Nuclear Data Evaluation of Light Nuclear Systems

Helmut LEEB
Working Group on Nuclear Physics and Astrophysics
Atominstitut, TU Wien, Austria

Research Topics

- **Nuclear Reaction Theory and Calculations**
  - reduced R-matrix analysis of light nuclear systems
  - development of R-matrix formalism for three-body breakup
  - extension of R-matrix theory to unresolved resonance regime
  - development of reaction code GECCCOS
- **Bayesian Evaluation Technique**
  - development of evaluation methods including model defects
  - formulation of evaluation technique for differential data and resonance data
  - large scale formulation of General Least Square Technique
  - development of general Bayesian evaluation code GENEUS
- **Neutron cross section measurements at n_TOF@CERN**
  - simultaneous (n,γ) and (n,f) cross section measurements of ^{233}U
  - neutron reaction measurements involving charged particles (n,p), (n,α)
  - development of diamond detectors
- **Specific Topics in Quantum Mechanics**
  - ultracold neutrons in the gravitational field
  - supersymmetric quantum mechanics, phase determination in neutron reflectivity

Impact of Neutron-induced Reactions of Light Nuclear Systems

Aging of Structure Materials due to radiation:

- embrittlement of structure materials due to radiation – composition of steel

$n + {}^{16}O \rightarrow {}^{13}C + {}^{4}He$
$n + {}^{12}C \rightarrow {}^{9}Be + {}^{4}He$
$n + {}^{16}O \rightarrow {}^{16}N + p$
$n + {}^{12}C \rightarrow {}^{12}B + p$

} gas producing reactions

Impact on Fusion Research – e.g. for the Breeding Blanket

- absorbing the energy of the neutrons produced by the D-T reaction in the plasma
- breeding of tritium fuel
- shielding to protect the outside of the reactor from radiation

One concept for the breeding blanket is based on Li and Be ceramics

$n + {}^{6}Li \rightarrow {}^{4}He + t$	Q=+4.783 MeV	tritium breeding
$n + {}^{9}Be \rightarrow {}^{4}He + {}^{4}He + n + n$	Q=-1.6651 MeV	neutron multiplier
$d + t \rightarrow {}^{4}He + n$	Q=17.580 MeV	fusion reaction (E_n=14.06 MeV)

Light Nuclear Systems

The quality of evaluated nuclear data files for light nuclear systems is not fully satisfactory – are limited in energy range and completeness

Major Challenges:

- no quantitatively reliable microscopic models
- resonance range extends to rather high energies
- occurence of dominant non-binary channels at low energy
- application of the statistical nuclear model is questionable
- reliable uncertainty information is still an open problem

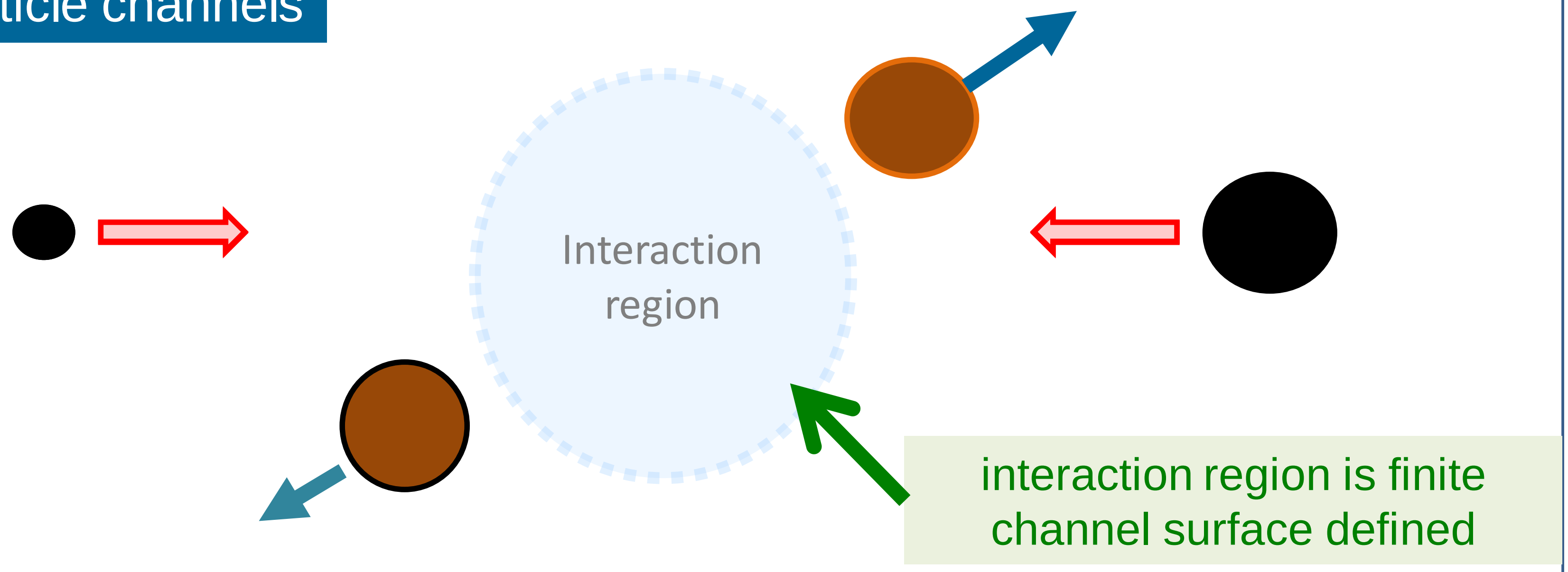
⇓

usually **R-matrix theory** is used (key: finite interaction volume)

- no microscopic basis → no predictive power
- limited to binary channels
- limited in energy range (number of width parameters)

Problem of R-matrix Theory

2-particle channels

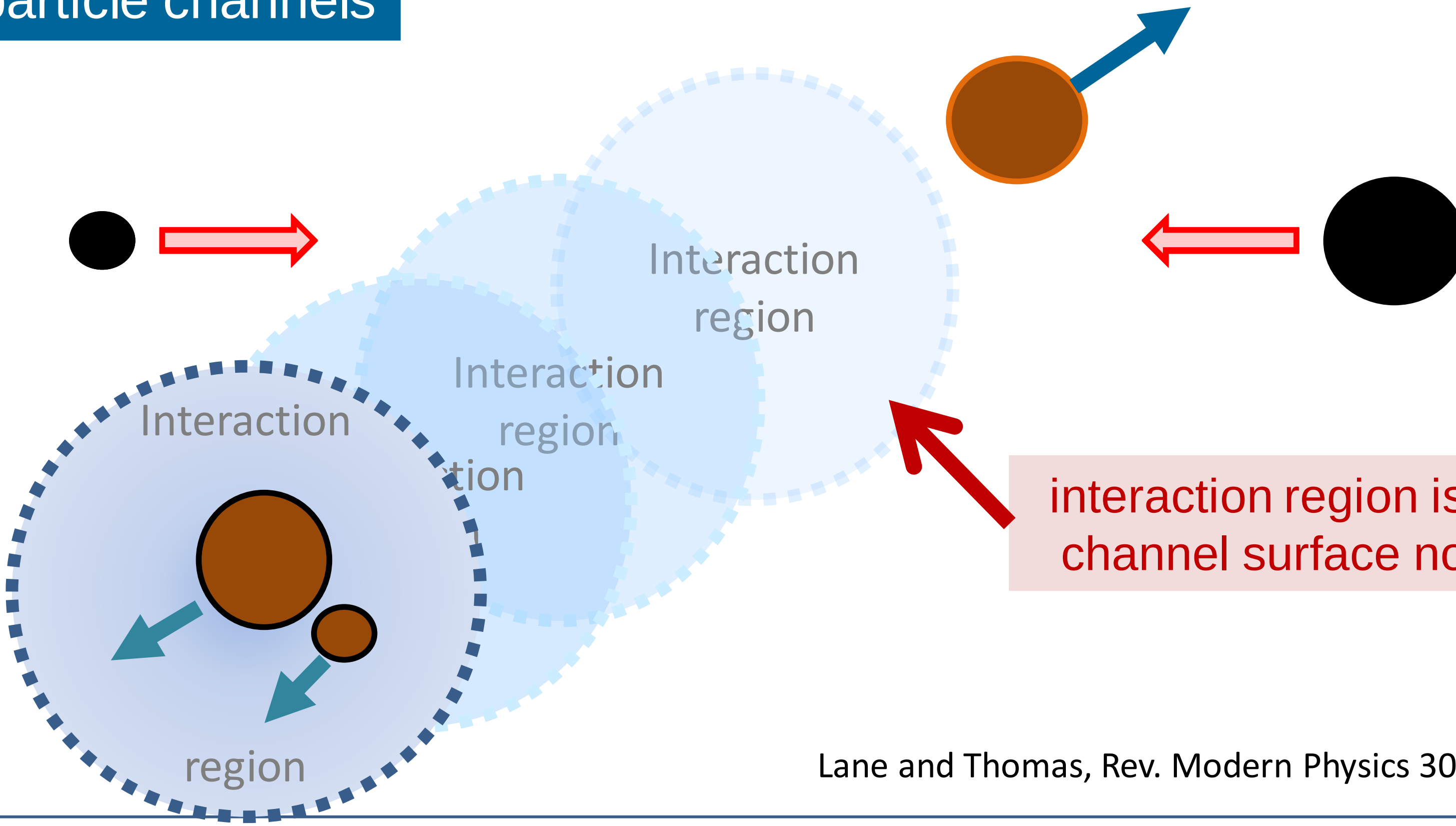


Lane and Thomas, Rev. Modern Physics 30, 257 (1958)

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_\lambda^c \gamma_\lambda^{c'}}{E_\lambda - E} \quad , \qquad \left(R_{cc'}\right) \Leftrightarrow \left(S_{cc'}\right)$$

Problem of R-matrix Theory

3-particle channels

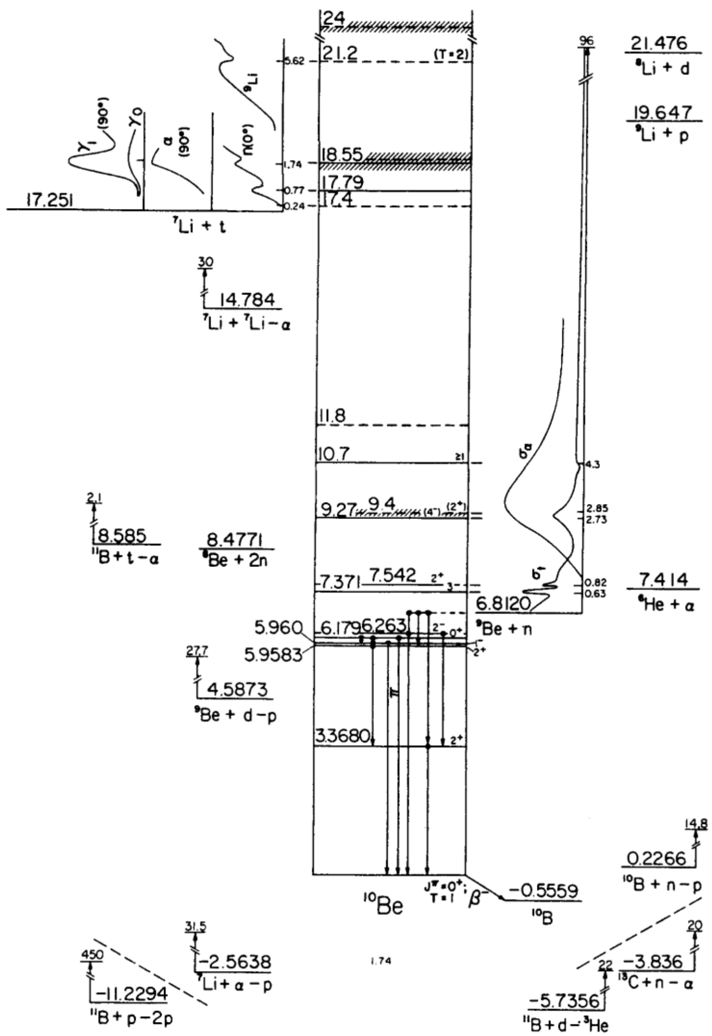


interaction region is not finite
channel surface not defined

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

Neutron-induced Reactions of ^{9}Be

level scheme of ^{10}Be

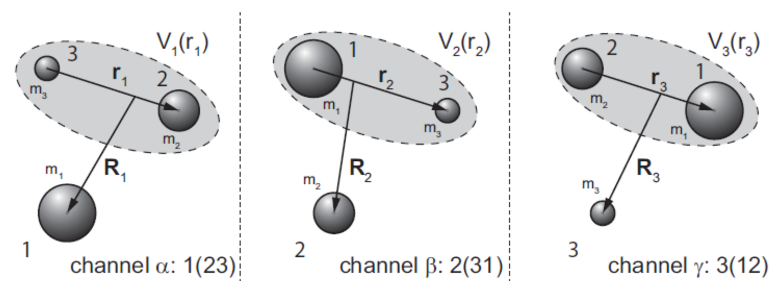


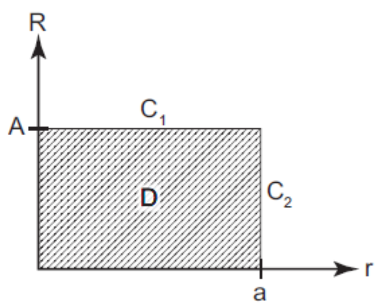
^{9}Be(n,n)^{9}Be	Q= 0.0000 MeV
^{9}Be(n,α)^{6}He	Q= -0.5971 MeV
^{9}Be(n,2nα)^{4}He	Q= -1.6636 MeV
^{9}Be(n,nα)(^{5}He)	Q= -2.3073 MeV
^{9}Be(n,n')^{9}Be*	various Q-values
^{9}Be(n,t)^{7}Li	Q=-10.4373 MeV
^{9}Be(n,p)^{9}Li	Q=-12.8248 MeV
^{9}Be(n,tα)t	Q=-12.9049 MeV
^{9}Be(n,d)(^{8}Li)	Q=-14.6615 MeV
^{9}Be(n,t)(^{8}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

Basics of the 3-body R-matrix formalism

- First idea by W. Glöckle in 1974 (Z. Physik 271, 1974)
  - ‘Channel surface’ introduced in Jacobi coordinate space
  - Based on the Faddeev equations in coordinate space
  - Theory for three identical particles
  - Equal two-body interactions between them
  - Restricted to s-waves
- Extension to general masses and interactions (Raab, diploma thesis. TU Wien, 2017)

Division of Jacobi-coordinate Space





$C_1:\ R = A\ \text{ and }\ 0 \le r \le a$

$C_2:\ r = a\ \text{ and }\ 0 \le R \le A$

The range r_0 of the potential determines *a* and *A*

Set of basis functions in the domain D:

$$u_i(r_i, R_i) = \sum_\mu c_\mu^{(i)} \varphi_\mu(r_i, R_i)$$

wave function component i in the domain D

$$\varphi_\mu(r, R) = X_{\mu_1}(r) Y_{\mu_2}(R)$$

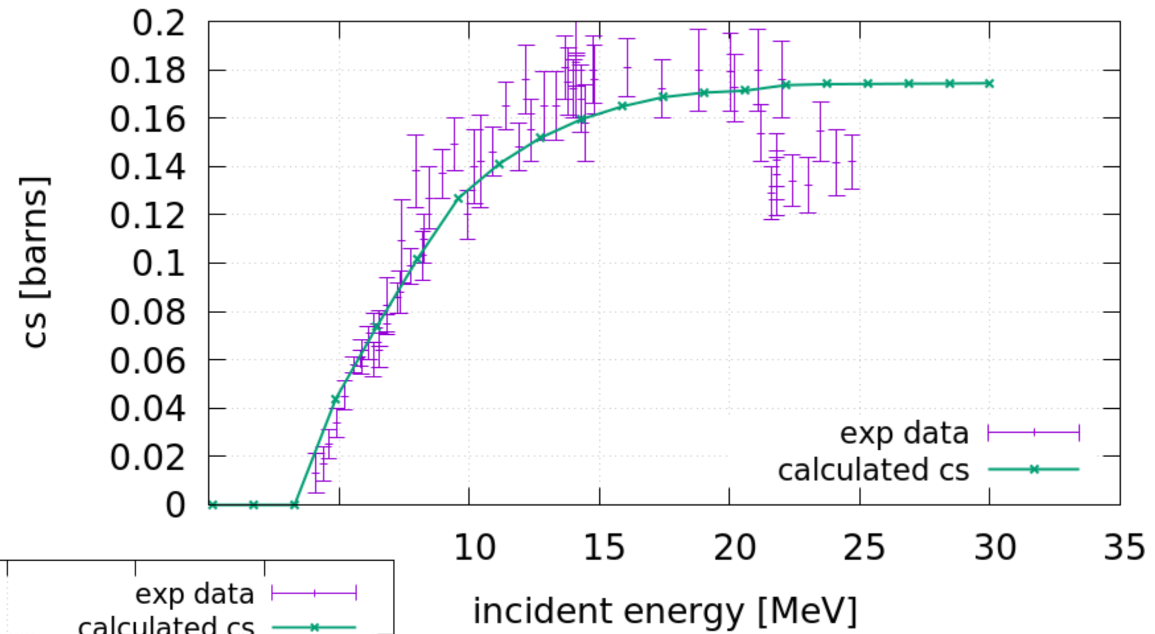
basis functions

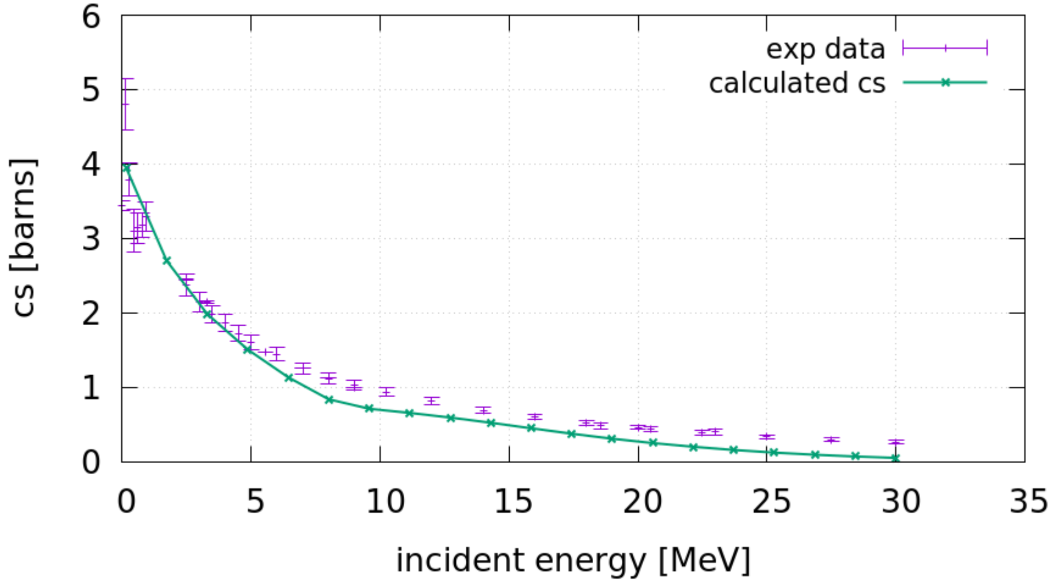
$$\left[-\frac{1}{2\mu_{jk}}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_i(r) - \epsilon_{\mu 1}^{(i)}\right] X_{\mu_1}(r) = 0$$

$$\left[-\frac{1}{2\mu_{i(jk)}}\frac{\mathrm{d}^2}{\mathrm{d}R^2} - \epsilon_{\mu 2}^{(i)}\right] Y_{\mu_2}(R) = 0$$

Results for n-d collisions

n-d breakup channel:



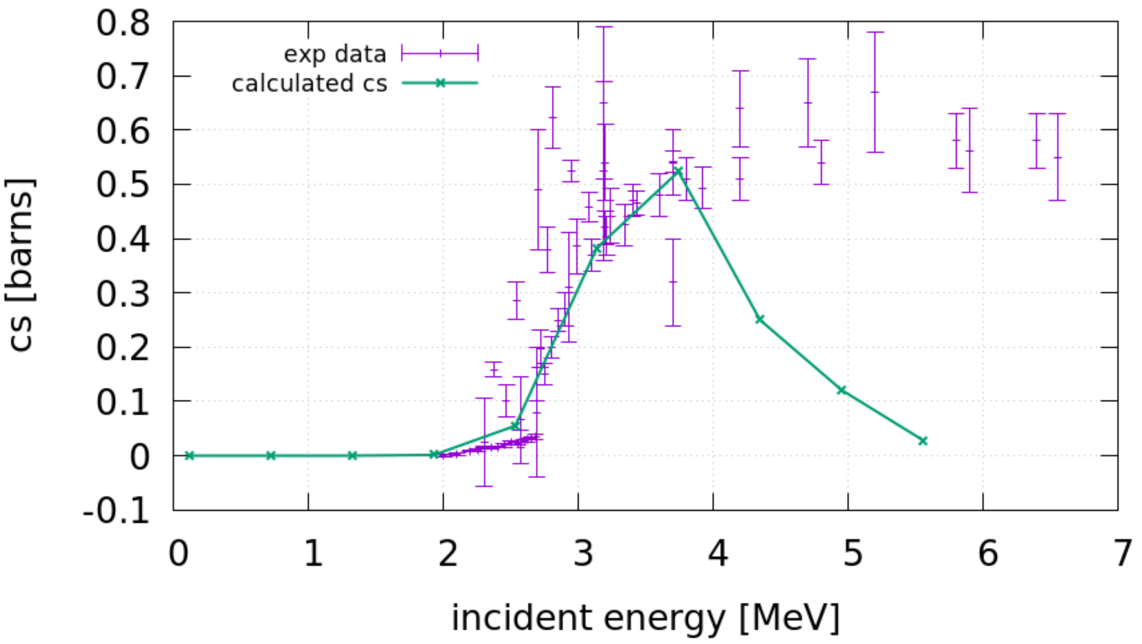


n-d elastic scattering

R-matrix calculation of $n+{}^{9}Be \rightarrow 2\alpha+2n$

- reaction considered as $n+{}^{9}Be \rightarrow ({}^{8}Be)+n+n$
- ${}^{9}Be$ is an l=1 neutron bound state of ${}^{8}Be$ at E_b=1.665 MeV in a Wood-Saxon potential
- the same neutron-neutron potential as in the n-d case is used
- approximation of the l=1 partial wave of ${}^{9}Be$

Breakup cross section: a_i=16 fm, A_i=13.4 fm



Subsystem 1:
bound state and 12 basis states, 0.1-6 MeV
Subsystem 2:
12 basis states, 0,1-25 MeV

Total: 156 basis states

An exact R-matrix formulation for 3-body breakup is required.
Already derived by our group and implementation is currently in progress.

Reduced R-Matrix Analysis

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

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

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

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

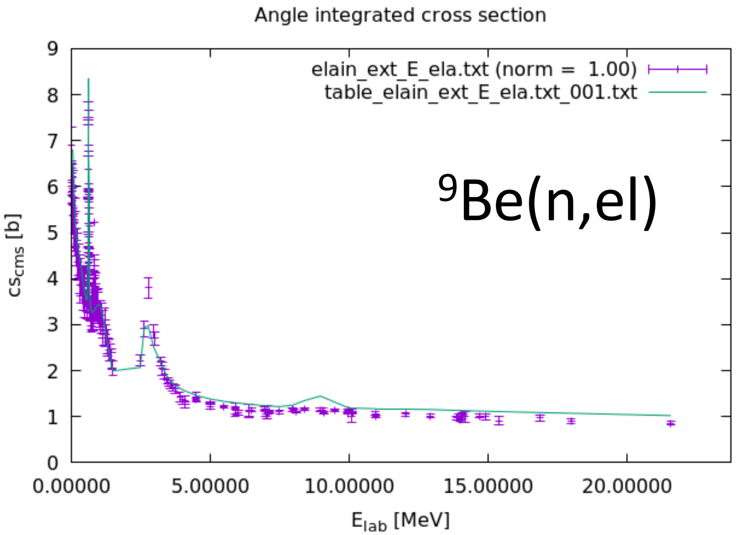
Property of *L(k_m a)*:

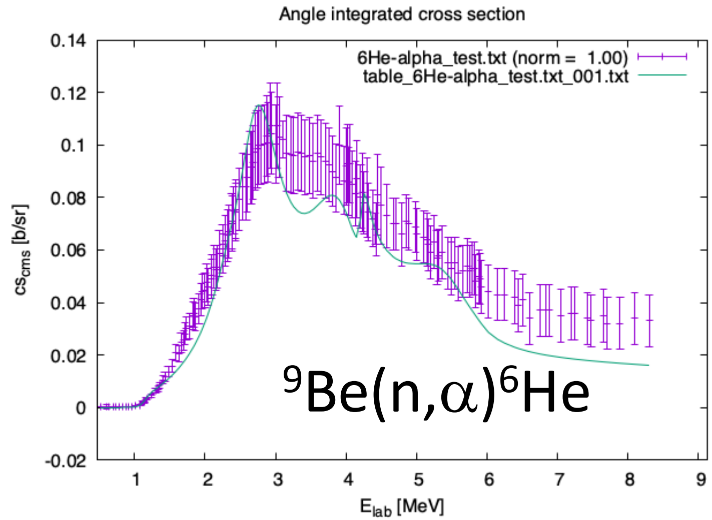
$L(k_m a)$ guarantees the correct threshold behaviour

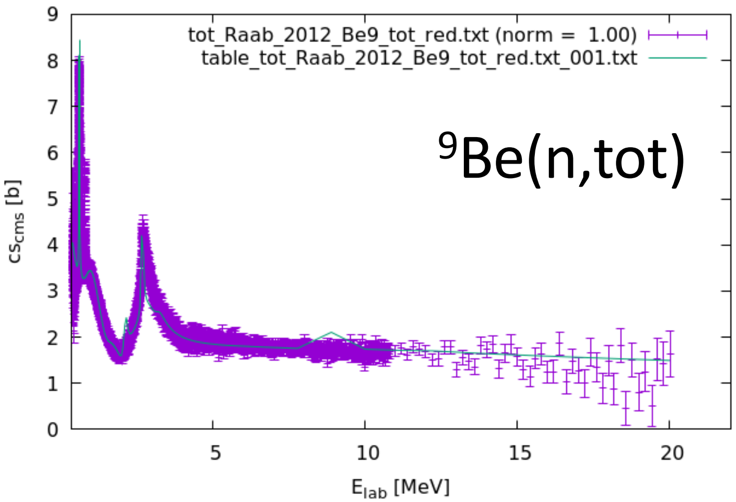
$L(k_m a)$ is real valued below threshold

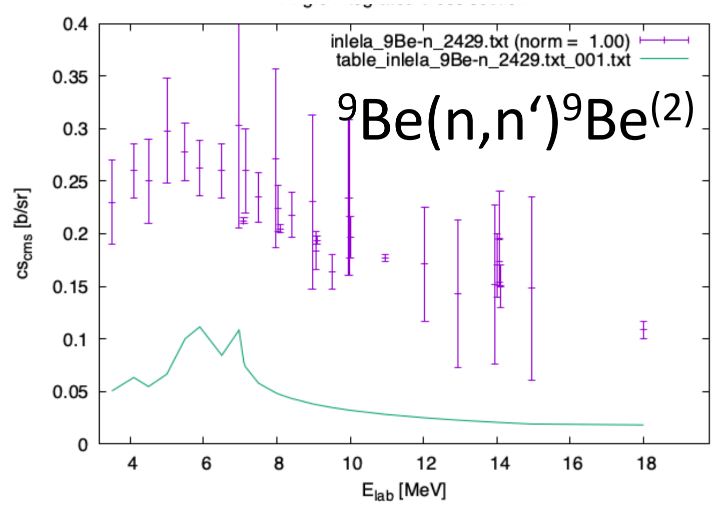
$L(k_m a)$ is complex above threshold

Reduced R-Matrix Analysis using one-pole formula



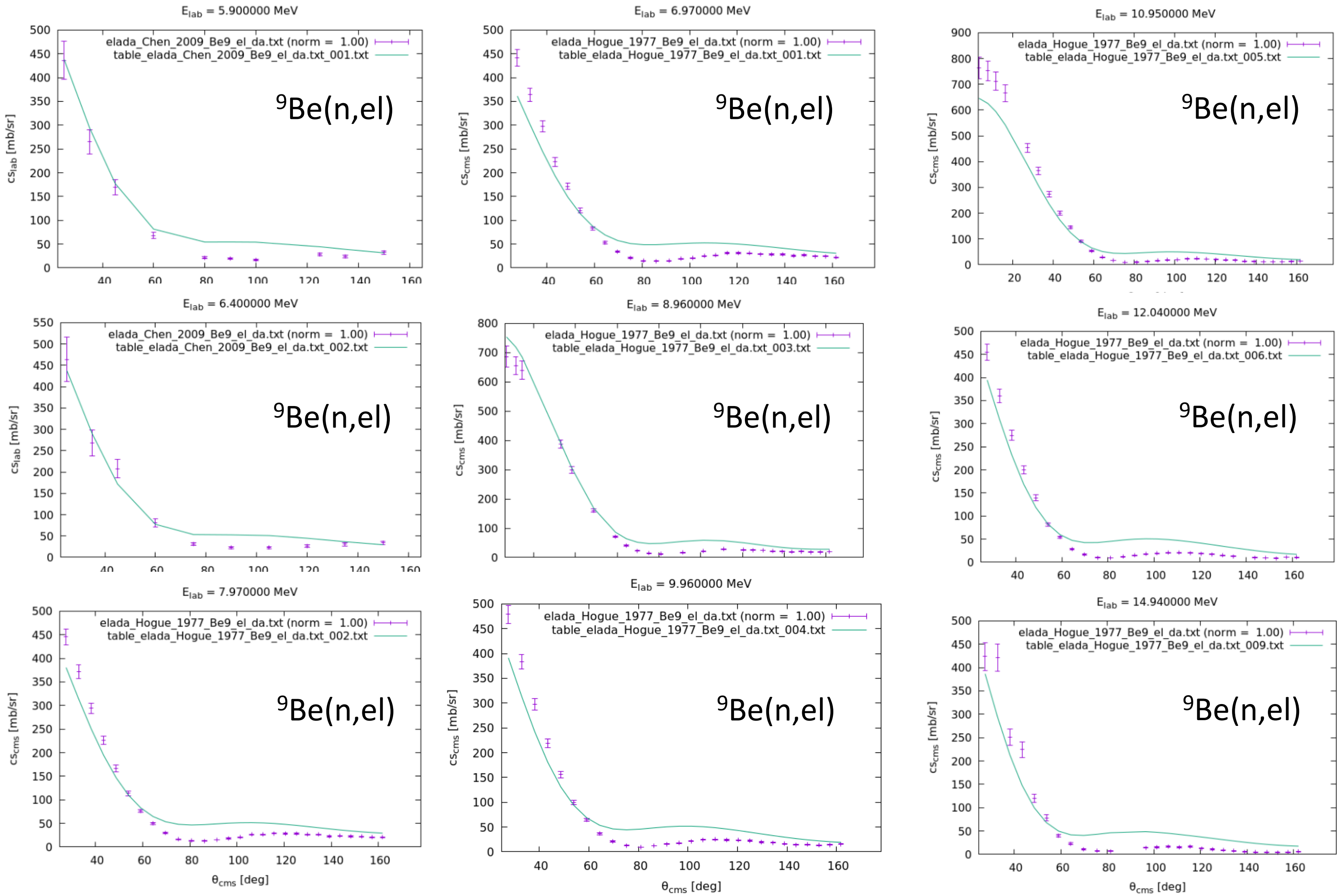




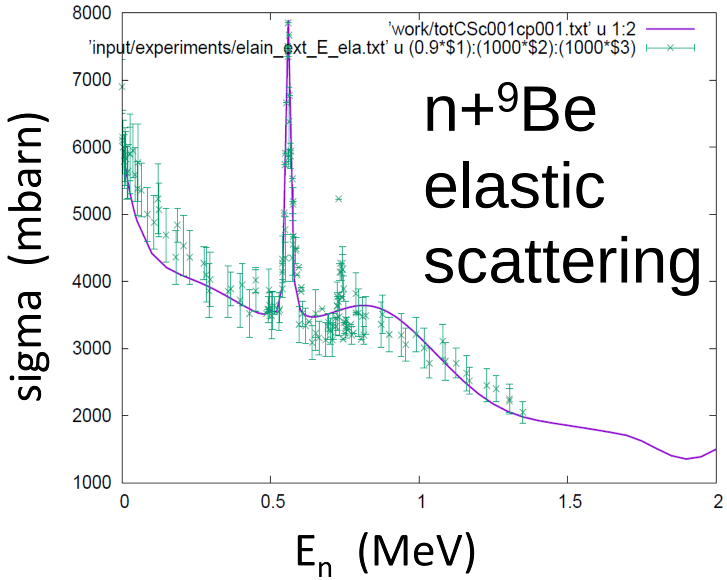


Reduced R-Matrix Analysis n+^{9}Be

elastic differential cross section



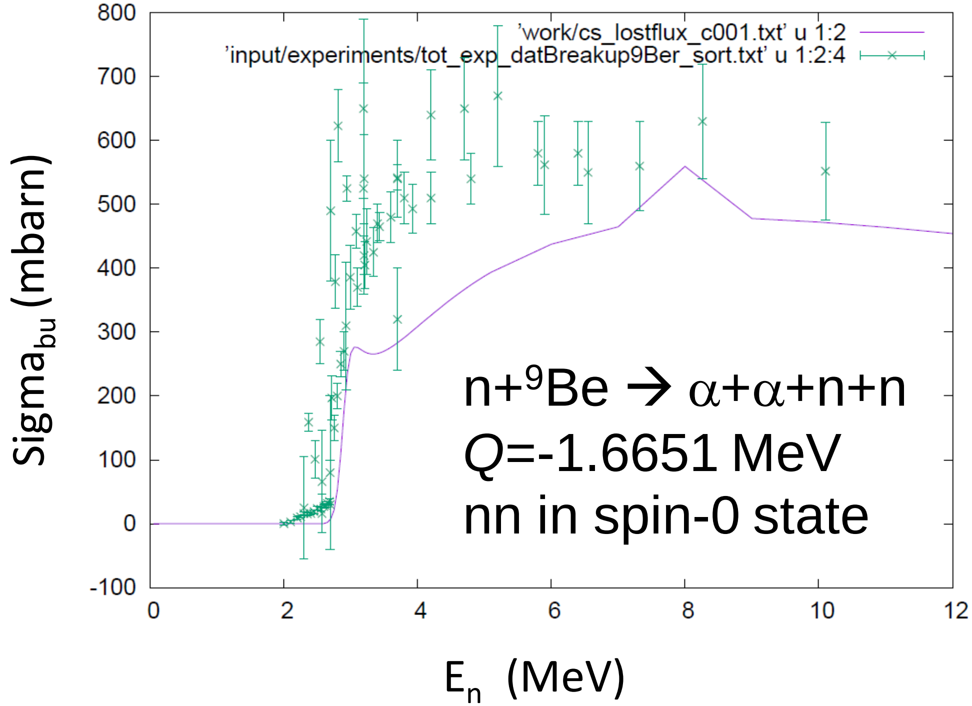
Reduced R-Matrix Analysis n+^{9}Be



The breakup cross section can be determined from the defect of unitarity. In principle the integral cross sections of different ignored channels can be disentangled.

Analysis performed with 26 pole terms and more than 260 reduced widths – several have large values + 26 normalisations and *a*-values

interference effects



Bayesian Evaluation Technique

Bayesian Statistics

Bayes Theorem (1761):

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

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

Evidence
normalisation

likelihood
Experimental information

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

Novel Evaluation Concept:
Statistically consistent Treatment of Model Defects

Standard Evaluation:

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

Experiment vector Model vector Uncertainty vector of experiment

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

Model defect

described by Gaussian process

Extended Evaluation:

Concept of non-perfect model can be applied in many fields of physics, e.g. optimizing Skyrme forces, etc.

PhD thesis of Georg Schnabel (TU Wien, June 2015)

Bayesian Evaluation Technique

R-matrix – subject to model defects?

Experience: excellent description of experimental data achieved

Expected: almost rigorous for binary entrance and exit channels
Doubts: 3- and many-body breakup, β- and γ-emitting channels

Possible sources of uncertainties

Key quantities in R-matrix theory: a_c, B_c, $\{E_n, \gamma_{nc}\}$
subject to **parameter uncertainties** → $R_{cc'} = \sum_{n=1}^{\infty} \frac{\gamma_{nc}\gamma_{nc'}}{E_n - E}$

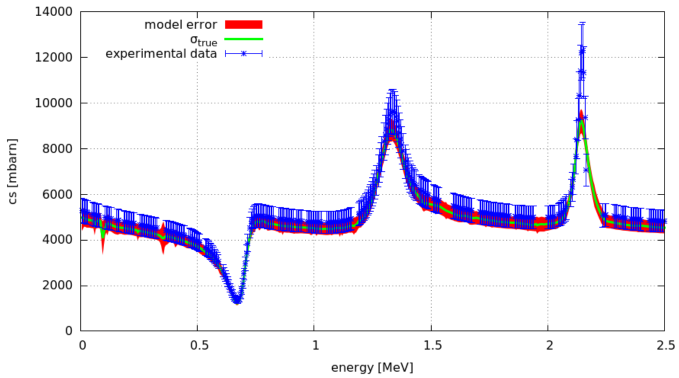
Possible Model Deficiencies:

- only finite number of pole terms included
- violation of unitarity (missing channels, perturbative contributions, …)
- use of approximations
- unrealistic a_c and/or background contribution

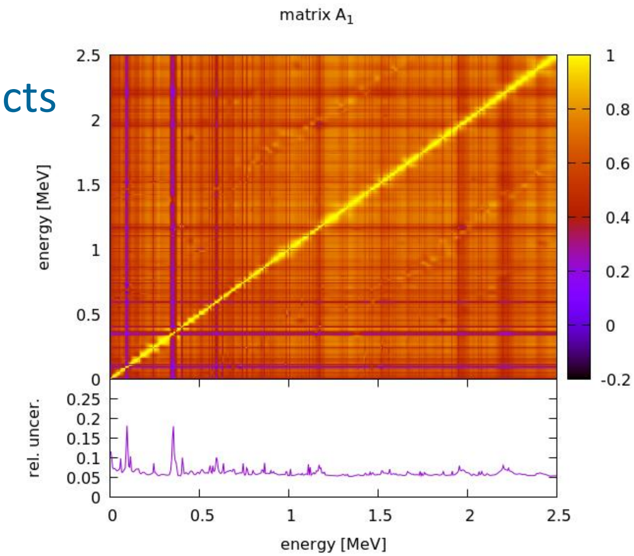
Model defects in the resonance regime via Gaussian processes
requires suitable covariance matrix for model defects (Raab et al., WONDER 2018)

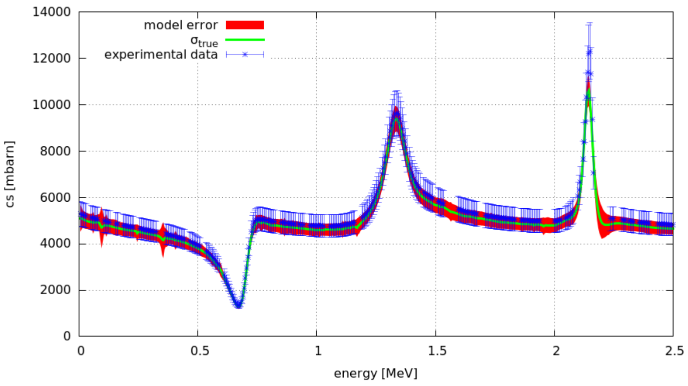
$$K_0(E_i, E_j) = \delta_1^2 \sigma_M(E_i)\sigma_M(E_j)\exp\left[-\frac{(E_i - E_j)^2}{2\lambda_1^2}\right] + \delta_2^2 \frac{d\sigma_M}{dE}(E_i)\frac{d\sigma_M}{dE}(E_j)\exp\left[-\frac{(E_i - E_j)^2}{2\lambda_2^2}\right]$$

Model Defects of R-Matrix Analysis:
Schematic Example

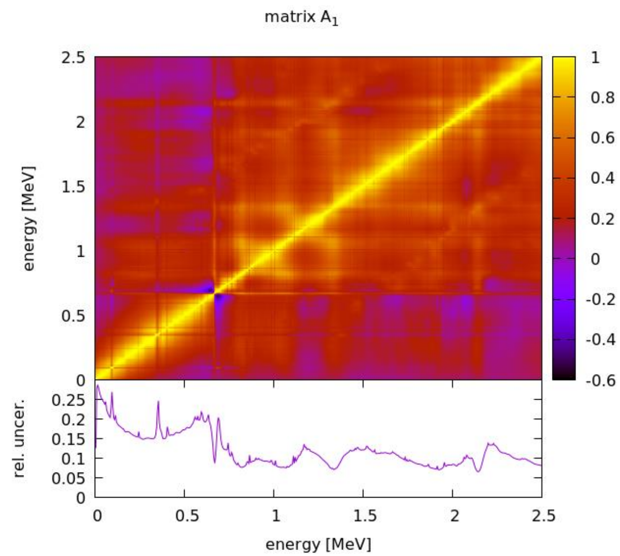


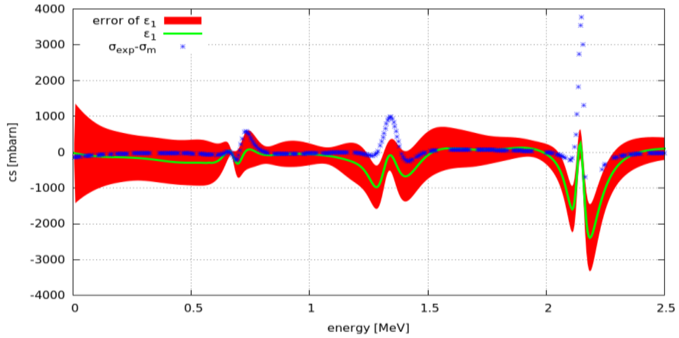
without model defects





with model defects





difference between built-in model defect and the extracted mean for the model defect

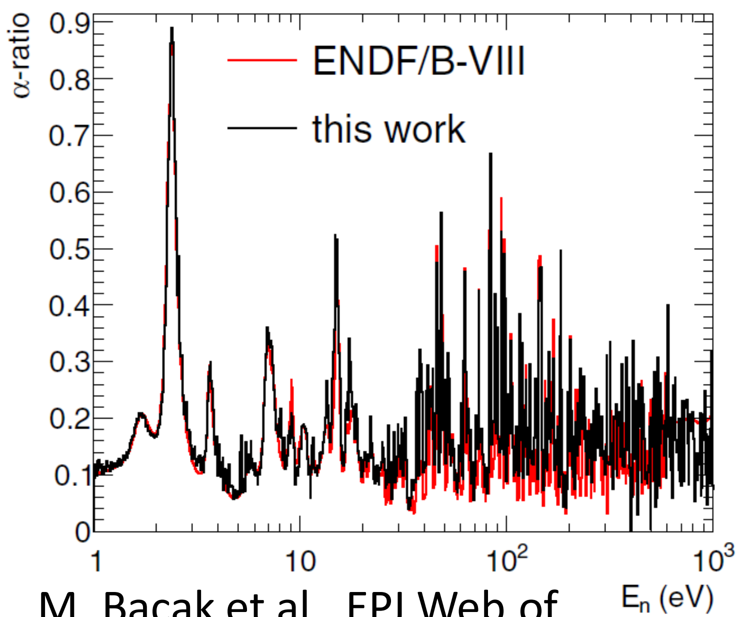
Experiments n_TOF@CERN with involvement of Team of TU Wien

n_TOF Team of TU Wien:

Atominstitut: M. Bacak*, E. Jericha, H. Leeb (*PhD student (until 2019)

Simultaneous measurement of ^{233}U(n,γ) and ^{233}U(n,f)

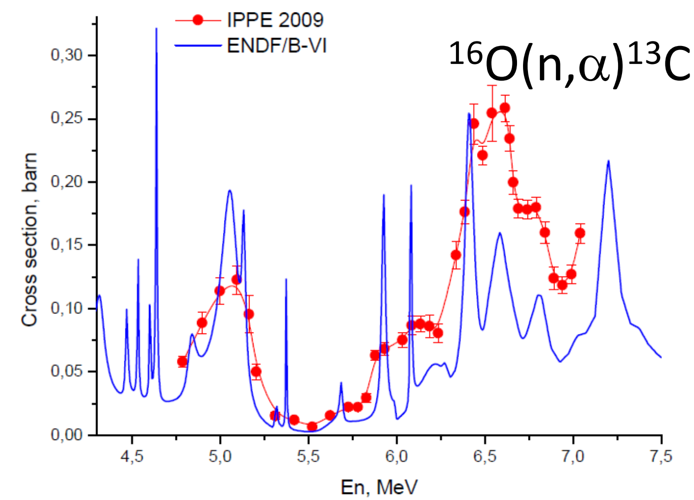
M. Bacak, PhD thesis (TUW, CEA-Saclay,2019) of



M. Bacak et al., EPJ Web of Conferences, ND2019_01043

The (n,α) cross section measurement for light isotopes

gas targets: ^{16}O, ^{10}B, ^{12}C, ^{14}N, ^{19}F



International Research Projects

Running Projects

- SANDA, Euratom Project, HORIZON 2020
- EUROfusion Nuclear Data, HORIZON EUROPE Project
- Matching Grants, Austrian Academy of Sciences – Fusion Research
- INDEN-LE, IAEA, Evaluation of Light Nuclear Systems
- IAEA, Technical Working Group on R-Matrix Calculations for charged particle systems.

Participant in completed Projects

EC-Projects: ENSAR, EURONS
ESF Eurocores Project EXNUC

Euratom Projects CHANDA, ANDES, IP-EUROTRANS, n_TOF-ADS
EUROfusion Grants and F4E Projects on Nuclear Data Files

Bachelor, Master and PhD students

Bachelor Students

About 10 Bachelor theses per year

Master Students

Tanja Stary (current)

Tobias Wojta (current)

PhD Students

Thomas Srdinko (current)

Current positions of former PhD Students

Marco Pigni (staff member. ORNL, Oak Ridge)

Denise Neudecker (staff member, LANL, Los Alamos)

Georg Schnabel (staff member, ND Group, IAEA)

Verena Kleinrath (staff member, LANL, Los Alamos)

Michael Bacak (n_TOF, CERN)

Benedikt Raab (PostDoc, Stanford)

Outlook

Physics

- Development of a combined R-matrix formalism for 2- and 3-body channels
- Extension of R-matrix analyses to the regime of unresolved resonances

Code Developments

- Extension of the reaction code GECCCOS

  to a unique and user-friendly R-matrix tool for 2- and 3-body channels
  (especially suited for analyses of light systems)

- Completion of the general evaluation code system GENEUS

  implementation of recently developed large scale techniques
  simultaneous consistent evaluations of isotope groups and reactions
  capability to manage input and output via data bank system

Thank you for your attention