A versatile R-matrix module including alternative parametrizations

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R-matrix challenges

Conventional R-matrix formalism excellent tool to describe experimental data, especially in the resolved resonance region

Fitting parameters (E_λ, $\gamma_{\lambda c}$) control observables indirectly:

- a variation in $\gamma_{\lambda c}$ may also shift resonance position in cross section
- formal resonance position E_λ not necessarily at cross section resonance
- possible interference effects between resonances

→ **fitting process challenging**

Helpful techniques available

Brune Parametrization

by C. R. Brune Phys. Rev. C 66, 044611 (2002)

- reformulation of conventional R-matrix
- resonance positions and widths coincide with observed values
  → **simplification of fitting process**
- Observables directly obtainable
- Transformation to and from conventional R-matrix parameters possible

Park Parametrization

by T.-S. Park Phys. Rev. C 104, 064612 (2021)

- **Similar to Brune** parametrization
- Level dependent Boundary condition, non-orthogonal basis functions
- Formal reduced widths and positions equal to observed ones by design
  → **simplification of fitting process**
- No direct transformation to conventional R-matrix

GECCCOS development

Implemented features (ongoing)

- **Calculable R-matrix via Lagrange-mesh technique**
  by P. Descouvemont and D. Baye, Rep. Prog. Phys. 73, 036301 (2010)
- **Phenomenological R-matrix:**
  standard options for a_c, B_c available
- **Hybrid approach**
  background via potential, resonances phenomenological
- **Transformation of the matching radius**
- **Newly added option: Park parametrization**
- **Reduced R-matrix** (T. Stary [Master Thesis])
  Introduced by A.M. Lane, R.G. Thomas in Ref. Modern Physics 30 (1958) 257 chapter10
  Restricts dimension of R-Matrix to included channel subset
  Automatically accounts for thresholds for not included channels
- **R-matrix Faddeev approach for three-body breakup channels (H. Leeb) (numerical implementation in progress)**

Conventional R-matrix

- **Idea: split configuration space at channel radius with smooth transition**
  (E.P.Wigner, L. Eisenbud, P.L. Kapur, R.E. Peierls, A.M. Lane, R.G. Thomas)

$$u_c^{\text{int}}(r) = \sum_{j=1}^{N} g_{cj}\, \varphi_j(r)$$

set of *N* basis functions
with $\phi_j(r=0)=0$,
no condition at *r=a*.

$$u_{cc_0}^{ext}(r) = v_c^{-1/2}\left[I_c(k_c r)\delta_{cc_0} - U_{cc_0} O_c(k_c r)\right] \text{ for } E > E_c$$

bound state wave functions are
proportional to the Whittaker function.
The collision matrix *U* is unknown.

0 r=a r

- There is only one wave function → **smooth transition between regions**

$$u_c^{\text{int}}(a) = u_c^{\text{ext}}(a) \qquad \frac{\partial}{\partial r} u_c^{\text{int}}(r)\Big|_{r=a} = \frac{\partial}{\partial r} u_c^{\text{ext}}(r)\Big|_{r=a}$$

- **R-matrix maps derivative of wave function to value at channel radius**

$$u_{c'}(a'_c) = \sum_c \sqrt{\frac{\mu'_c a'_c}{\mu_c a_c}} R_{c'c} \left[a_c \frac{du_c(r)}{dr} - B_c u_c(a_c)\right]_{r=a_c}$$

$\boldsymbol{B}_c$… boundary param.
$\boldsymbol{\mu}_c$… reduced mass
in channel c

Conventional R-matrix

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

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

$\gamma_{\lambda c}$ … n-th reduced width in channel c
E_λ … n-th pole energy in channel c

Fitting parameters for phenomenological R-matrix

- **Directly related to the collision Matrix**

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

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

$\Rightarrow$

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

With collision matrix all observables can be obtained

Conventional R-matrix

- **Introducing the quantities**

$$L_c = a_c \left(\frac{1}{O_c} \cdot \frac{\partial O_c}{\partial r_c} \right)_{r_c = a_c} = S_c + i\ P_c \quad \text{and} \quad \Omega_c = \sqrt{\frac{I_c}{O_c}}$$

L_c: Outgoing logarithmic derivative; S_c: shift factor; P_c: penetration factor

- **The collision matrix may be alternatively written in terms of a matrix *A***

$$U_{c'c} = \Omega'_c \left(\delta_{c'c} + 2i \sqrt{P'_c} \sum_{\lambda'\lambda} \gamma_{\lambda'c'} A_{\lambda'\lambda} \gamma_{\lambda c} \sqrt{P_c} \right) \Omega_c$$

where the identity can be found

$$\sum_{\lambda'\lambda} \gamma_{\lambda'c'} A_{\lambda'\lambda} \gamma_{\lambda c} = \gamma^T \mathbf{A} \gamma = \left(\left[\mathbf{1} - \mathbf{R}(\mathbf{L} - \mathbf{B}) \right]^{-1} \mathbf{R} \right)$$

The collision matrix in terms of the matrix *A also links conventional, Brune and Park R-matrix parametrizations*

Park's Parametrization

T.-S. Park Phys. Rev. C 104, 064612 – (2021)

- **Drop orthogonality requirement for basis functions in inner region → Boundary parameter *B* becomes level dependent**

- **non-orthogonality term can be written as**

$$J_{\lambda\lambda'} = -\frac{1}{E_\lambda - E} \sum_c \gamma_{\lambda c} \left(B_{\lambda c} - B_{\lambda' c}\right) \gamma_{\lambda' c} \quad \text{for } \lambda \neq \lambda'$$

- **Alternative R-matrix objects are introduced**

$$\mathcal{R}_{cc'} = \sum_{\lambda'\lambda} \gamma_{\lambda' c'} \left(J^{-1}\right)_{\lambda'\lambda} \frac{1}{E_\lambda - E} \gamma_{\lambda c}$$

$$\mathcal{R}^B_{cc'} = \sum_{\lambda'\lambda} \gamma_{\lambda' c'} \left(J^{-1}\right)_{\lambda'\lambda} \frac{1}{E_\lambda - E} \gamma_{\lambda c} B_{\lambda c}$$

- **To align observed resonance positions with formal positions E_λ**

$$B_{\lambda c} = S_c(E_\lambda) \qquad J_{\lambda\lambda} = 1 - \sum_c \gamma^2_{\lambda c} \left.\frac{dS_c(E)}{dE}\right|_{E=E_\lambda}$$

Park‘s Parametrization

T.-S. Park Phys. Rev. C 104, 064612 (2021)

- **Collision matrix can again be written as**

$$U_{c'c} = \Omega'_c \left(\delta_{c'c} + 2i\sqrt{P'_c} \sum_{\lambda'\lambda} \gamma_{\lambda'c'} A_{\lambda'\lambda} \gamma_{\lambda c} \sqrt{P_c} \right) \Omega_c$$

but the relation between matrix *A* and Park’s R-matrix parametrization now reads

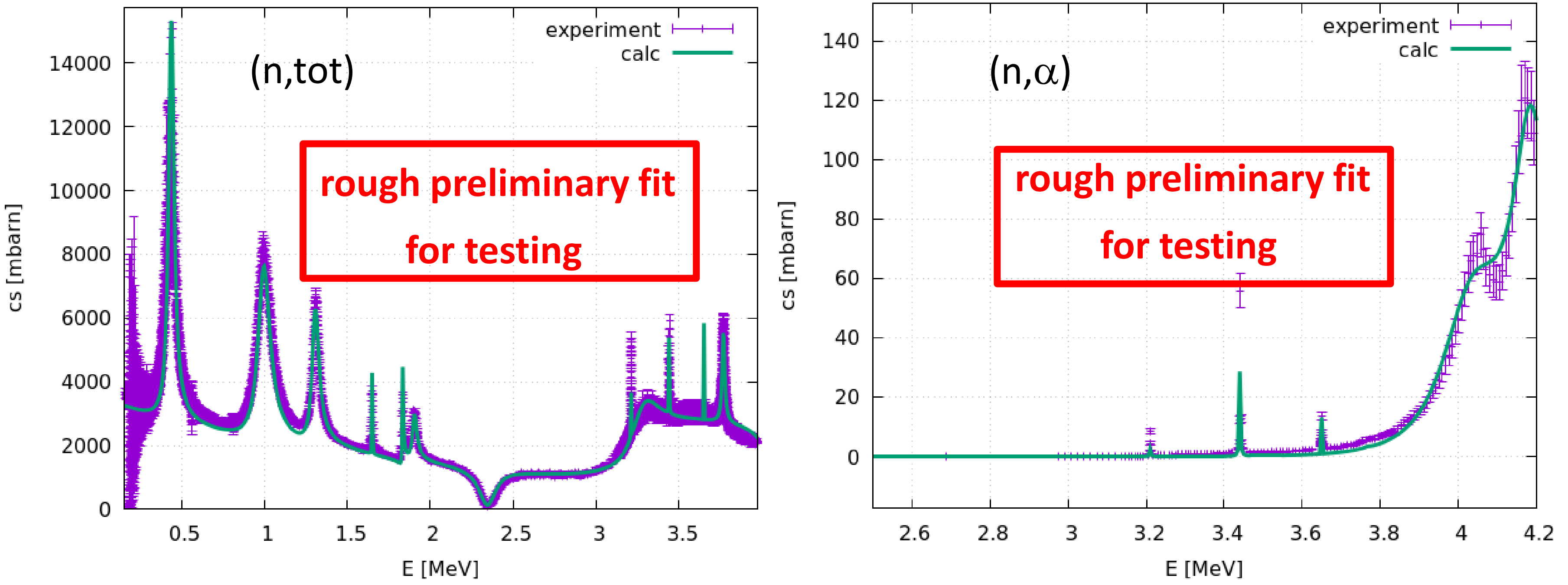
$$\sum_{\lambda'\lambda} \gamma_{\lambda'c'} A_{\lambda'\lambda} \gamma_{\lambda c} = \gamma^T \mathbf{A} \gamma = \left(\left[\mathbf{1} - \boldsymbol{\mathcal{R}}(\mathbf{S} + i\mathbf{P}) + \boldsymbol{\mathcal{R}}^B \right]^{-1} \boldsymbol{\mathcal{R}} \right)$$

Neat detail: the fundamental R-matrix relation looks very familiar

$$u_{c'}(a'_c) = \sum_c \sqrt{\frac{\mu'_c a'_c}{\mu_c a_c}} \left(\mathcal{R}_{c'c} a_c \frac{du_c(r)}{dr} - \mathcal{R}^B_{c'c} u_c(a_c) \right)_{r=a_c}$$

Example (n+^{16}O)

- **Test for angle integrated cross section (n,tot) and (n,α)**
- **Behavior confirmed:**
  → observed resonance position = formal E_λ
  → positions constant during change of reduced width $\gamma_{\lambda c}$



Reconstruction

Starting with collision matrix expression

$$U_{c'c} = \Omega'_c \left(\delta_{c'c} + 2i\sqrt{P'_c} \sum_{\lambda'\lambda} \gamma_{\lambda'c'} A_{\lambda'\lambda} \gamma_{\lambda c} \sqrt{P_c} \right) \Omega_c$$

Conventional R-Matrix

Park's Parametrization

$$\left([\mathbf{1} - \mathbf{R}(\mathbf{L} - \mathbf{B})]^{-1} \mathbf{R} \right) = \left([\mathbf{1} - \boldsymbol{\mathcal{R}}(\mathbf{S} + i\mathbf{P}) + \boldsymbol{\mathcal{R}}^B]^{-1} \boldsymbol{\mathcal{R}} \right)$$

after a few basic rearrangements

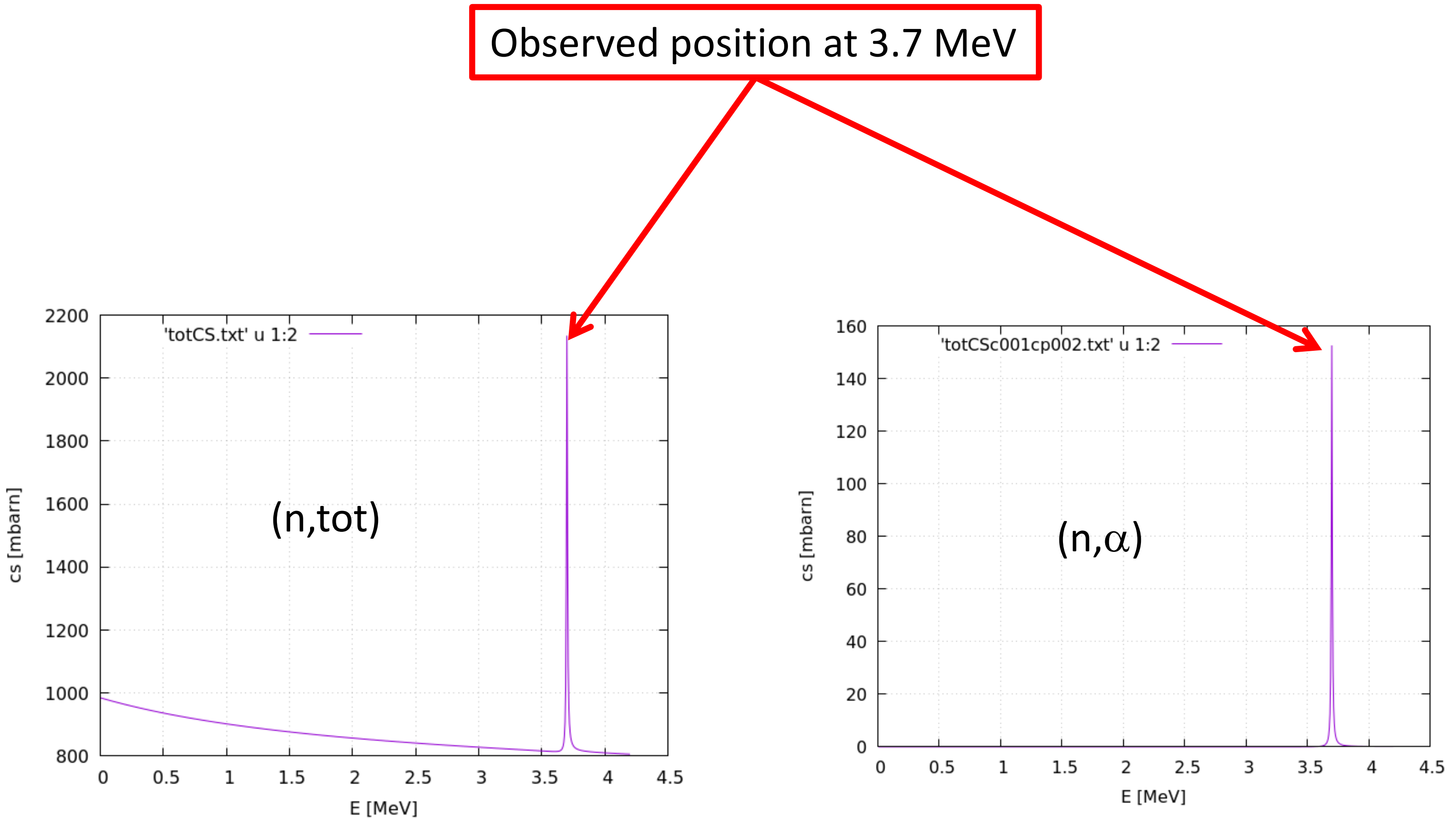
$$\mathbf{R} = [\mathbf{1} + \boldsymbol{\mathcal{R}}^B - \boldsymbol{\mathcal{R}}\mathbf{B}]^{-1} \boldsymbol{\mathcal{R}}$$

- Conventional R-matrix parameters not immediately available
- Allows for pointwise reconstruction of R-matrix values

Reconstruction

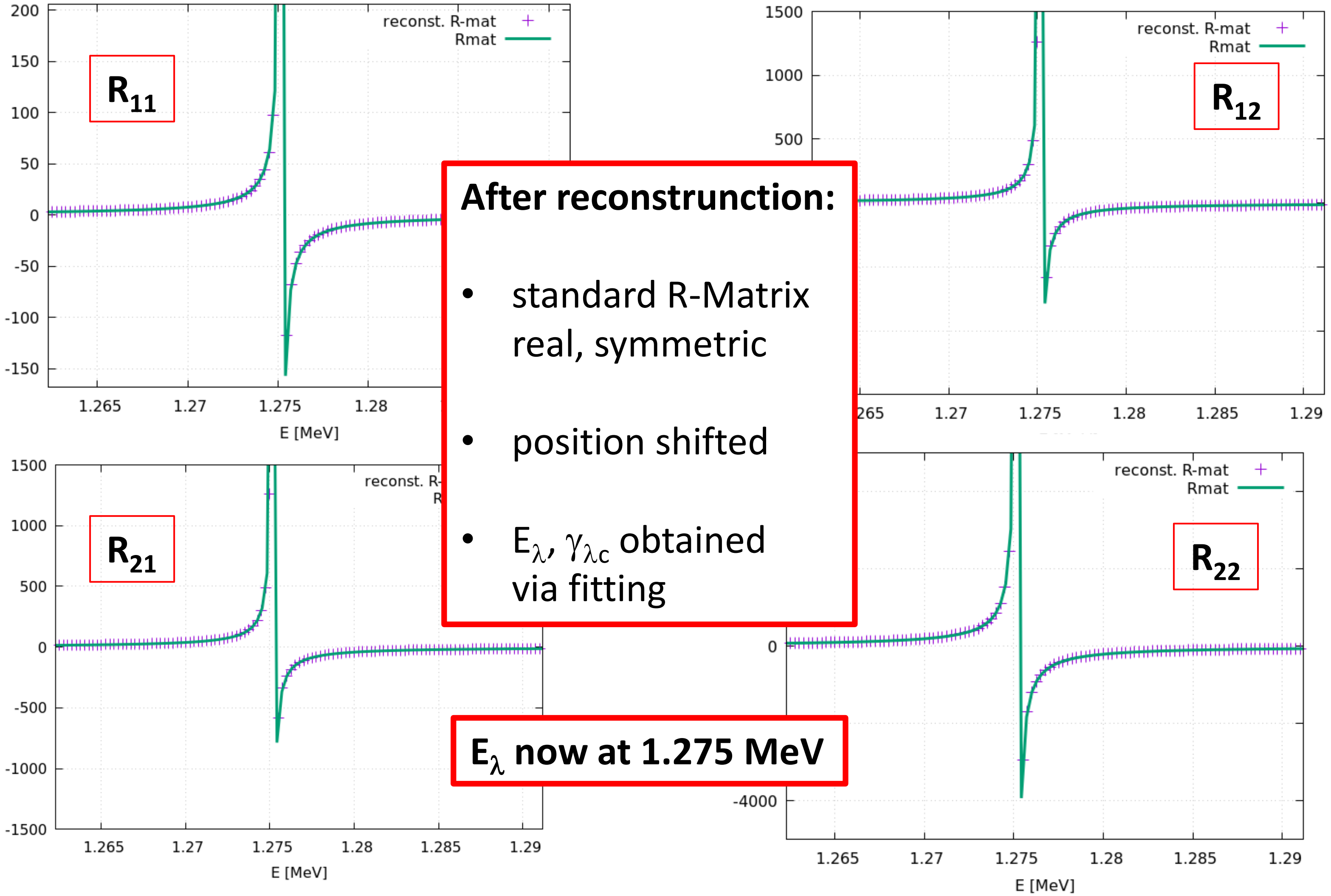
- **Park parametrization with one pole:**

  J=3/2+ E_1 = 3.7 MeV $\gamma_{1,1}$ = 0.2 $\gamma_{1,2}$ = 1.0



Reconstruction

- Back to conventional R-matrix



After reconstrunction:

- standard R-Matrix real, symmetric
- position shifted
- E_λ, $\gamma_{\lambda c}$ obtained via fitting

E_λ now at 1.275 MeV

Summary

- **alternative R-matrix parametrizations (Brune and Park) handy tools for nuclear data analysis**
- **parameter fitting becomes much more convenient**
- **added support for Park parametrization in GECCCOS**
- **successfully tested Park's parametrization on (n+^{16}O) for two channels up to 4 MeV**

Outlook

next steps

- **Including both Brune and Park parametrization in evaluation pipeline of GECCCOS**
- **automate conventional R-matrix parameter reconstruction for Park**
- **… more testing and comparing with different experiment data sets**

other topics within the group:

- **Including methods to treat 3-body processes**
  - Glöckle type R-matrix (see poster F.W. Wührleitner [Master thesis in progress])
  - Solution of Faddeev equation for separable potentials (T. Wojta [Master thesis in progress])
- **Code efficiency optimization**
- **Improving usability (Grapical Interface)**

Thank you for your attention