Adaptive R-matrix Approach for Light Nuclei

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Motivation

- R-matrix approach which leads to a smooth transition to the statistical model
- General scope: continuous evaluation over the boundaries of the validity of different reaction theories/models
- Complement to TALYS code with resonance regime and capability for light nuclei → TALYS output → ENDF-file generated via TEFAL
- Physical division between mean-field contributions and multi-particle features

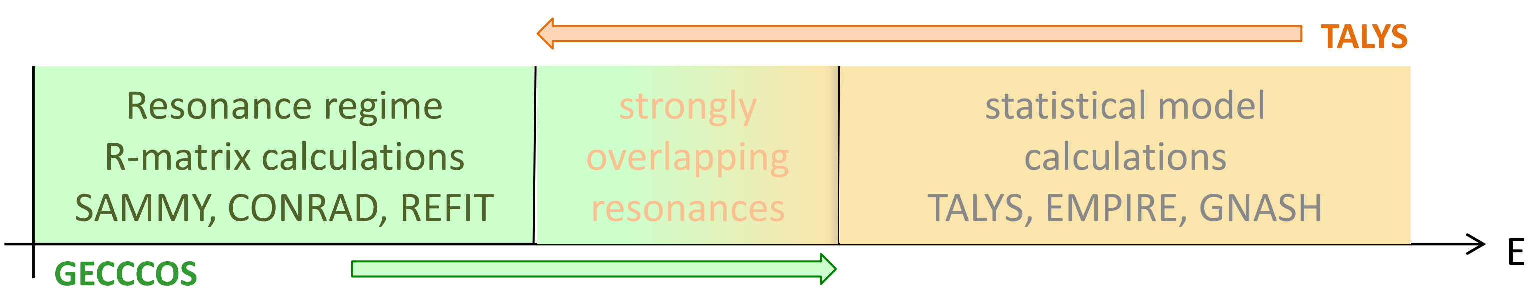
Goals and Challenges

Present drawbacks

- ***Problem of Consistency:*** the evaluation of reactions involving light nuclei represents the challenge of consistency, because reliable theories are missing
- ***Missing microscopic basis:*** in the absence of a proper theory of resonances, phenomenological R-matrix fits to experimental cross section data are usually performed at the cost of losing predictive power.
- ***Problem of matching:*** evaluation methods in the resonance region and at higher energies are based on completely different concepts;

Focus of the Work

Development of a R-matrix based method to gain a **continuous transition** between the resonance regime and standard reaction calculations (statistical model and coupled-channel)



Idea

R-matrix theory has two facets:

Phenomenological approach:

- R-matrix as a series of pole terms
- Positions and widths found via fitting procedure
- Excellent description of experimental data

Application in transition energy region:
→strongly overlapping resonances
→interference effects

↓

Single pole approximation not well suited

Solution of coupled-channel equations:

- Elegant formalism
- Numerically efficient
- Predictive power, if all potentials well-known

At present:
N-body nucleon nucleon interactions cannot be fully included in coupled channels

↓

Lack of microscopic description

Hybrid Approach

to combine best of both

Starting Point

P. Descouvemont and D. Baye, Rep. Prog. Phys. 73, 036301 (2010)

Coupled-channel system:

$$\sum_d \left[\left(T_c + E_c - E \right) \delta_{cd} + \mathrm{V}_{\mathrm{cd}} \right] u_d = 0$$

Problem:
although the Hamiltonian is hermitean on the line, this is not true for [0,a]

Bloch-Operator $\hat{L} = \sum_d |d\rangle \hat{L}_{\mathrm{d}} \langle d|$ with $\hat{L}_d = \frac{\hbar^2}{2\mu_d} \delta(r-a) \left(\frac{d}{dr} - \frac{B_d}{r} \right)$

$$\sum_d \left[\left(T_c + \hat{L}_c + E_c - E \right) \delta_{cd} + \mathrm{V}_{\mathrm{cd}} \right] u_d^{\mathrm{int}}(r) = \hat{L}_c \, \mathrm{u}_{\mathrm{c}}^{\mathrm{ext}}(r)$$

Bloch-Schrödinger equation

R-Matrix: $R_{cd}(E) = \frac{\hbar^2}{2a\sqrt{\mu_c \mu_d}} \sum_{i,j=1}^{N} \varphi_i(a) \left(C^{-1} \right)_{ci,dj} \varphi_j(a)$

$$C_{ci,dj} = \langle \varphi_i | T_c + \hat{L}_c + E_c - E | \varphi_j \rangle \delta_{cd} + \langle \varphi_i | V_{cd} | \varphi_j \rangle$$

pseudo-potential (background)

Because of hermiticity:

$$R_{cd}(E) = \sum_p \frac{\gamma_{pc} \gamma_{pd}}{E_p - E} \quad \text{with} \quad \gamma_{pc}' = \sqrt{\frac{\hbar^2}{2a\mu_c}} \sum_{i=1}^{N} v_{pci} \, \varphi_i(a)$$

Pseudo Potential

- defined in (relative) channel coordinates
- In principle related to microscopic nucleon-nucleon interaction (except elastic and inelastic channel) [*pseudo* potential]
- Should include all necessary channels to maintain unitarity of S-matrix up to overlap region with statistical model calculations (TALYS)
- **→ Large scale calculations necessary to manage all channels and observables in resonance regime up to overlap region**

Hybrid Approach

Pseudo-Potential leads to: $$C_{ci,dj} = \langle \varphi_i | T_c + \hat{L}_c + E_c | \varphi_j \rangle \delta_{cd} + \langle \varphi_i | V_{cd} | \varphi_j \rangle$$

Diagonalisation ↓ E_p, v_{pc}

$$S_{cd}^{bg}(E) \Leftarrow R_{cd}^{bg}(E) = \sum_p \frac{\gamma_{pc}\gamma_{pd}}{E_p - E} \Leftarrow \gamma_{pc} = \sqrt{\frac{\hbar^2}{2a\mu_c}} \sum_{i=1}^{N} v_{pci}\, \varphi_i(a)$$

Hybrid R-matrix approach:

$$R_{cd}(E) = R_{cd}^{bg}(\mathrm{E}) \quad + \quad \sum_p \frac{\gamma_{pc}\gamma_{pd}}{E_p - E}$$

↓ background pseudo-potential expected to be smooth

↓ pole terms should primarily describe many-body resonances

Background and Resonances

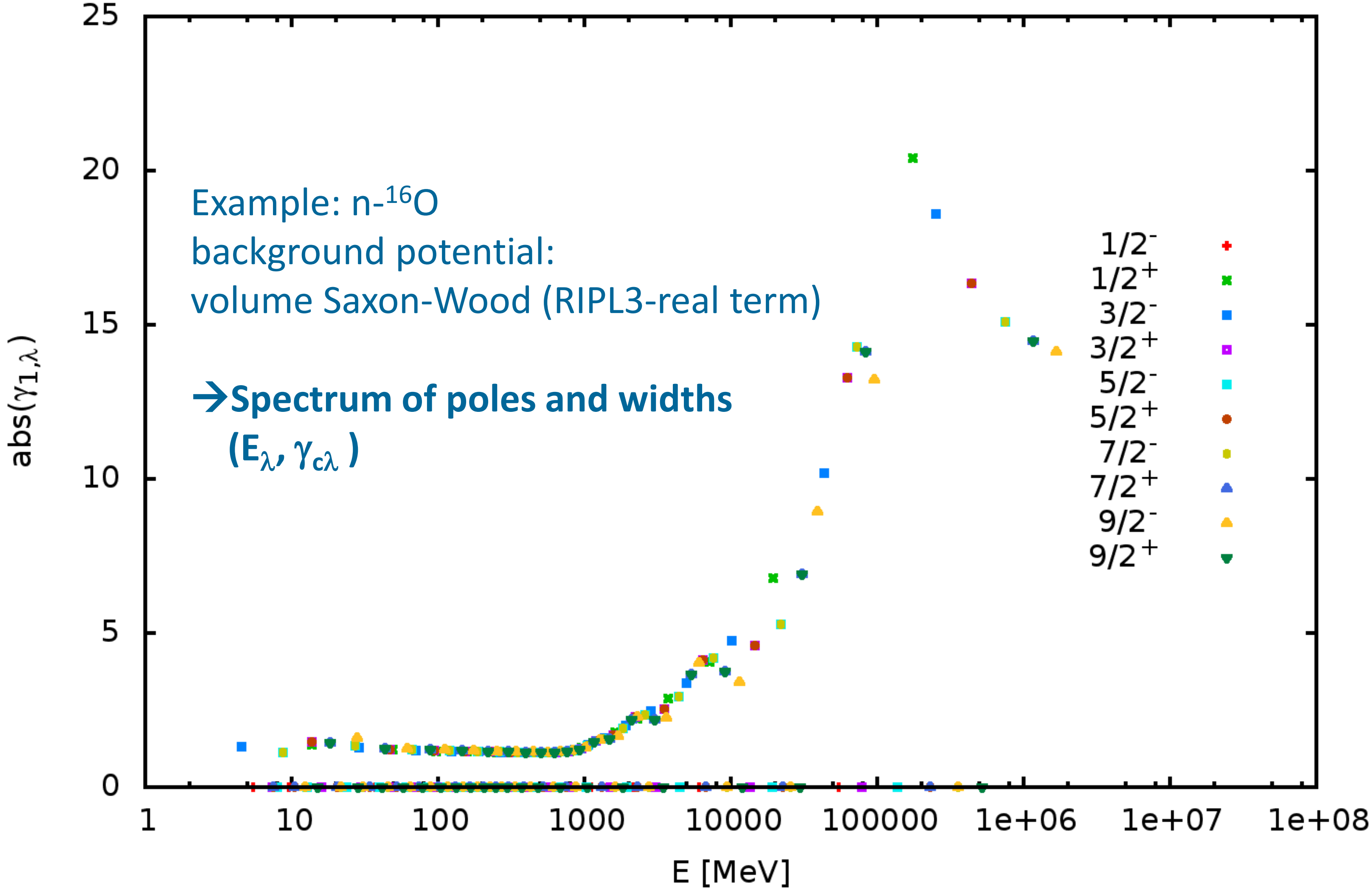
Background Potential:

- Describe effects achievable by single particle potential
- Shall provide the “mean field”

Additional Resonance Terms

- Shall cover remaining peaks and details in cross section structure
- Account for e.g. nuclear n-body effects not covered by the potentials within the coupled-channel equations

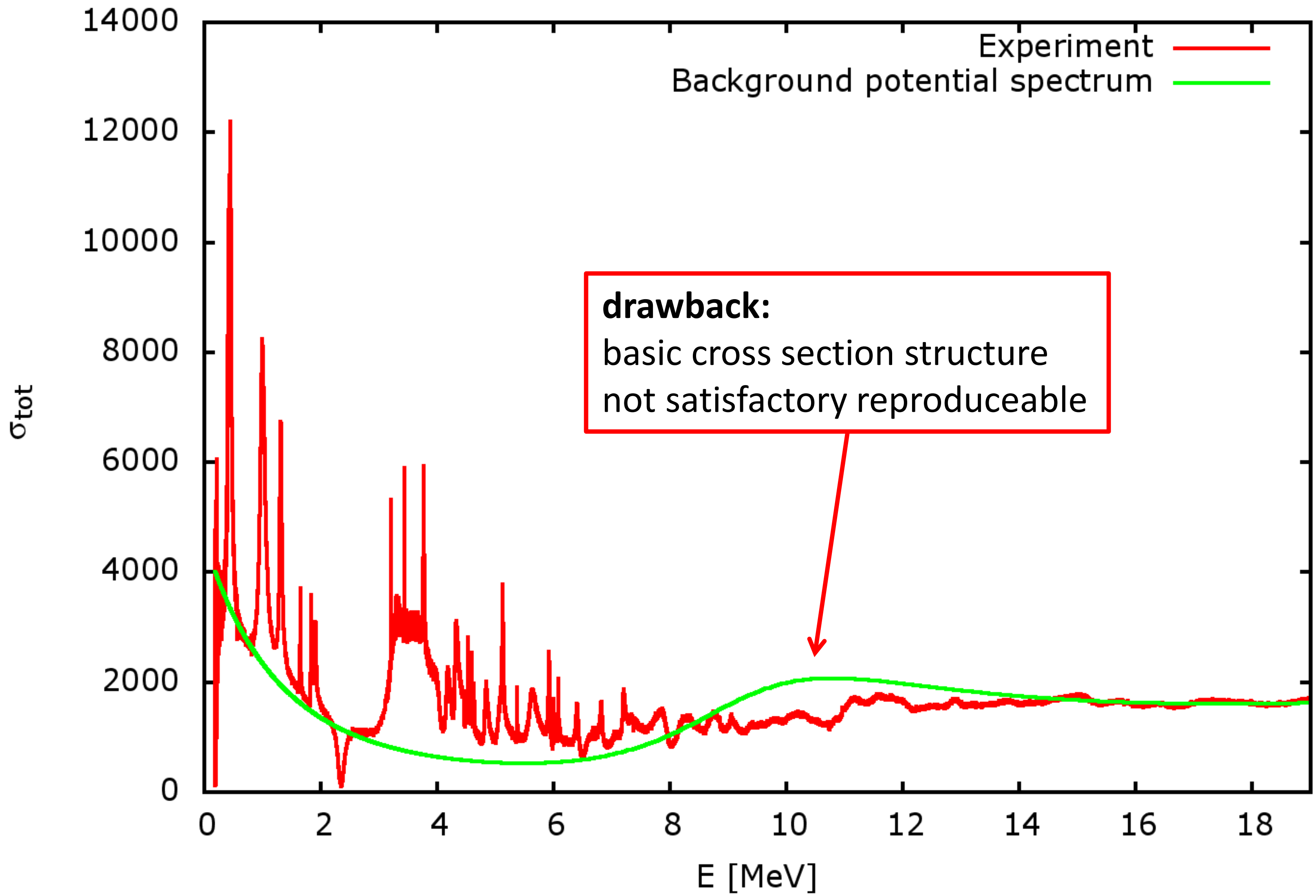
Spectrum of Background Poles



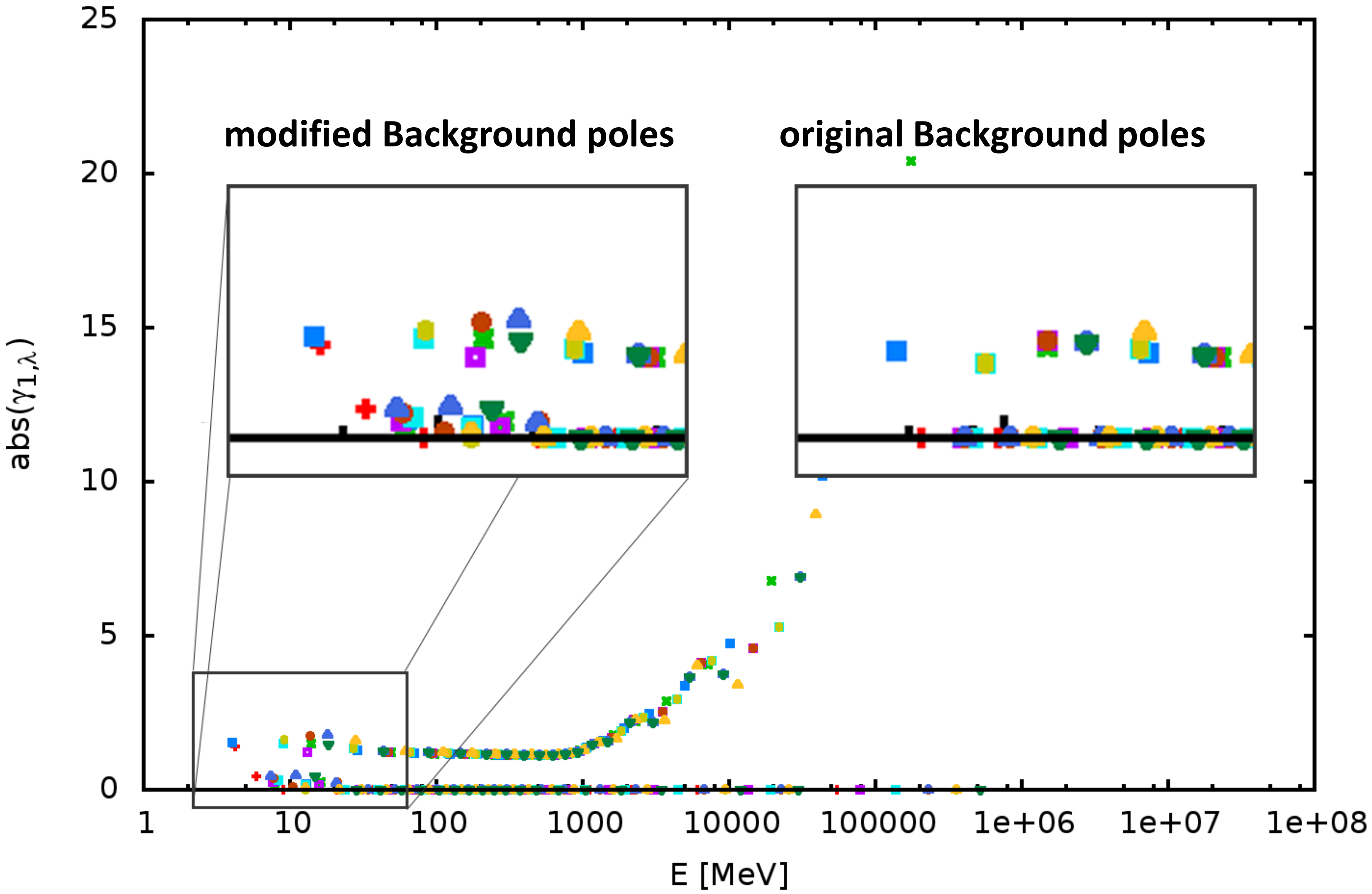
Example: n-^{16}O
background potential:
volume Saxon-Wood (RIPL3-real term)

→**Spectrum of poles and widths (E_λ, $\gamma_{c\lambda}$)**

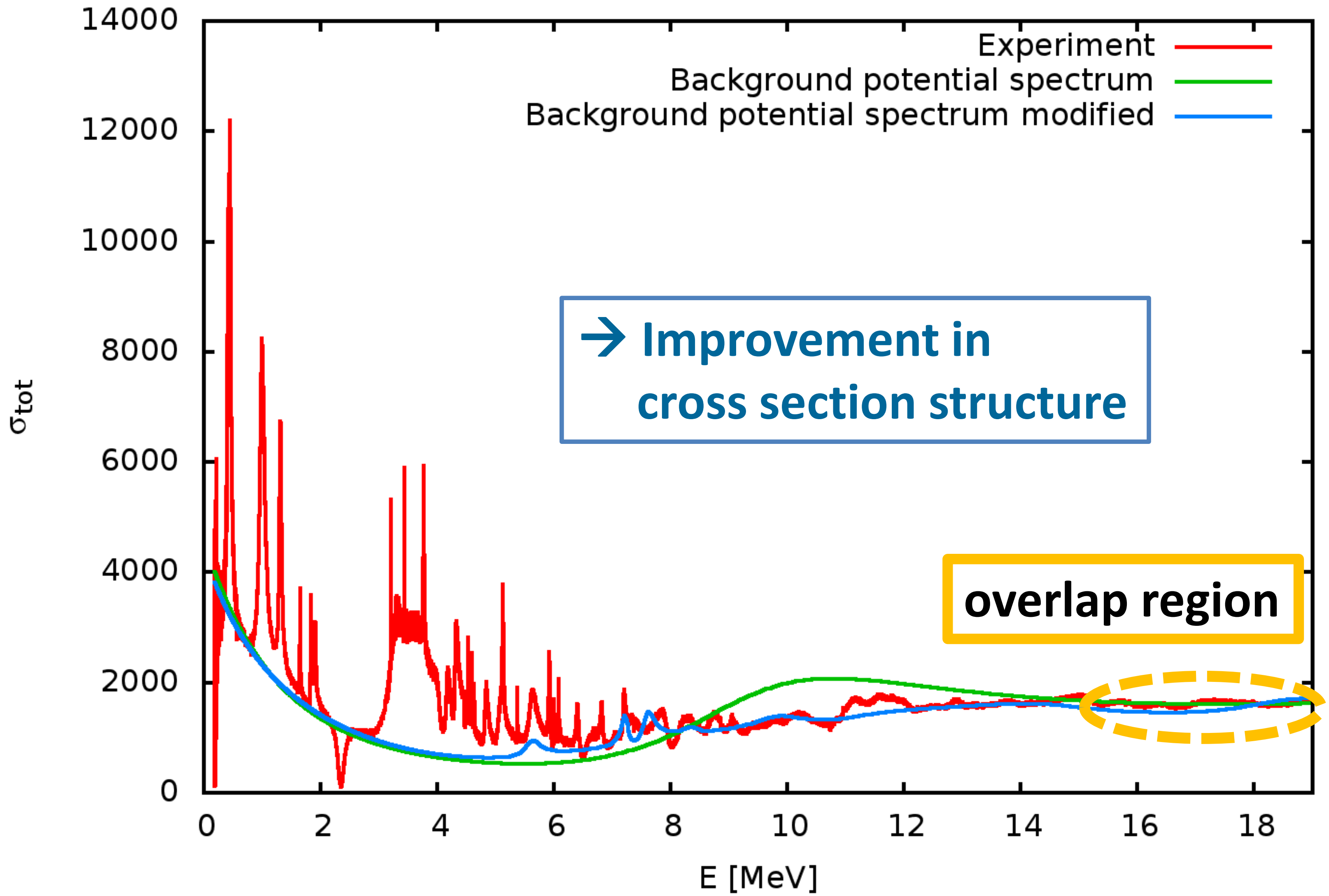
Total Cross Section



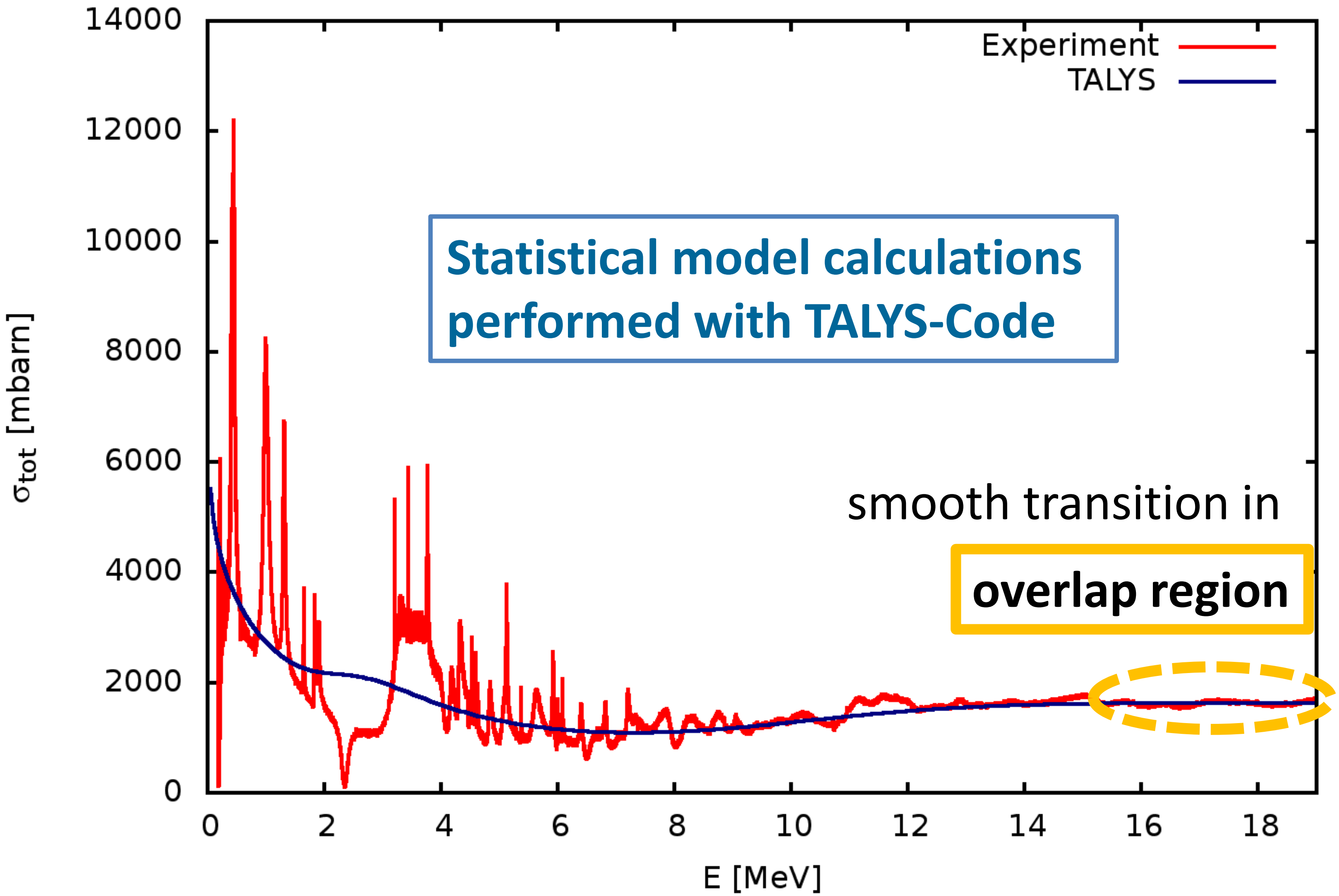
Modified Spectrum of Background Poles



Total cross Section



Transition to TALYS



Modified Background Spectrum

- Simple real Woods-Saxon shape cannot reproduce the basic cross section structure

- Background poles and widths are only *L*-dependent
  (→ overlapping poles and widths in different partial waves for
  same angular momentum *L*)

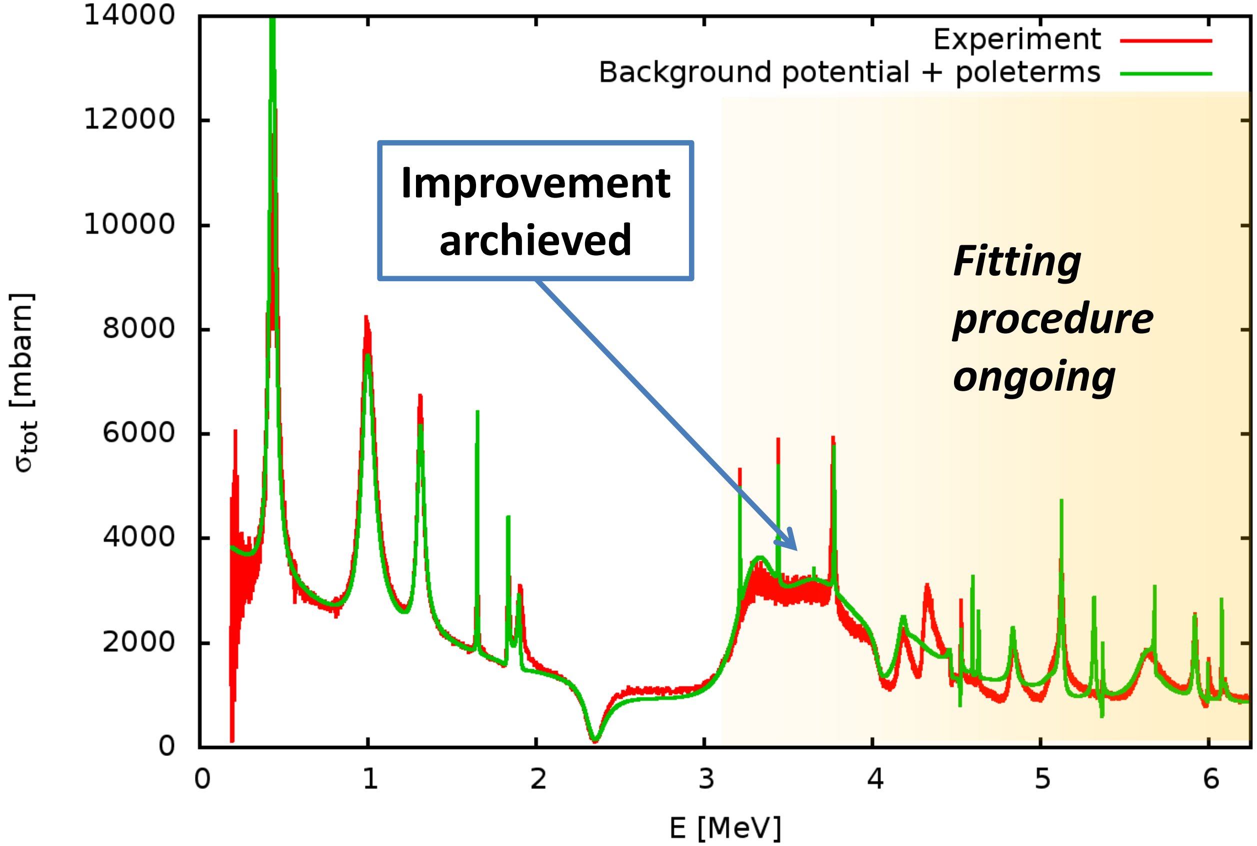
- Modification of poles and widths introduces
  additional J-dependency (e.g. spin-orbit) in pseudo potential
  → improved cross section shape

A potential parametrization which delivers modified poles and widths directly would be desireable – **work in progress**

Modified Background with Pole Terms

Until now:

- reproduction of total cross section structure 0.2 - 3 MeV
- modified background potential + pole terms
- matching radius a = 6 fm

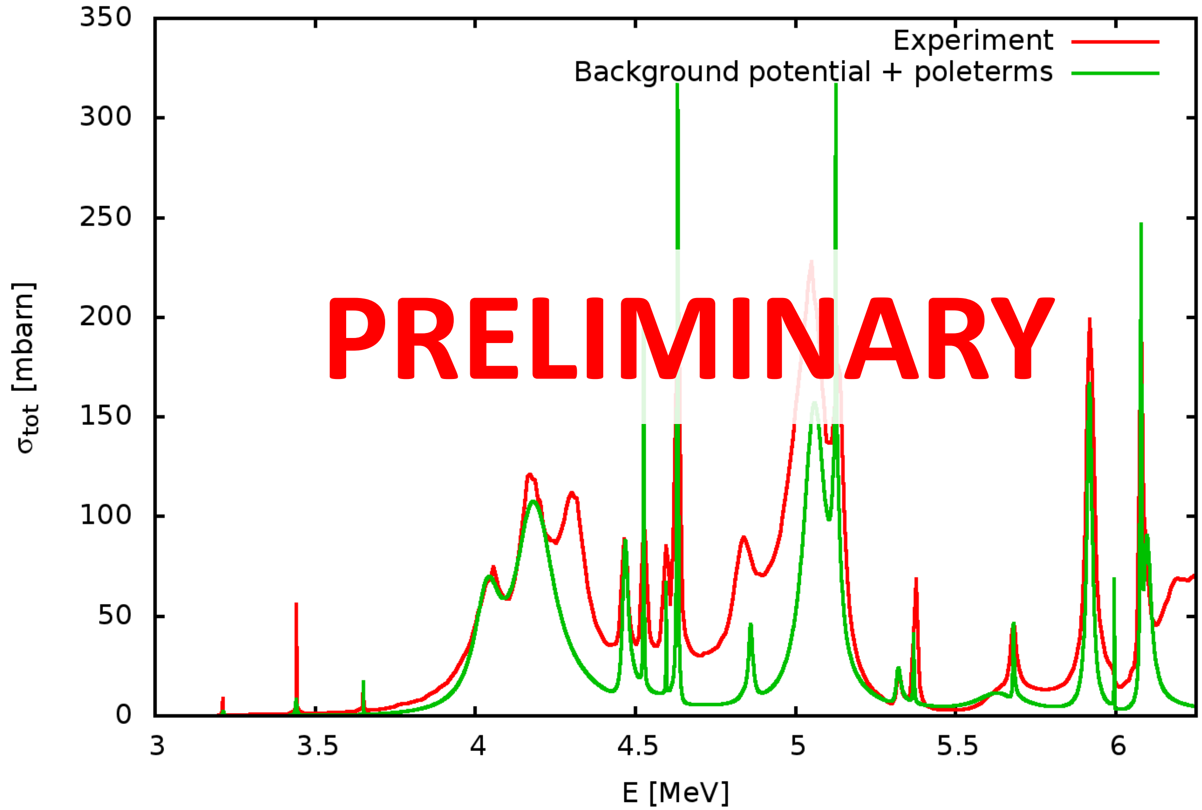


fitting of reaction channels (e.g. nα) with modified background – **work in progress**

Preview: (n,α)-channel

Until now:

- Inclusion of poles for (n,α)-coupling
- modified background potential + pole terms
- matching radius a = 6 fm
- Pole positions reproduced



early stage, fitting with modified background poles

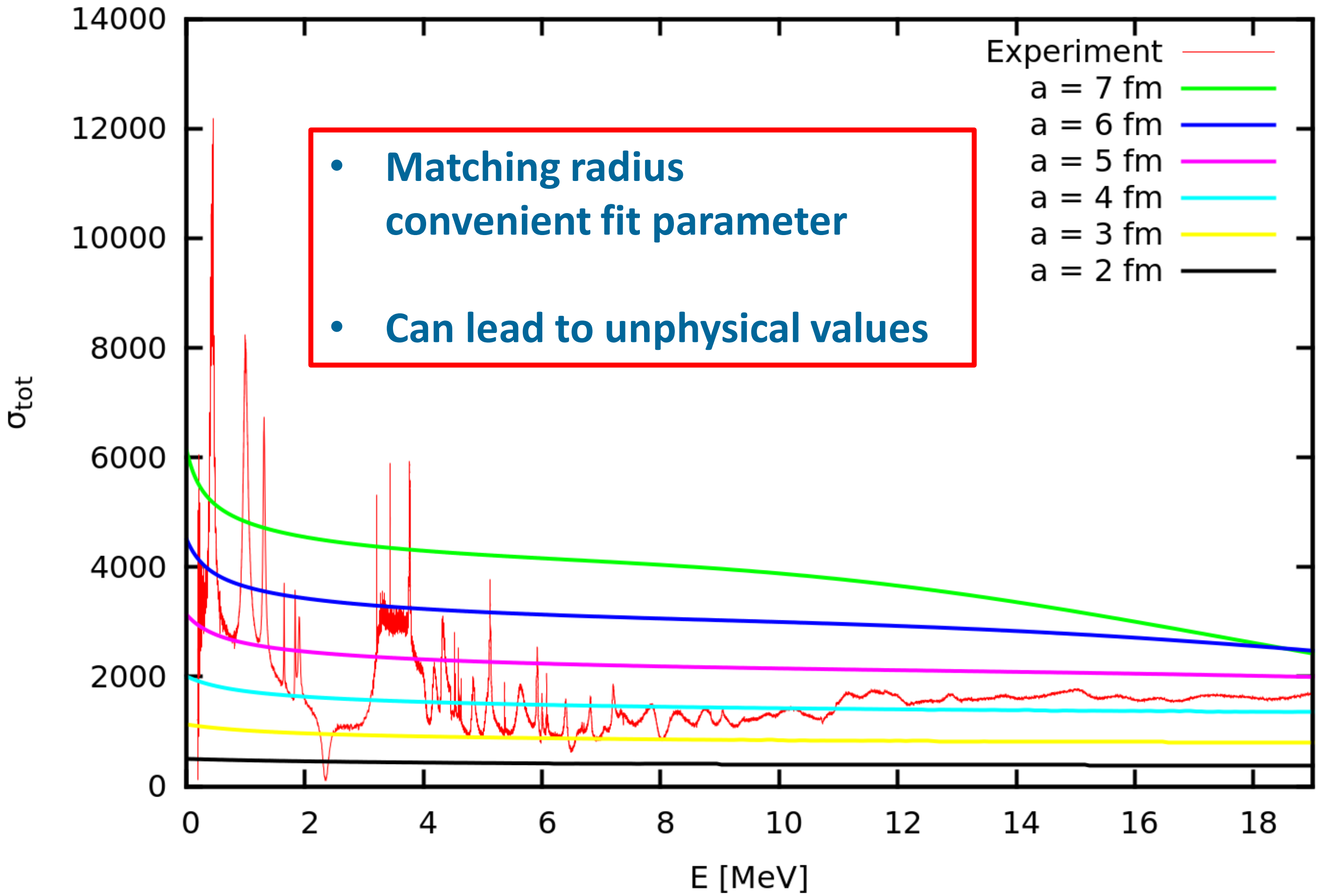
→work in progress

Current challenges

- Background poles help to maintain physical reasonable matching radii
- Source for interference effects
- Only few background poles within relevant region
- However, large impact on cross sections on wide range
- **Proper combination of background poles and resonance poles crucial**

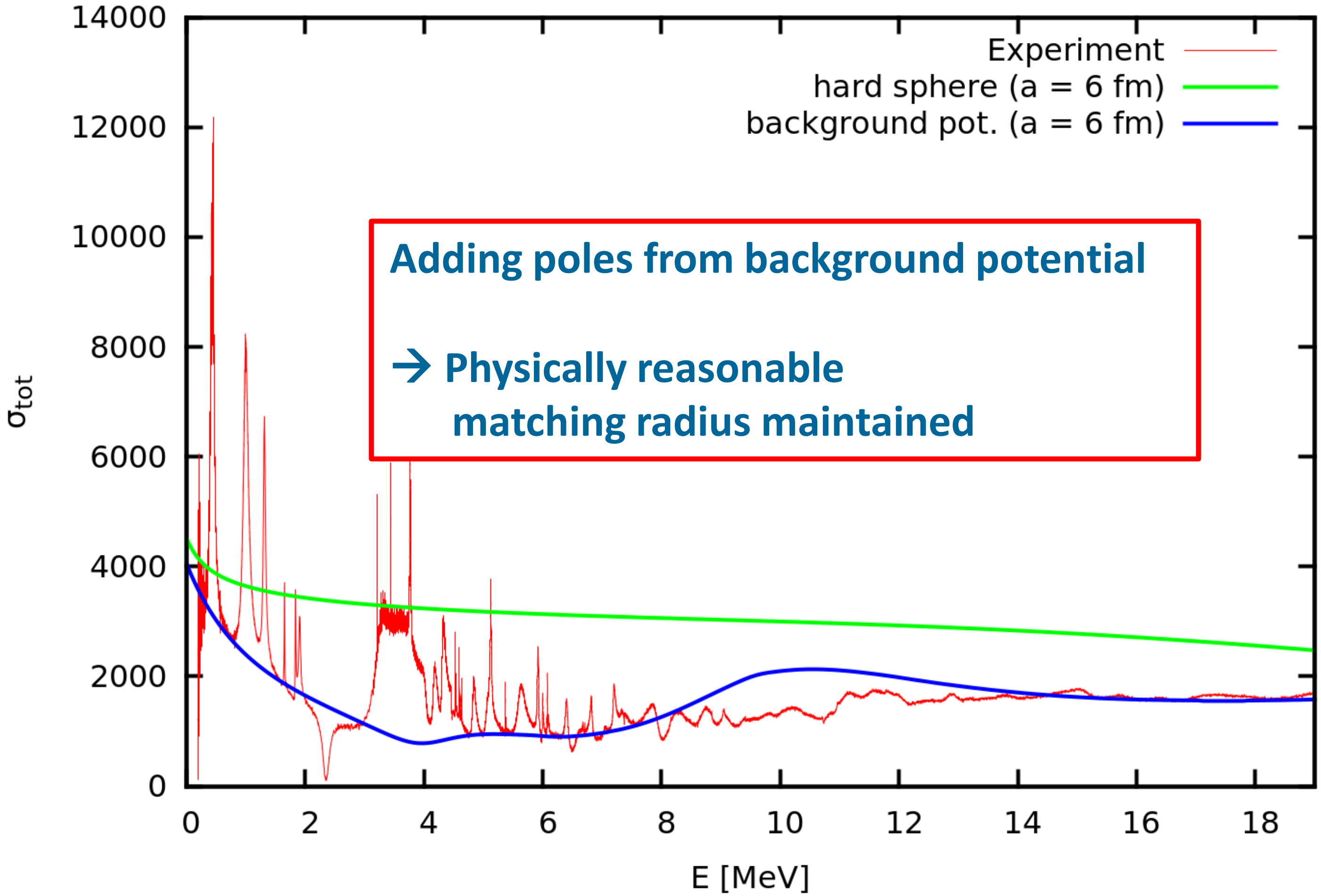
Matching Radius

Hard sphere scattering cross section for various matching radii *a*

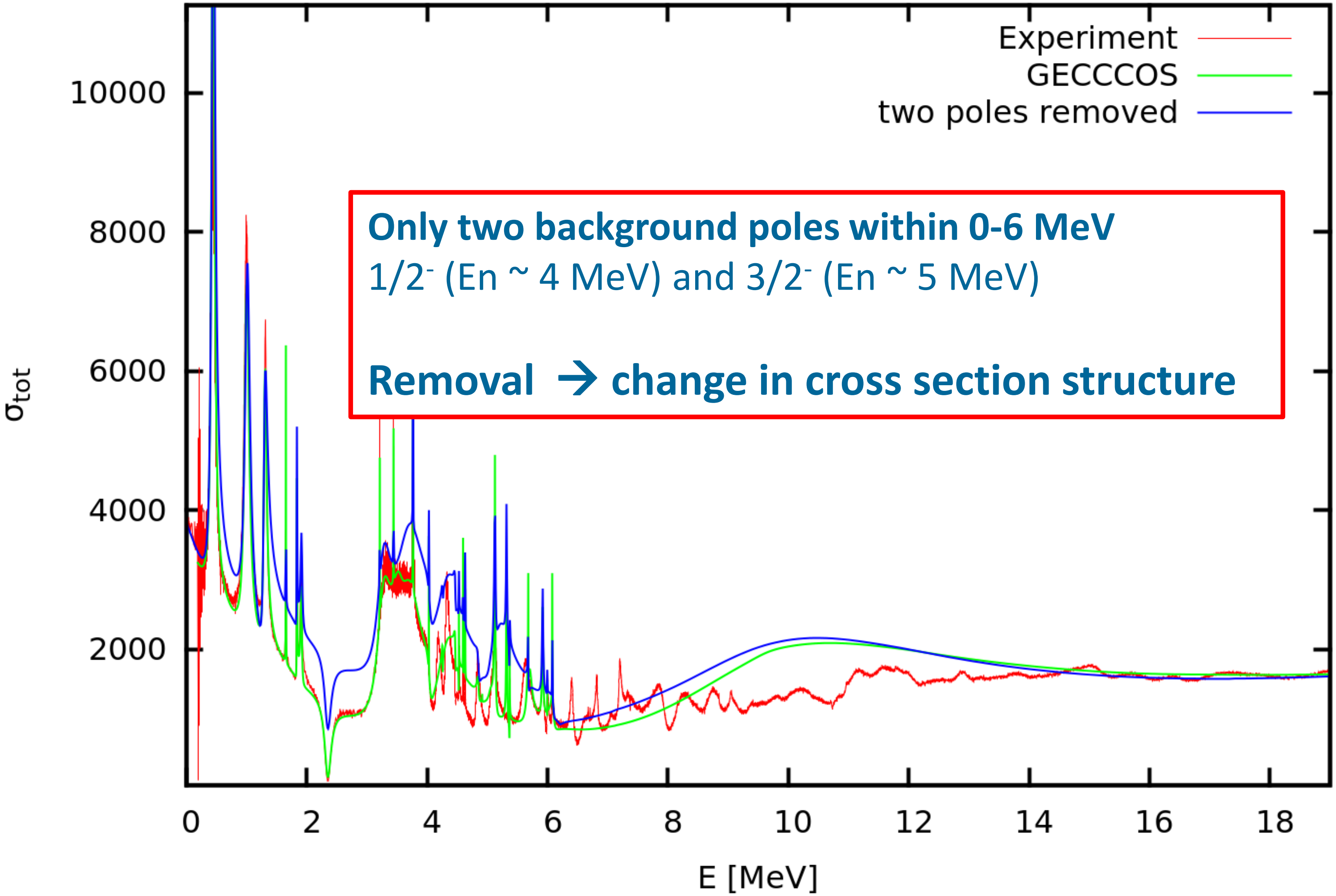


- **Matching radius convenient fit parameter**
- **Can lead to unphysical values**

Background Potential



Impact of background poles on cross section structure



Only two background poles within 0-6 MeV

$1/2^-$ (En ~ 4 MeV) and $3/2^-$ (En ~ 5 MeV)

Removal → change in cross section structure

Impact of background poles on cross section structure

- Few background poles have huge impact on the cross section shape
- Fitting routines have to deal with interferences between background poles and resonance poles
- **Proper combination of background poles and resonance poles crucial**

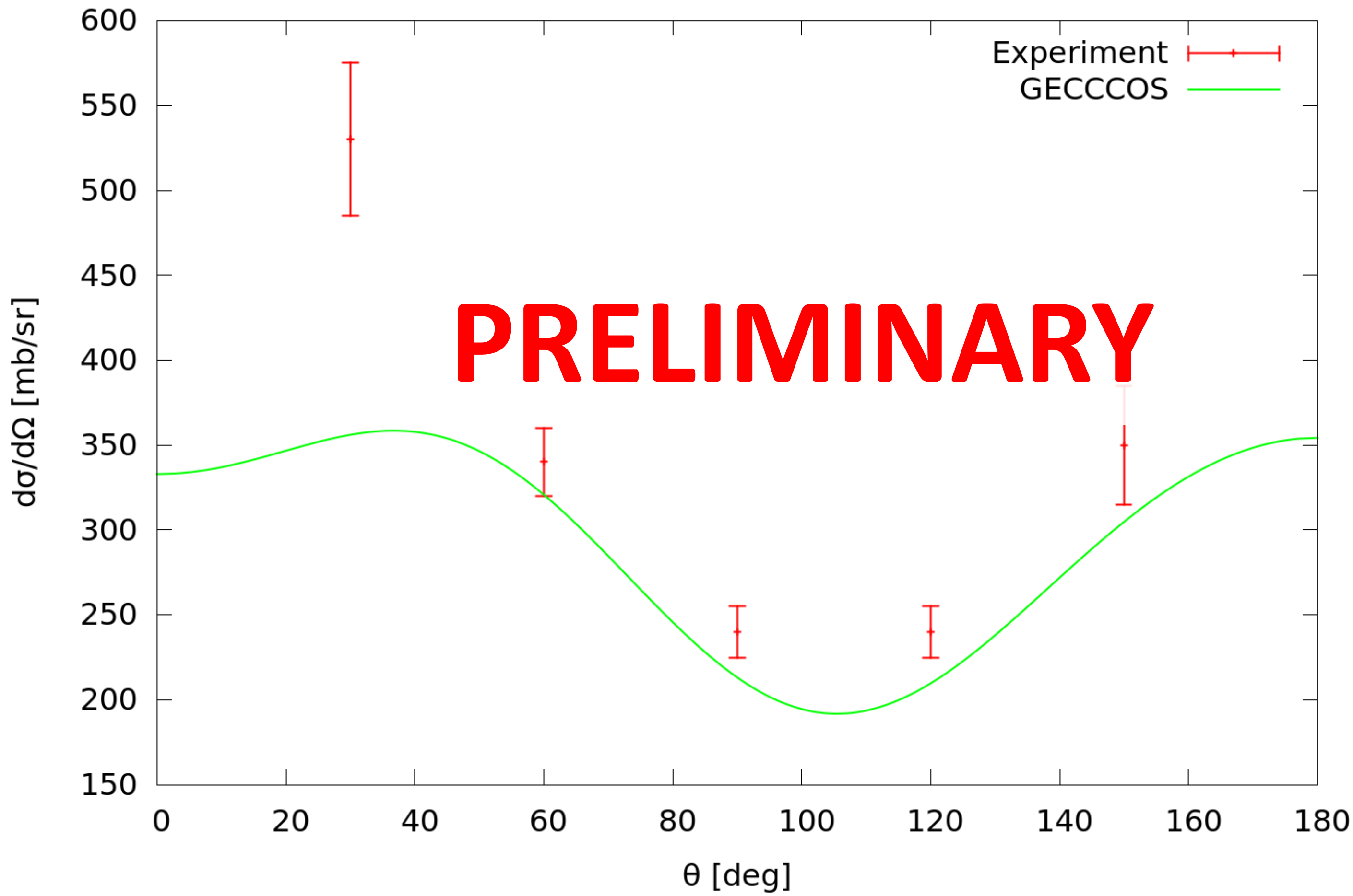
Differential Data

- For reference to verify partial wave composition
- Not yet fully part of fitting porcedure
- **Preliminary – work in progress**

Differential Data

Example: elastic cross section at E= 0.9 MeV

- Near peak of resonance
- Some features reproduced
- Small angle scattering → need for further optimization

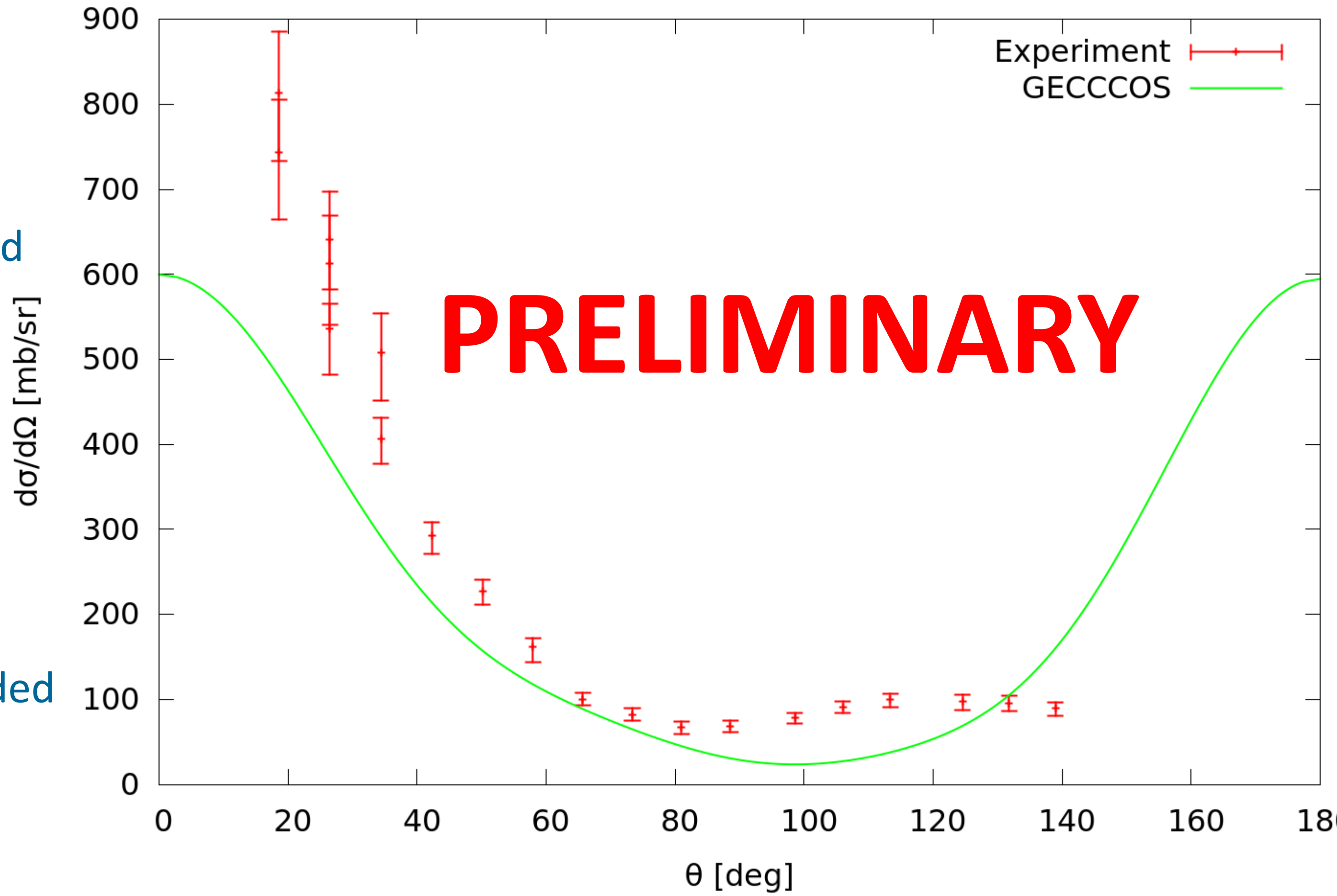


work in progress

Differential Data

Example: elastic cross section at E= 4.34 MeV

- Near peak of resonance
- Not fully optimized in integrated cross section
- Some features reproduced
- → further optimization needed



work in progress

Summary

Proof of concept:

- Background potential leads to reasonable shape for total cross section while maintaining physically reasonable matching radius

- Additional pole terms reproduce the pole signature of the cross sections in elastic and (n,α)-cross sections
- for quantitative description multiparameter fitting routines necessary **(ongoing)**
  (potential parameters, background poles/widths, resonance poles/widths
  → for each channel)

Current challenges:

- Nonlinear behaviour of cross sections with regard to R-matrix pole terms (height and positions of resonances are subject to interference effects)
  → requires study of background pole terms
  → demanding for versatile fitting routines
  → association of modified potential to optimized background poles → spin dependence
  (perturbative approach: small variation of few poles per partial wave)

Outlook

Ongoing Work:

- Optimization for all involved channels (including differential data) up to about 6 MeV (n-^{16}O elastic, α-^{13}C elastic, n-α coupling)
- Inclusion of inelastic and higher nα (nα_1, nα_2, …) up to about 10 MeV

Future Developments:

- **proper treatment of (n,γ)- reactions**
  (so far ignored – because (n,γ)-contribution for ^{16}O negligible);
  perturbative calculation already performed
- **proper treatment of 3-body channels**
  (e.g. (n,2n), (n,np), (n,nα) – formulating 3-body Faddeev approach
  for practical applications
  → important for transition region about 15 MeV (Master thesis in progress).
- **Completion of polarization parameters** (prepared)
- **relativistic corrections**

Thank you for your attention