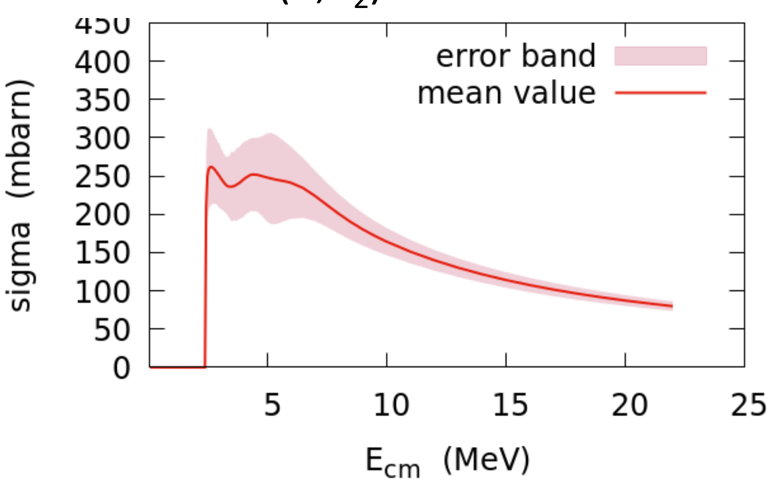
^{9}Be(n,n)^{9}Be elastic



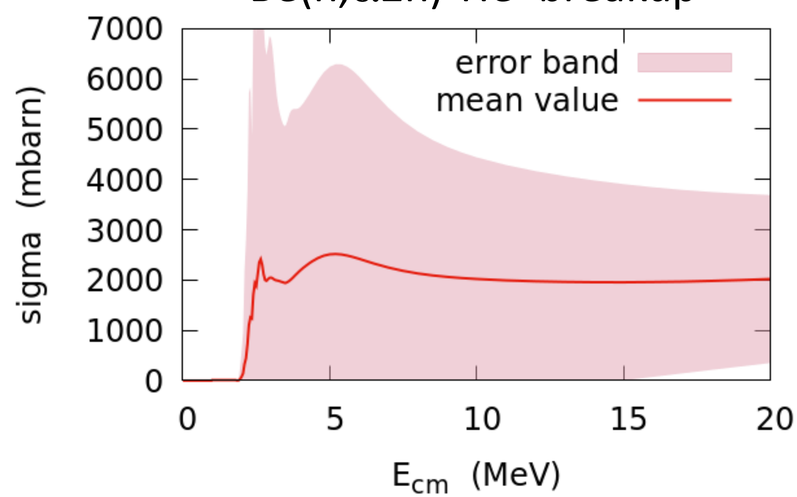
^{9}Be(n,^{4}He)^{6}He



^{9}Be(n,n$_2$)^{9}Be inelastic



^{9}Be(n,α2n)^{4}He breakup



Standard Bayesian Analysis in the Resonance Region

Standard Evaluation:

$$\vec{\sigma}_{\mathrm{exp}} = \vec{\sigma}_{\mathrm{mod}} + \vec{\varepsilon}_{\mathrm{exp}}$$

Experiment vector — Model vector — Uncertainty vector of experiment

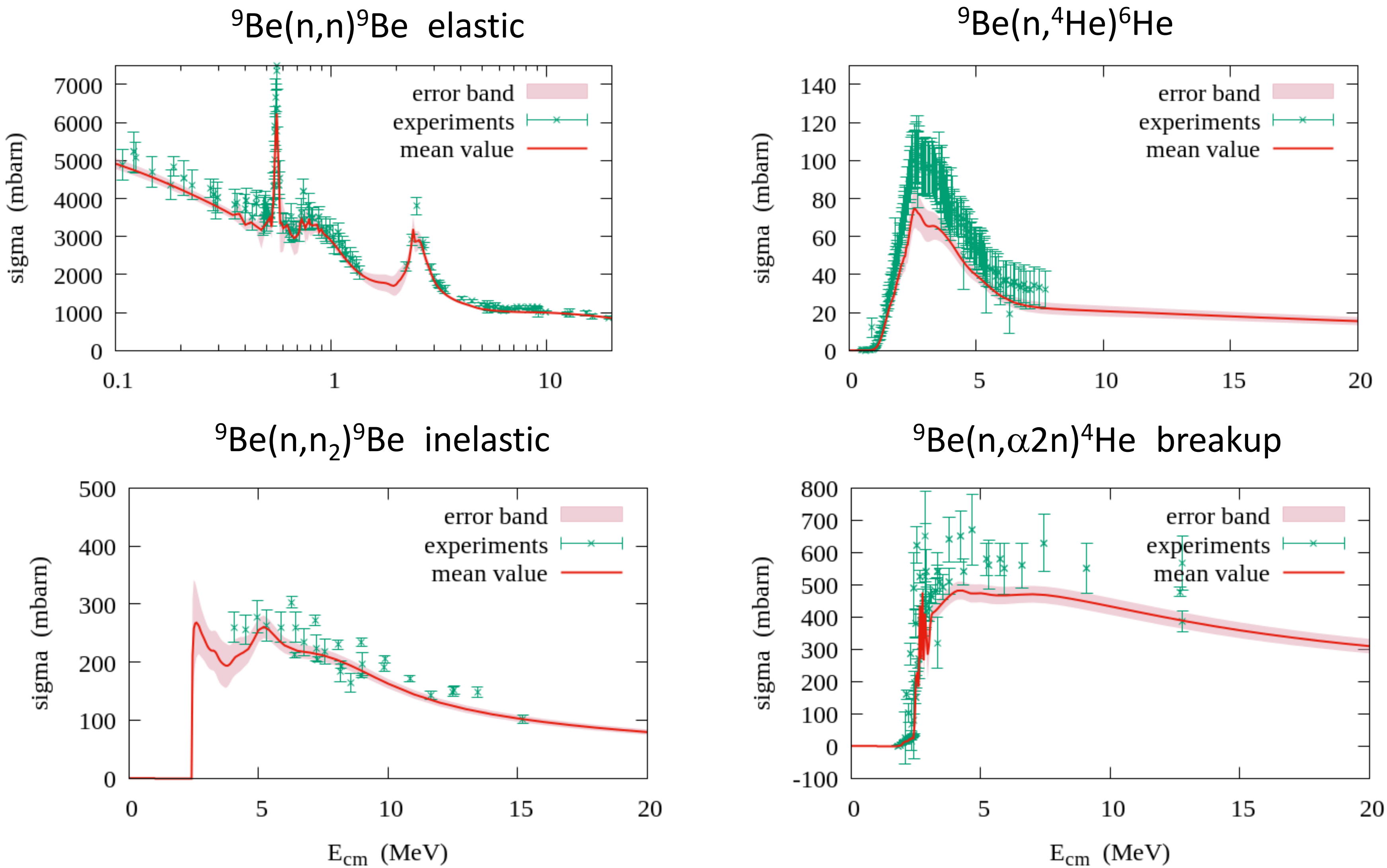
Generalised Least Square (GLS): Using multi-variate normal distributions allows linearization of Bayesian Theorem for update:

$$\vec{\sigma}_1 = \vec{\sigma}_0 + \mathbf{A}_0\mathbf{S}^T\left(\mathbf{S}\mathbf{A}_0\mathbf{S}^T + \mathbf{B}\right)^{-1}\left(\vec{\sigma}_{\mathrm{exp}} - \mathbf{S}\vec{\sigma}_0\right)$$

$$\mathbf{A}_1 = \mathbf{A}_0 - \mathbf{A}_0\mathbf{S}^T\left(\mathbf{S}\mathbf{A}_0\mathbf{S}^T + \mathbf{B}\right)^{-1}\mathbf{S}\mathbf{A}_0$$

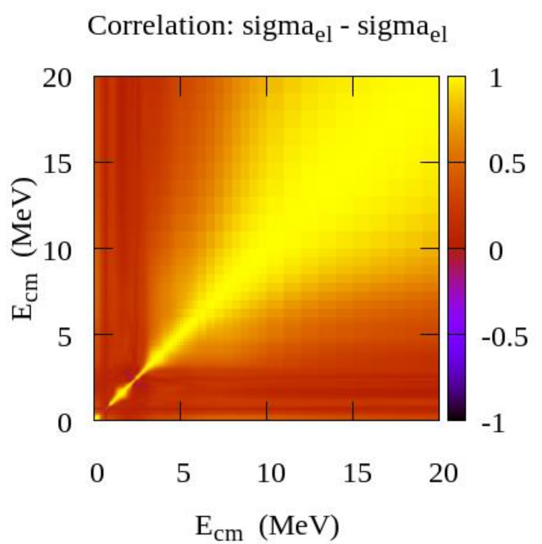
Sensitivity Matrix: $\vec{\sigma}_{\mathrm{int}} = M_{\mathrm{surr}}\left(\vec{\sigma}_{\mathrm{mod}}\right) = \mathbf{S}\vec{\sigma}_{\mathrm{mod}}$

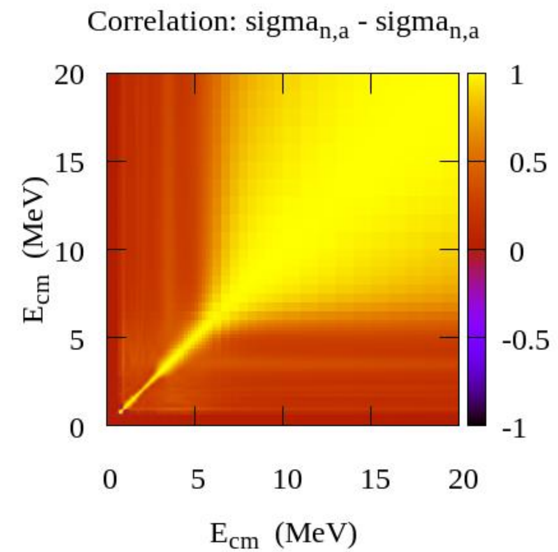
Bayesian Evaluation of n+^{9}Be via GLS

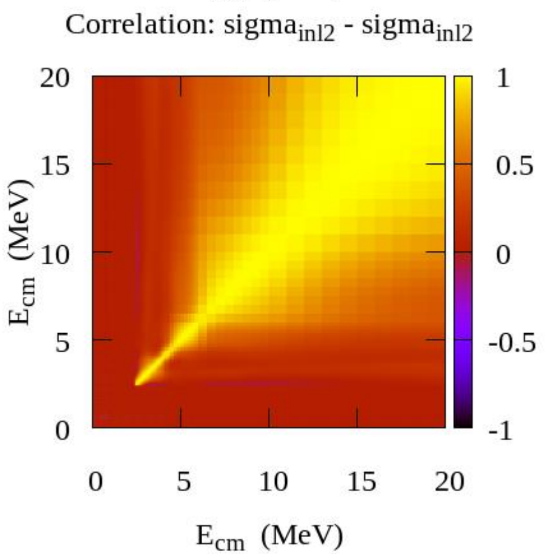


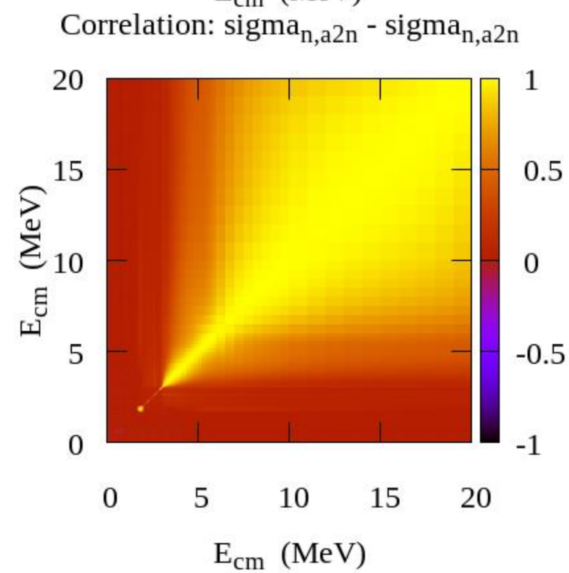
Bayesian Evaluation of n+^{9}Be via GLS

Correlations

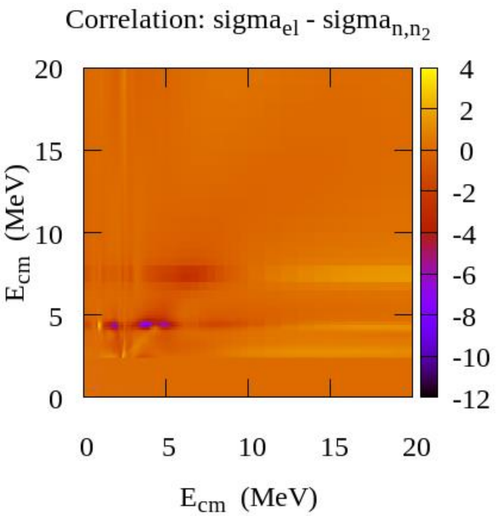


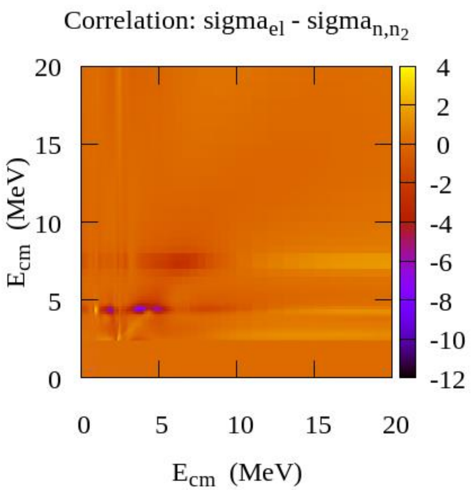


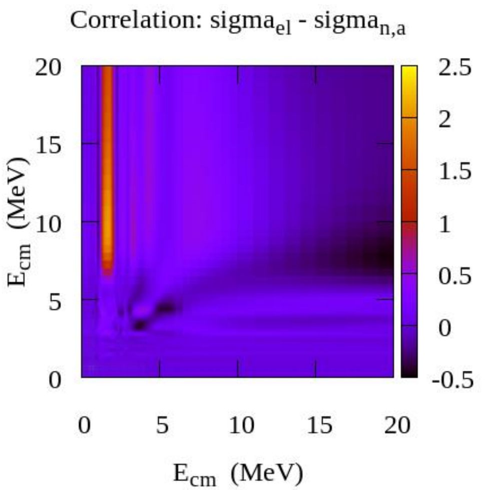


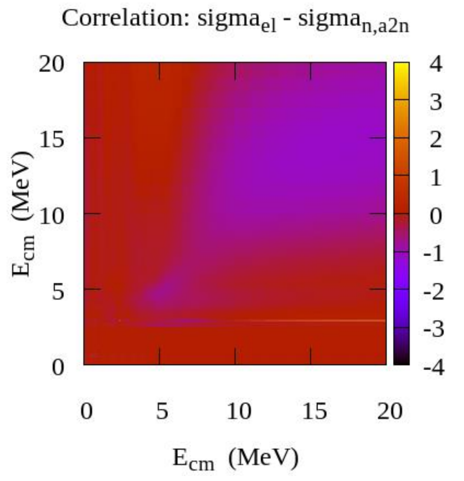


Bayesian Evaluation of n+^{9}Be via GLS
Cross Reaction Correlations









Summary and Outlook

Challenges in light nuclear data evaluation:

- ✓ Inclusion of dominant breakup channels
- ✓ definition of a quasi a-priori
- ✓ execution of Bayesian evaluation technique in the resonance range
- extension of R-matrix to higher energy (in progress)
- inclusion of model defects into the Bayesian evaluation procedure

Standard Evaluation: $\vec{\sigma}_{\mathrm{exp}} = \vec{\sigma}_{\mathrm{mod}} + \vec{\varepsilon}_{\mathrm{exp}}$

Experiment vector — Model vector — Uncertainty vector of experiment

$$\vec{\sigma}_{\mathrm{exp}} = \vec{\sigma}_{\mathrm{mod}} + \vec{\varepsilon}_{\mathrm{mod}} + \vec{\varepsilon}_{\mathrm{exp}}$$

Extended Evaluation:

Model defects via Gaussian process

Raab et al., WONDER 2018

The Nuclear Data Team at TU Wien

End

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Thank you for your attention