Novel Developments In R-Matrix Theory

Atominstitut, TU Wien:

H. Leeb, B. Raab, T.Stary, Th. Srdinko

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014-2018 and 2019-2020 under grant agreement No 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

support by the KKKÖ Matching Grant MG 2018-7 of the Austrian Academy of Sciences is acknowledged.

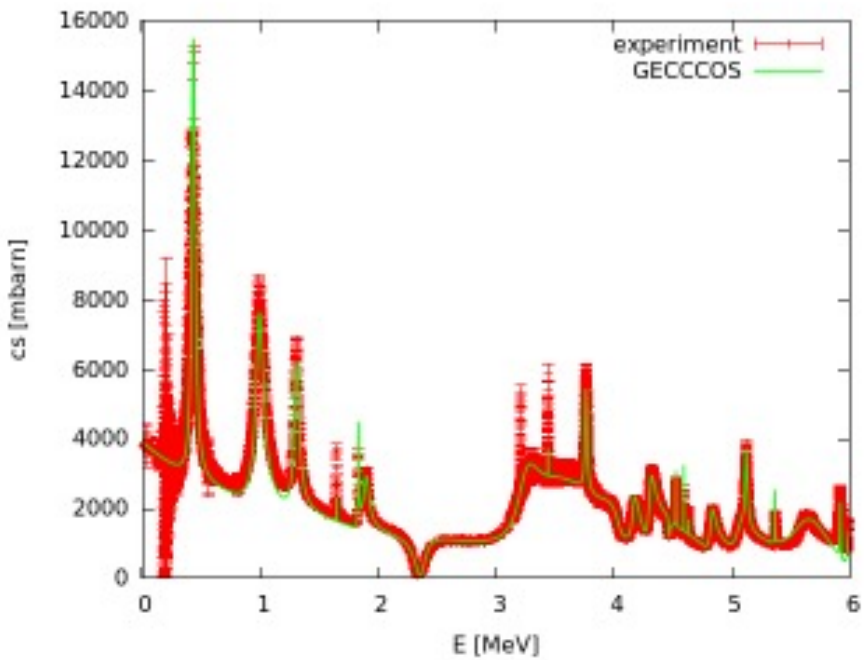
Motivation - Background

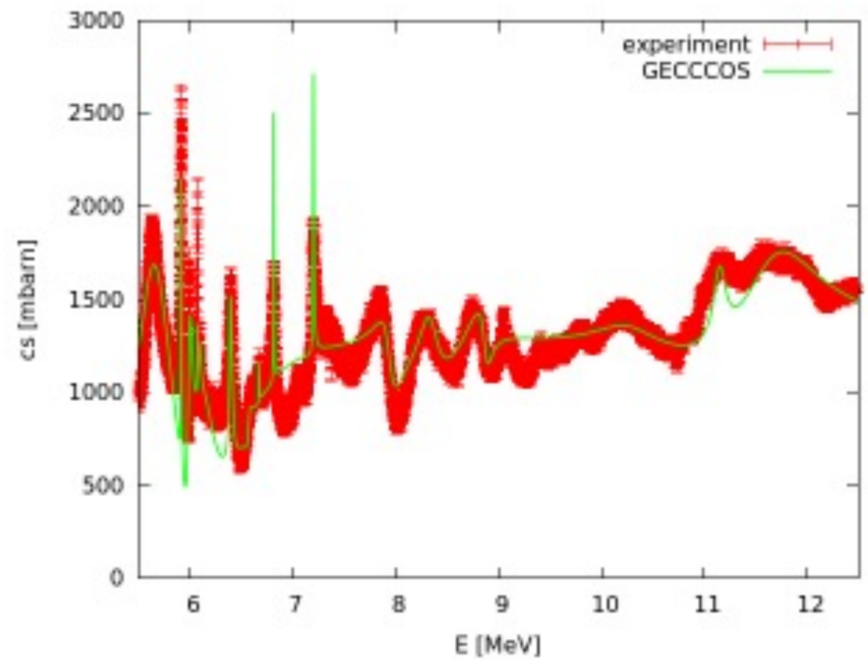
There is a worldwide effort to determine the best knowledge of nuclear reaction cross sections (nuclear data libraries)

- This is an important prerequisite for the development of new technologies in various fields (fusion research, advanced reactor techniques, medicine, safety issues, space science, materials testing,…
- General problem is the resonant behaviour at low incident collision energy, reflecting the many-body character of nuclei. (Especially, in light nuclear systems.)

The total n+^{16}O cross section

Example: Neutron Cross Sections on ^{16}O





Challenges in Light Nuclear Systems

Problems:

- Resonance range up to relatively high incident energies
- No predictive quantitative microscopic models

⇩

R-Matrix Theory

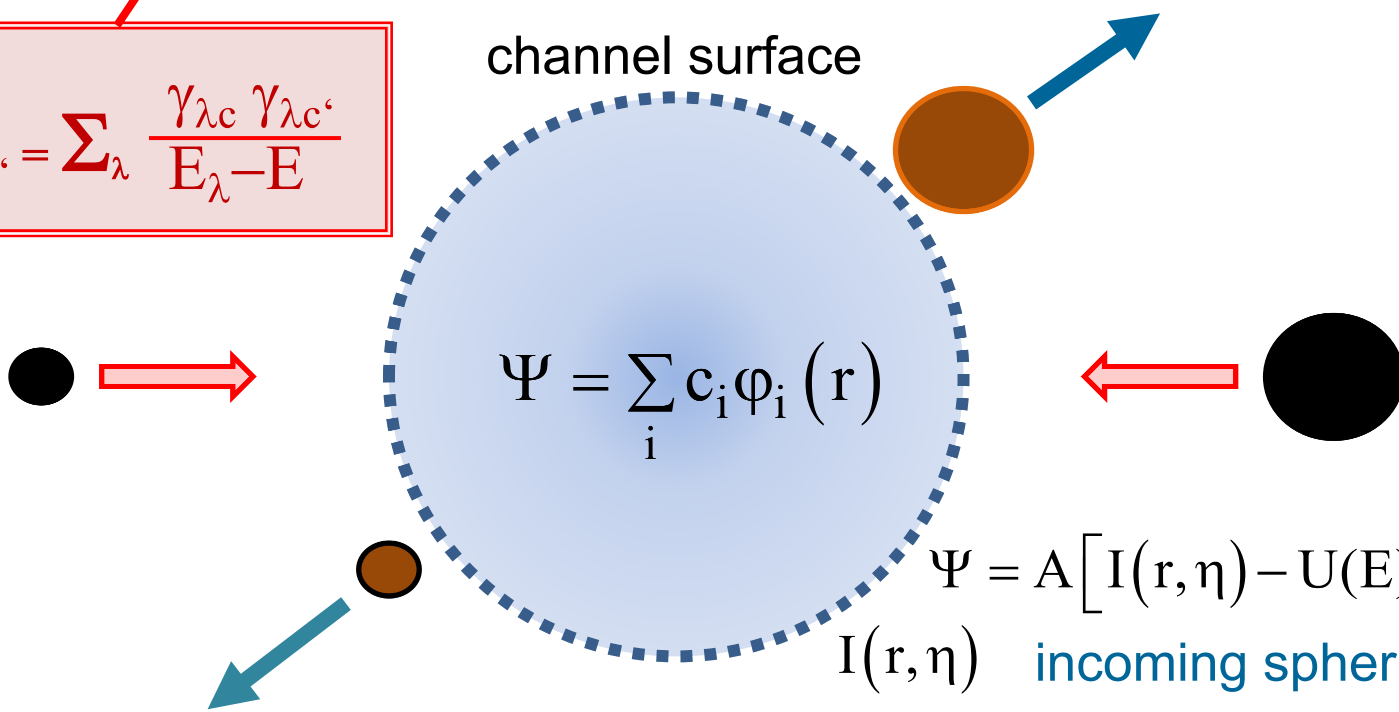
No microscopic information,but satisfies all conservation rules
Proposed by Eisenbud and Wigner in the fifities of the last century

Standard R-Matrix Formalism: wave function

2-particle channel: cm-system

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

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



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

$I(r,\eta)$ 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,…

New R-Matrix Code: GECCCOS

GECCCOS (GEneral Coupled-Channel COde System)
A new comprehensive R-matrix code developed by T. Srdinko at TU Wien

New features compared with existing R-Matrix codes (SAMMY, AZUR, …)
but also compared to special codes like EDA, FRESCO, RAC, …

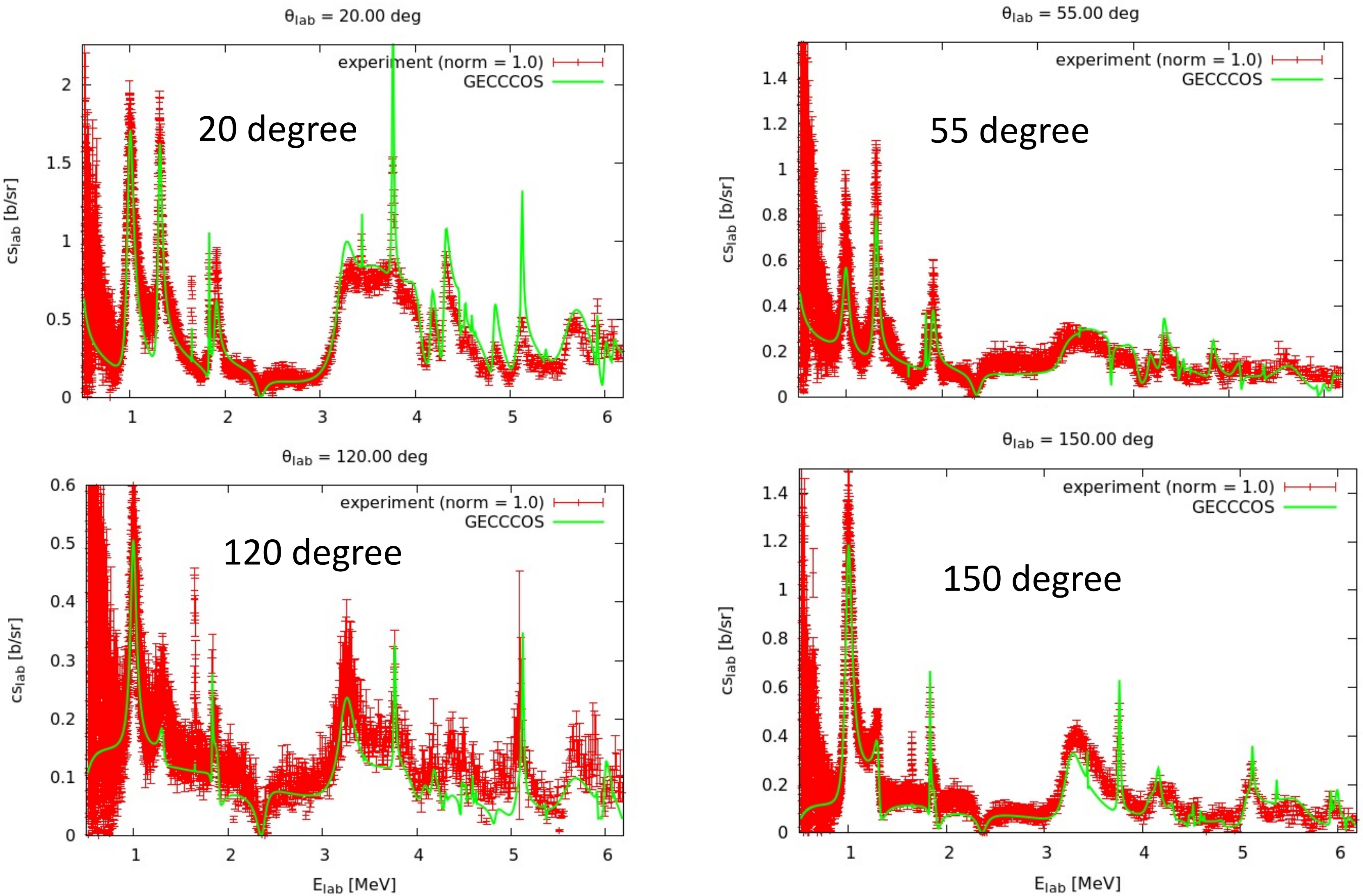
New Features:

- ✓ Capability of calculabe R-Matrix calculations
- ✓ Possibility of hybrid R-Matrix approach
- ✓ Analysis procedures based on different optimization procedures
- ✓ Allowing for combined analysis of observables and S-matrices
- ✓ Transformation of R-matrices to different matching radii

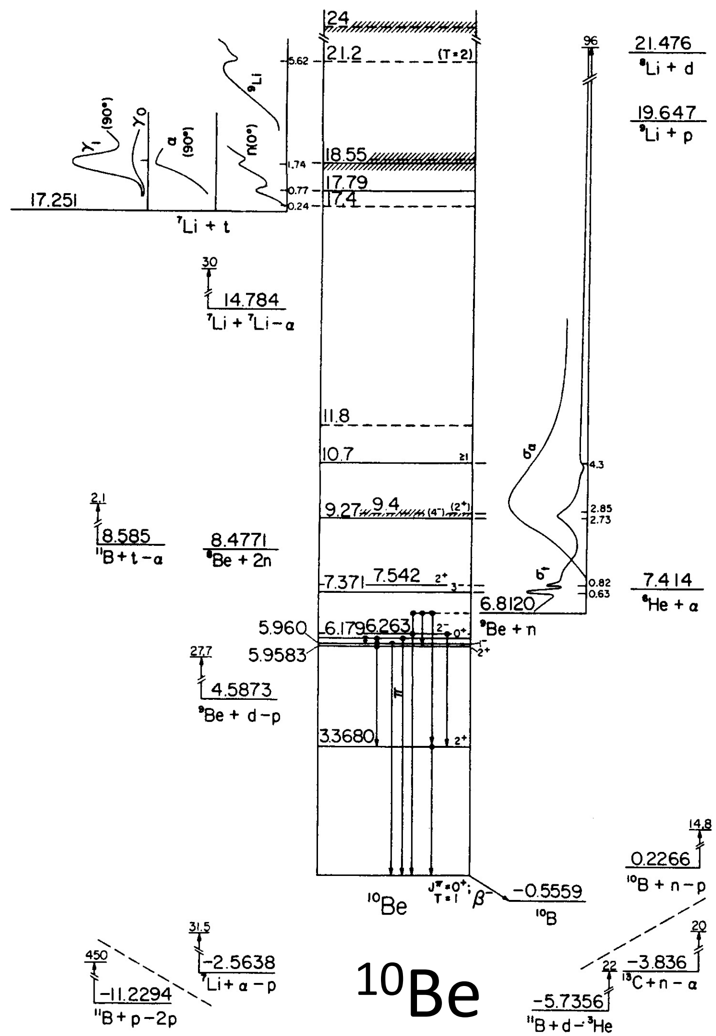
Current Developments

- ➢ Development of R-matrix formulations for three-body channels (breakup)
- ➢ Reduced R-matrix parametrisations accounting for thresholds of non-explicitly treated channel

Elastic excitation functions



Light Nuclear Systems: Further Challenge



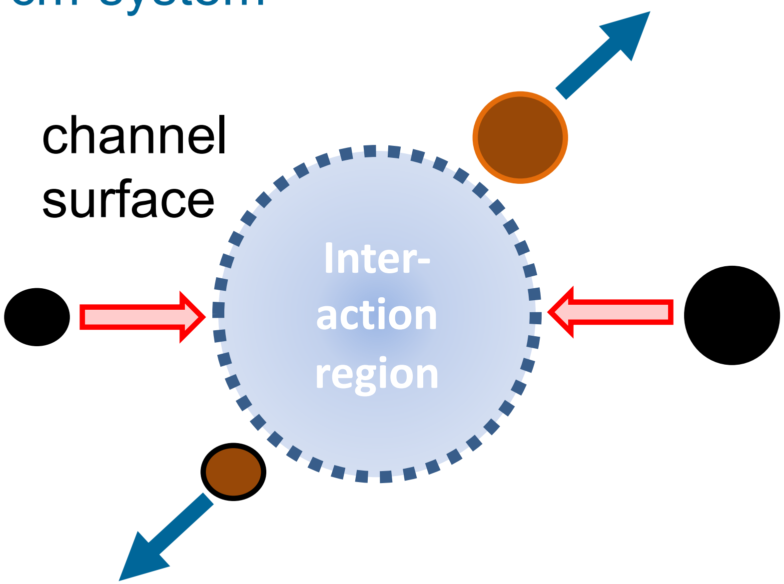
n-induced Reactions

$^{9}Be(n,n)^{9}Be$	Q= 0.0000 MeV
$^{9}Be(n,\alpha)^{6}He$	Q= -0.5971 MeV
$^{9}Be(n,2n\alpha)^{4}He$	Q= -1.6636 MeV
$^{9}Be(n,n\alpha)(^{5}He)$	Q= -2.3073 MeV
$^{9}Be(n,t)^{7}Li$	Q=-10.4373 MeV
$^{9}Be(n,p)^{9}Li$	Q=-12.8248 MeV
$^{9}Be(n,t\alpha)t$	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
$^{9}Be(n,\alpha)^{6}Li$	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
$^{9}Be(n,p\alpha)(^{5}H)$	Q=-23.1857 MeV

R-Matrix Formalism: Concept

Standard

2-particle channel:
cm-system



Lane, Thomas, Rev. Mod. Physics 30, 257 (1958)

Extension to 3-Particles

Problems:

- no fixed channel surface in space
- asymptotic form of wave function in 3-body breakup
- impact of off-shell behavior of 2-body *t*-matrix on breakup

Proposal of Glöckle: R-Matrix Formulation based on the Faddeev Equations (only s-waves)

- variable channel surfaces
- problem-adapted basis functions

$$\Psi^{(+)} = \Psi_1(r_1, R_1) + \Psi_2(r_2, R_2) + \Psi_3(r_3, R_3)$$

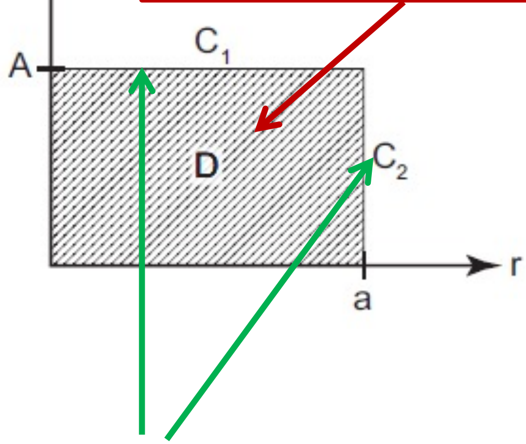
W. Glöckle, Z. Phys. **271**, 31 (1974)

$$\sum_d \left[\langle \varphi_i | \; \hat{C}_{cd} \; | \varphi_j \rangle \right] c_{d,j} = \sum_d \frac{\hbar^2}{2\mu_d a} \varphi_i(a) \left[a_d u'_{d,ext}(a) - B_d u_{d,ext}(a) \right]$$

Three-body formalism of Glöckle

R, r Jacobi-cordinates of three-body system

$$u_i(r_i,R_i)=\sum_\mu c^i_\mu \varphi_\mu(r_i,R_i)$$



boundary condiitons on C_1 and C_2

Faddeev equations in configuration space

$$\left[-\frac{d^2}{dr_1^2}-\frac{3}{4}\frac{d^2}{dR_1^2}+V(r_1)\right]u(r_1,R_1)=-V(r_1)\int_{-1}^{+1}dx\,\frac{r_1R_1}{r_2R_2}u(r_2,R_2)$$

expansion of wave function in D:
set of basis functions

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

$$\left[-\frac{1}{2\mu_{jk}}\frac{d^2}{dr^2}+V(r)-\varepsilon^i_{\mu_1}\right]X_{\mu_1}(r)=0\ ,$$

$$\left[-\frac{1}{2\mu_{i(jk)}}\frac{3}{4}\frac{d^2}{dR^2}-\varepsilon^i_{\mu_2}\right]Y_{\mu_2}(R)=0$$

algebraic system of linear equations for the coefficients c^i_μ

$$\mathbf{A}\cdot c=B[T_b,T(k)]$$

Calculation of cross sections

Breakup cross section:

$$\sigma_{breakup} = 16\pi \left(\frac{\mu_{1(23)}}{m_n}\right)^2 \frac{1}{Q^2} \int_{-1}^{1} \mathrm{d}x \int_{0}^{\sqrt{2\mu_{23}E}} \mathrm{d}k_1 Q_{k_1} k_1^2 \left| \frac{T_1(k_1)}{k_1} + \frac{T_2(k_2(x))}{k_2(x)} + \frac{T_3(k_3(x))}{k_3(x)} \right|^2$$

Elastic cross section:

$$\sigma_{elastic} = 2\mu_{1(23)} m_n \left(\frac{c^2}{\hbar^2 c^2}\right)^2 \frac{1}{Q^2} |T_b|^2$$

First system to be studied:Neutron-Deuteron system

- E_b=-2.225 MeV
- Potential of Reid soft core type:

$$V(r) = -10463\frac{e^{-\mu r}}{\mu r} - a\frac{e^{-4\mu r}}{\mu r} + b\frac{e^{-7\mu r}}{\mu r}$$

a and b determined by fitting to Nijmegen phase shift data and E_b

(Phys. Rev. C **48 (1974)**792)

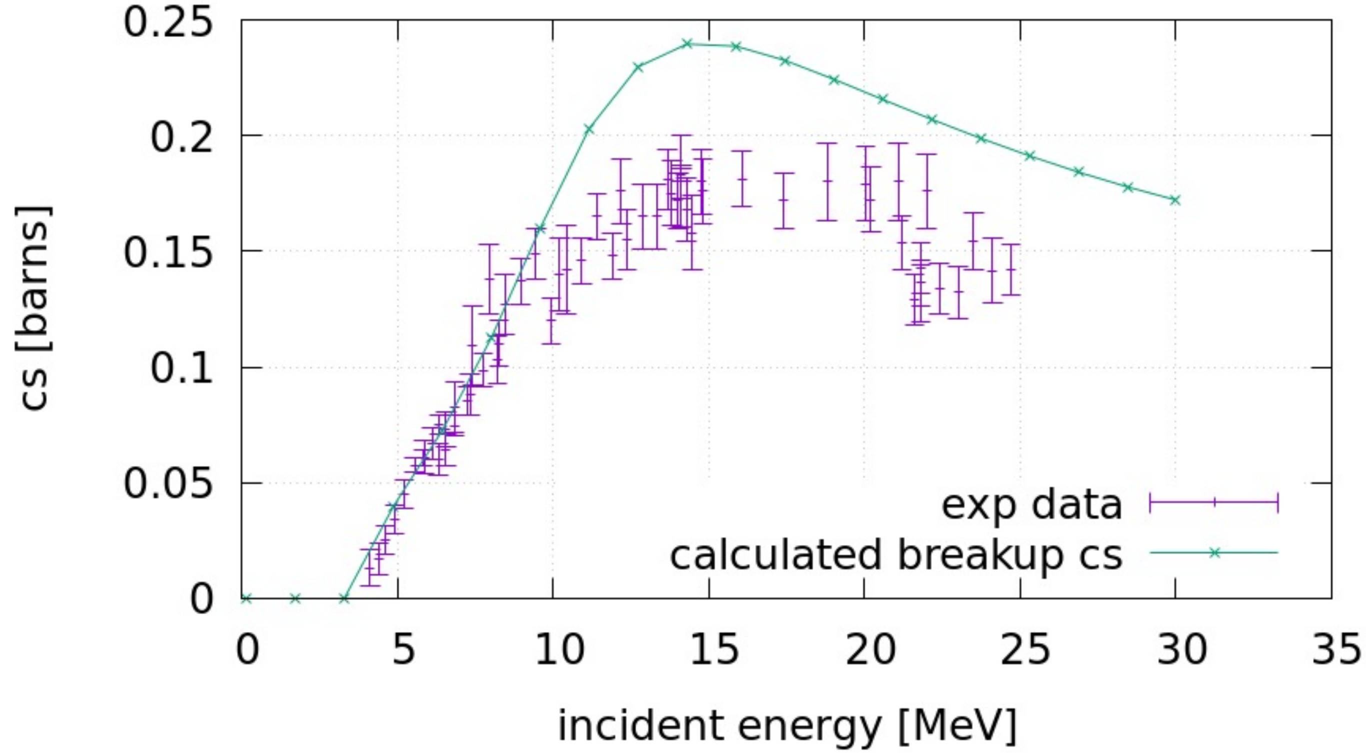
for np interaction: a=1650.6 MeV, b=5371.5 MeV

for nn interaction: a=1210,4 MeV, b=4257,5 MeV

Regularization of the system of linear equations

$\mathbf{A}\cdot c = B[T_b, T(k)] \rightarrow (\mathbf{A} + \eta)\cdot c = B[T_b, T(k)]$

3-Body R-Matrix Calculation: Deuteron Breakup n+d → n+n+p



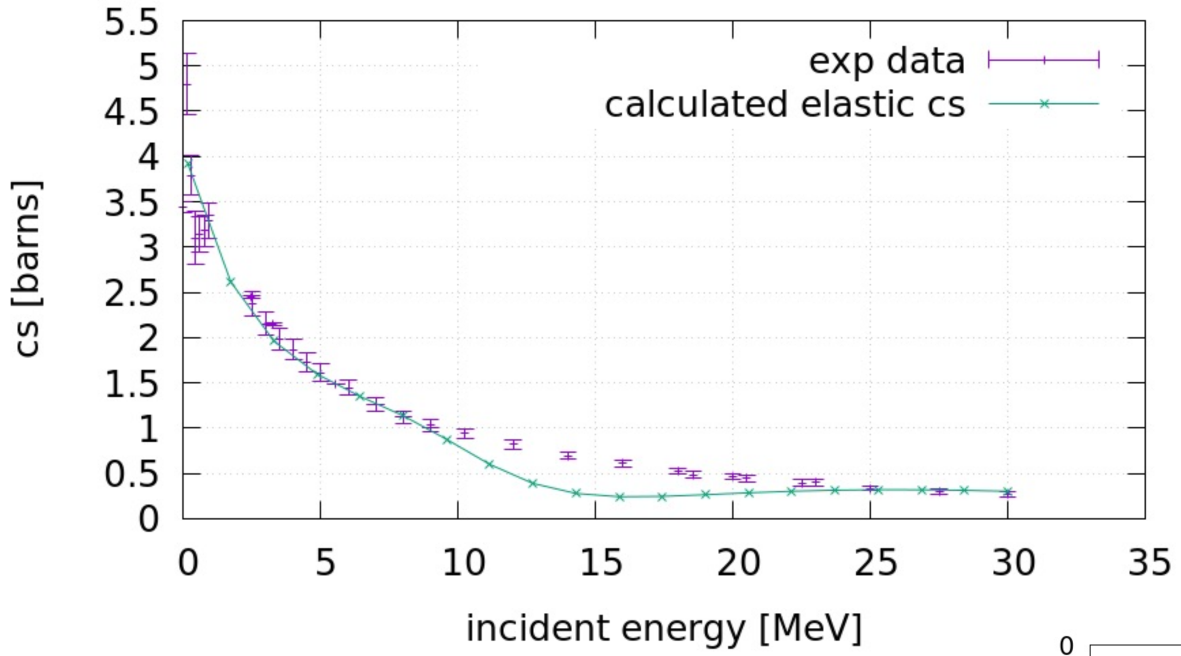
First calculation based on a three-body R-matrix:

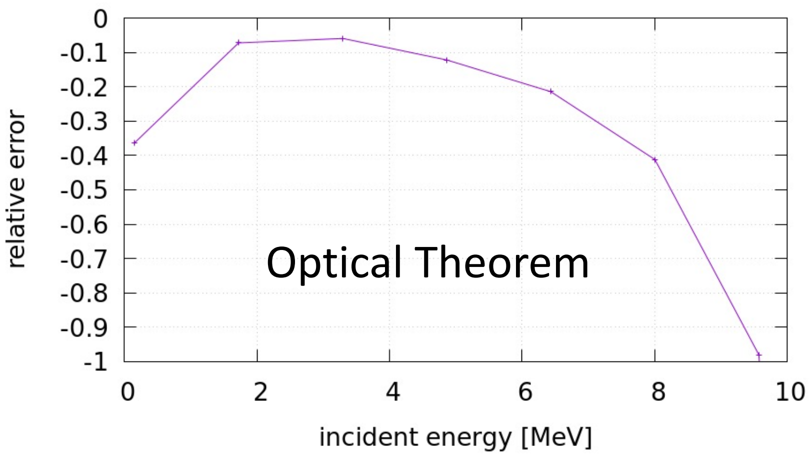
required substantial modifications of original Glöckle formalism:

- conditions on basis functions, bound state corrections, …
- regularisation of linear equations

PhD thesis B. Raab

3-Body R-Matrix Calculation: Elastic Scattering n+d → n+d





PhD thesis B. Raab

Summary and Outlook

Generation of basic tools for the evaluation of nuclear reaction data of light nuclear systems

- Construction of the novel R-Matrix Code GECCCOS
- Development and Implementation of the first R-Matrix analysis based on the Faddeev equations
- Novel Parametrisation of the Reduced R-Matrix for analyses of incomplete reaction data

The Nuclear Data Team at TU Wien

Helmut Leeb

Benedikt Raab
Thomas Srdinko

Tanja Stary
and BA students

Thank you for your attention

Reduced R-Matrix Formalism: Motivation

In nuclear physics the number of energetically open channels rises significantly with increasing energy.

⬇

Unitary treatment of R-matrix description becomes increasingly difficult

a) experimental data are only available for a limited number of channels
b) there are channels which cannot be described by R-matrix theory
c) R-matrix analyses become numerically involved

⬇

Lane and Thomas introduced the REDUCED R-MATRIX FORMALISM

A.M.Lane, R.G. Thomas, Rev. Modern Physics 30 (1958) 257 chapter 10

Development of adequate reduced R-matrix parametrisation

the $\mathbf{R}_{rr}$-submatrix is not unitary

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

the complete R-matrix is unitary

Maintaining the S-matrix elements of S_{rr} equivalent leads to the following relationship (Lane & Thomas)

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

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

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

Novel Parametrisation for Reduced R-Matrix Analyses

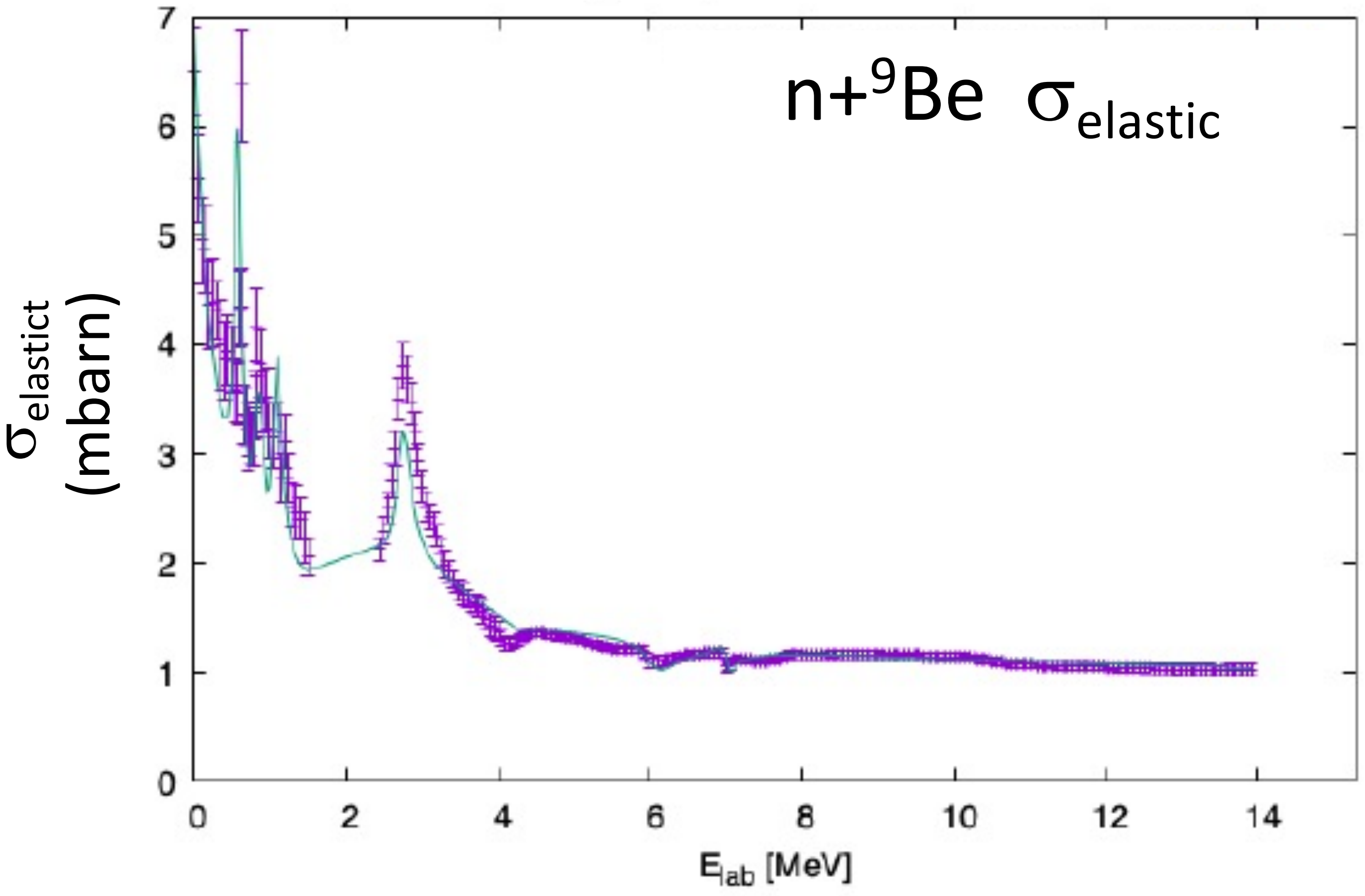
Proposal based on exact solutions for elimination of channels
In 2- and 3-channel systems

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

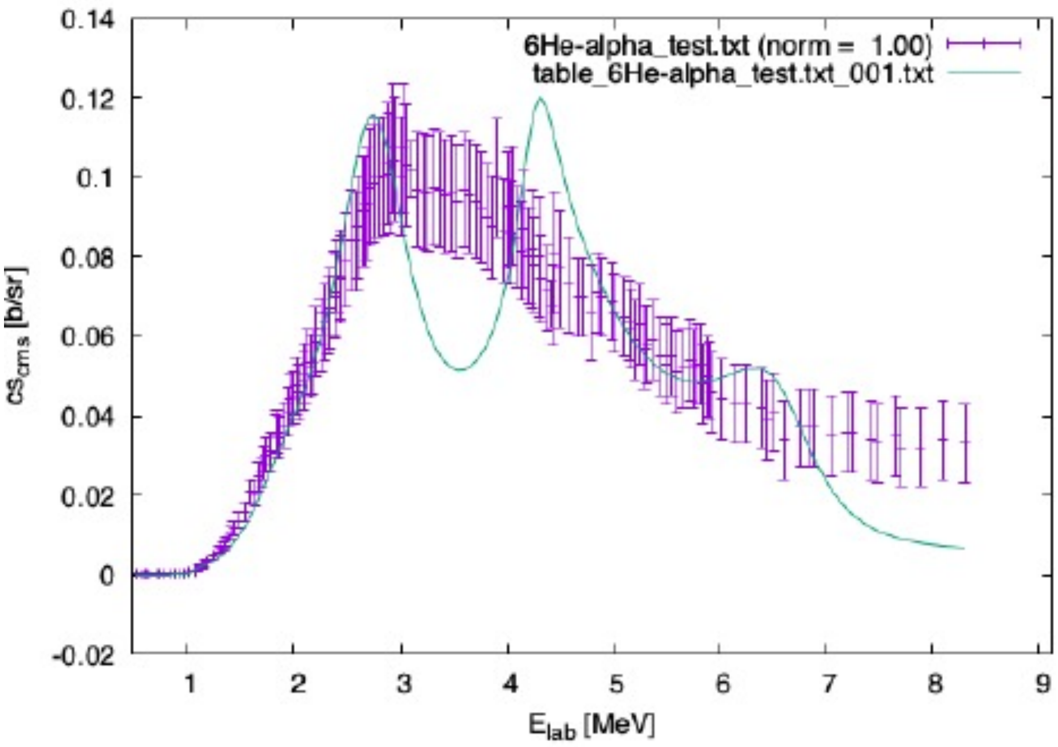
$$c,d = 1,2,\ldots, M_r \qquad L_m(k_m \cdot a) = k_m \cdot a \frac{O'(k_m \cdot a)}{O(k_m \cdot a)}$$

Important feature: $L(k_m a) = \begin{cases} \text{complex} & \text{above threshold} \\ \text{real} & \text{below threshold} \end{cases}$

Preliminary Reduced R-Matrix Analysis: n+^{9}Be elastic cross section



Preliminary Reduced R-Matrix Analysis: Reaction: $n+{}^9Be \rightarrow {}^6He+{}^4He$



Summary and Outlook

Generation of Basic Tools for the Evaluation of Nuclear Reaction Data of Light Nuclear Systems

- Construction of the novel R-Matrix Code GECCCOS
- Development the first R-Matrix Analysis based on the Faddeev equation
- Novel Parametrisation of the Reduced R-Matrix for analyses of incomplete reaction data

The Nuclear Data Team at TU Wien

Helmut Leeb

Benedikt Raab
Thomas Srdinko

Tanja Stary
and BA students

Thank you for your attention

Determination of R-Matrix

$$u_i(r_i,R_i)=\sum_\mu c^i_\mu \varphi_\mu(r_i,R_i) \qquad c^i_\mu=\int\int_D dr\, dR\; \varphi_\mu(r_i,R_i)\, u_i(r_i,R_i)$$

$$\begin{aligned}
1)\,&(E_\mu^{(i)}-E)\sum_{\mu'} C^{(i)}_{\mu\mu'}c^{(i)}_{\mu'}+\sum_{\substack{j=1\\ j\neq i}}^{3}\sum_{\mu'} V^{(j)}_{\mu\mu'}c^{(j)}_{\mu'}\\
&=\frac{1}{2\mu_{i(jk)}}QM_{\mu b}\cos(QA_i)-\mathrm{i}QM_{\mu b}\mathrm{e}^{\mathrm{i}QA_i}T_i^b\\
&-\frac{2}{\pi}\int_0^{\sqrt{2\mu_{jk}E}}\mathrm{d}k\left[\mathrm{i}Q_kM^{(-)}_{\mu k}\mathrm{e}^{\mathrm{i}Q_kA_i}+\frac{\mu_{i(jk)}}{\mu_{jk}}\mathrm{i}kM_{\mu Q_k}\mathrm{e}^{\mathrm{i}ka_i}\right]T_i(k)\\
&-\sum_{\substack{j=1\\ j\neq i}}^{3}\frac{\mathrm{i}\mathrm{e}^{\mathrm{i}\sqrt{2\mu_{j(ik)}E}\frac{m_i}{m_i+m_k}A_i/\sin\varphi_j^*}}{A_i^{3/2}}T_i\left(\sqrt{2\mu_{jk}E}\cos\varphi_j^*\right)\\
&\times\left(N_b(E)M_{\mu b}\frac{2\mu_{i(jk)}}{\mu_{j(ik)}\left(E-\frac{2Q^2}{\mu_{j(ik)}}\sin^2\varphi_j^*\right)}\int_0^{r_{0i}}\mathrm{d}r\; u_i^b(r)V_i(r)\right.\\
&\left.+\frac{2}{\pi}N_k(E)\int_{\sqrt{2\mu_{jk}E}}^{\infty}\mathrm{d}k\; M^{(-)}_{\mu k}\frac{1}{\frac{1}{\mu_{jk}}k^2-2E+2\frac{\mu_{j(ik)}}{\mu_{i(jk)}}E\left(\frac{m_i}{(m_i+m_k)\sin\varphi_j^*}\right)^2}\int_0^{r_{0i}}\mathrm{d}r\; u_k^{(-)*}(r)V_i(r)\right)
\end{aligned}$$

equation for the coefficients c_μ and the T-matrices

$$T_i^b\;,\;T_i(k)$$

Boundary conditions

$$2)\sum_{\mu} M_{\mu b} c_{\mu}^{(i)} \simeq \sin(QA_i) - 2\mu_{i(jk)} \mathrm{e}^{\mathrm{i}QA_i} T_i^b$$

$$3)\sum_{\mu} c_{\mu}^{(i)} \varphi_{\mu}(r_i, A_i) - u_i^b(r_i)\left[\sin(QA_i) - 2\mu_{i(jk)} \mathrm{e}^{\mathrm{i}QA_i} T_i^b\right]$$

$$\simeq (2\mu_{i(jk)})^{3/2} \sqrt{2\mu_{jk}} \sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} E^{1/4} \frac{\mathrm{e}^{\mathrm{i}\rho_A \sqrt{E}}}{\rho_A^{1/2}} \frac{A_i}{\rho_A} T_i\left(2\mu_{jk}\sqrt{E}\frac{r_i}{\rho_A}\right)$$

$$4)\sum_{\mu} c_{\mu}^{(i)} \varphi_{\mu}(a_i, R_i) \simeq (2\mu_{i(jk)})^{3/2} \sqrt{\frac{2}{\pi}} \mathrm{e}^{\mathrm{i}\frac{\pi}{4}} E^{1/4} \frac{\mathrm{e}^{\mathrm{i}\rho_a \sqrt{E}}}{\rho_a^{1/2}} \frac{R}{\rho_a} T_i\left(2\mu_{jk}\sqrt{E}\frac{a_i}{\rho_a}\right)$$

with $\rho_A = \sqrt{2\mu_{jk} r_i^2 + 2\mu_{i(jk)} A_i^2}$ $\quad \rho_a = \sqrt{2\mu_{jk} a_i^2 + 2\mu_{i(jk)} R_i^2}$

T-amplitudes

Transition amplitude from channel α to β:

$$T_{\beta\alpha} = \left\langle \phi_\beta \middle| V^\beta \middle| \Psi_\alpha^{(+)} \right\rangle$$

Comment:
Corresponds for reactions to the collision matrix element $U_{\beta\alpha}$ usually defined In three-body quantum Scattering theory

$$T_i^b = \int_0^\infty \mathrm{d}R \int_0^\infty \mathrm{d}r \, \frac{\sin(QR)}{Q} u_i^b(r) V_i(r) Q_i(r,R)$$

Elastic or rearrangement

$$T_i(k) = \int_0^\infty \mathrm{d}R \int_0^\infty \mathrm{d}r \, \frac{\sin(Q_k R)}{Q_k} u_k^{(-)*}(r) V_i(r) Q_i(r,R)$$

Breakup

with $$Q_i(r_i, R_i) = \int_{-1}^{1} \mathrm{d}x_i \; r_i R_i \frac{1}{2} \sum_{\substack{j=1 \\ j\neq i}}^{3} \frac{u_j(r_j, R_j)}{r_j(x_i) R_j(x_i)}$$