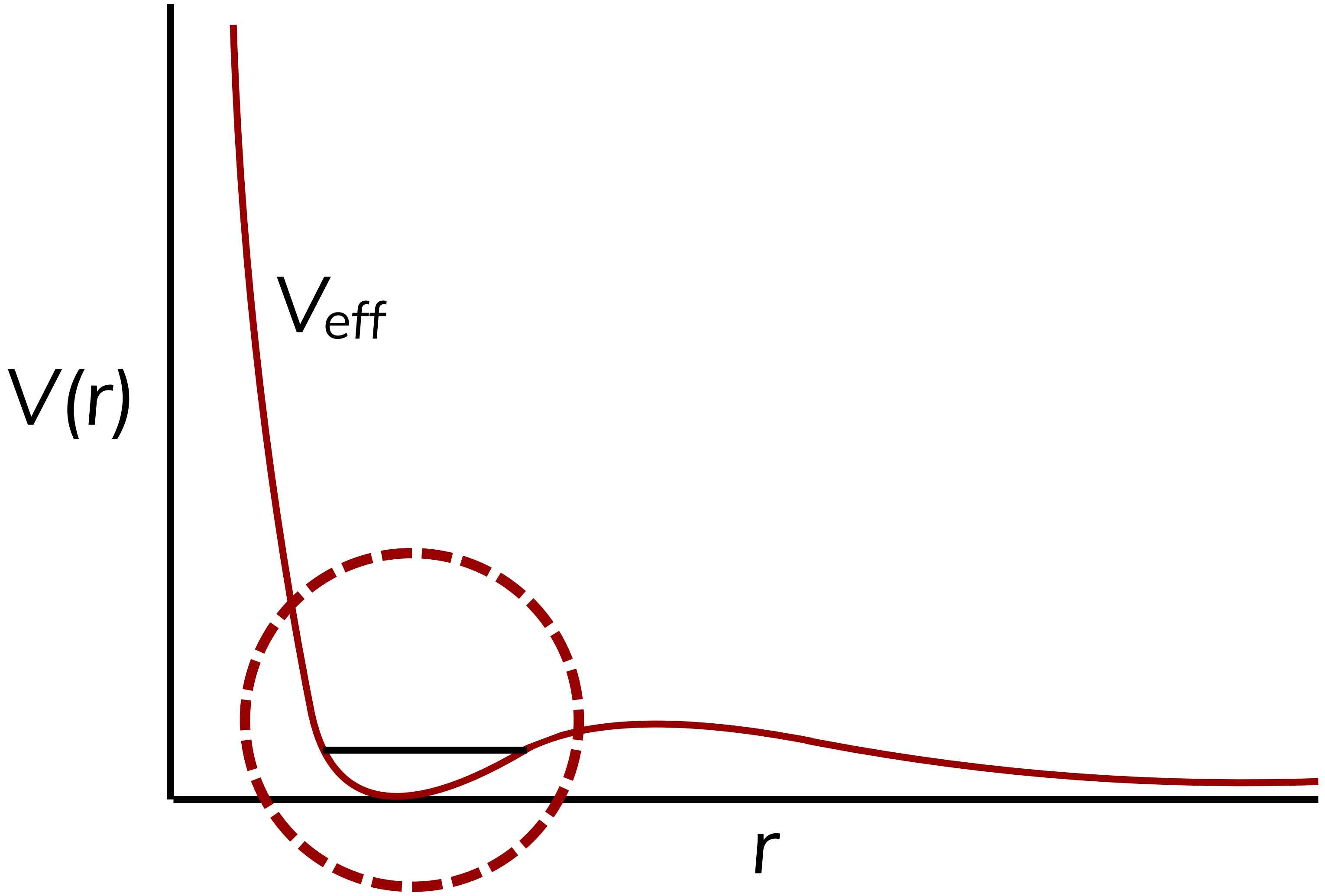
Reproduction and analysis of: *R-matrix type parametrization of the Jost function for extracting the resonance parameters from scattering data*†

Juliana Prada Suarez
Cristian Eduardo Martinez Torres



Universidad Nacional de Colombia
Facultad de Ciencias
Departamento de Física
Introducción a la Teoría de Reacciones Nucleares

OUTLINE

1. Author’s motivation and problem
2. Some approaches to the problem
3. Author’s proposed approach
4. Theoretical background
5. Understanding the method
6. Results
7. Conclusions

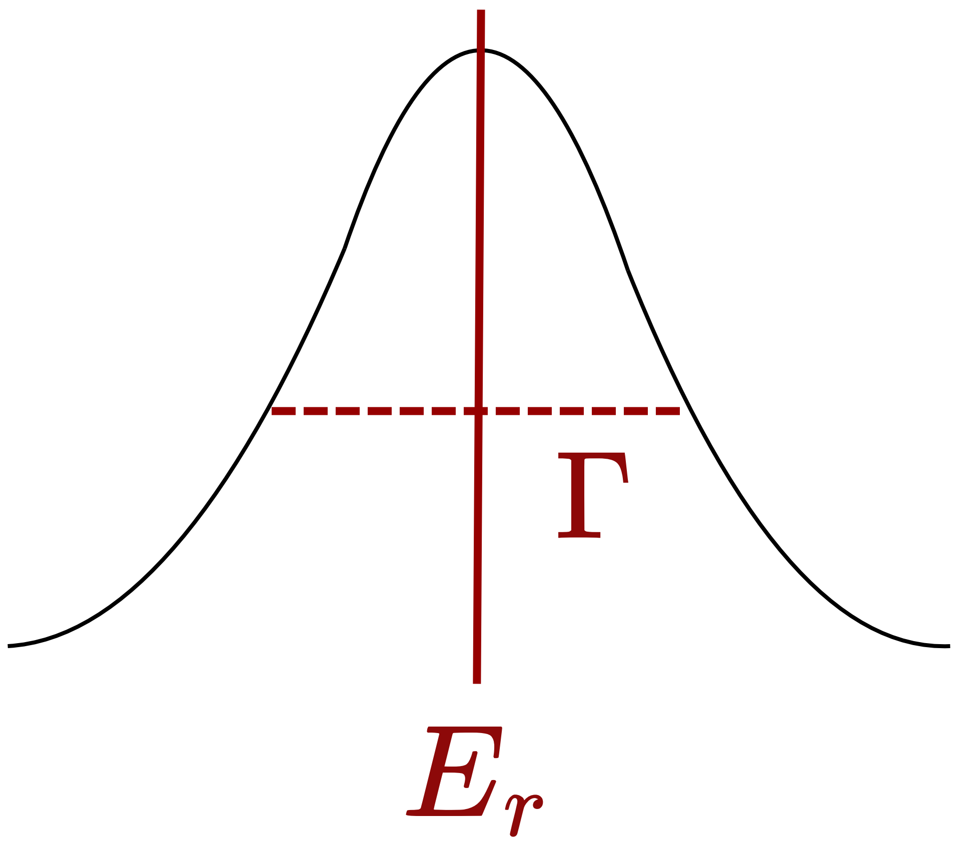
Reference list

† Vaandrager, P., Lekala, M. L., & Rakityansky, S. A. (2025). R-matrix type parametrization of the Jost function for extracting the resonance parameters from scattering data. European Physical Journal A, 61, 79.

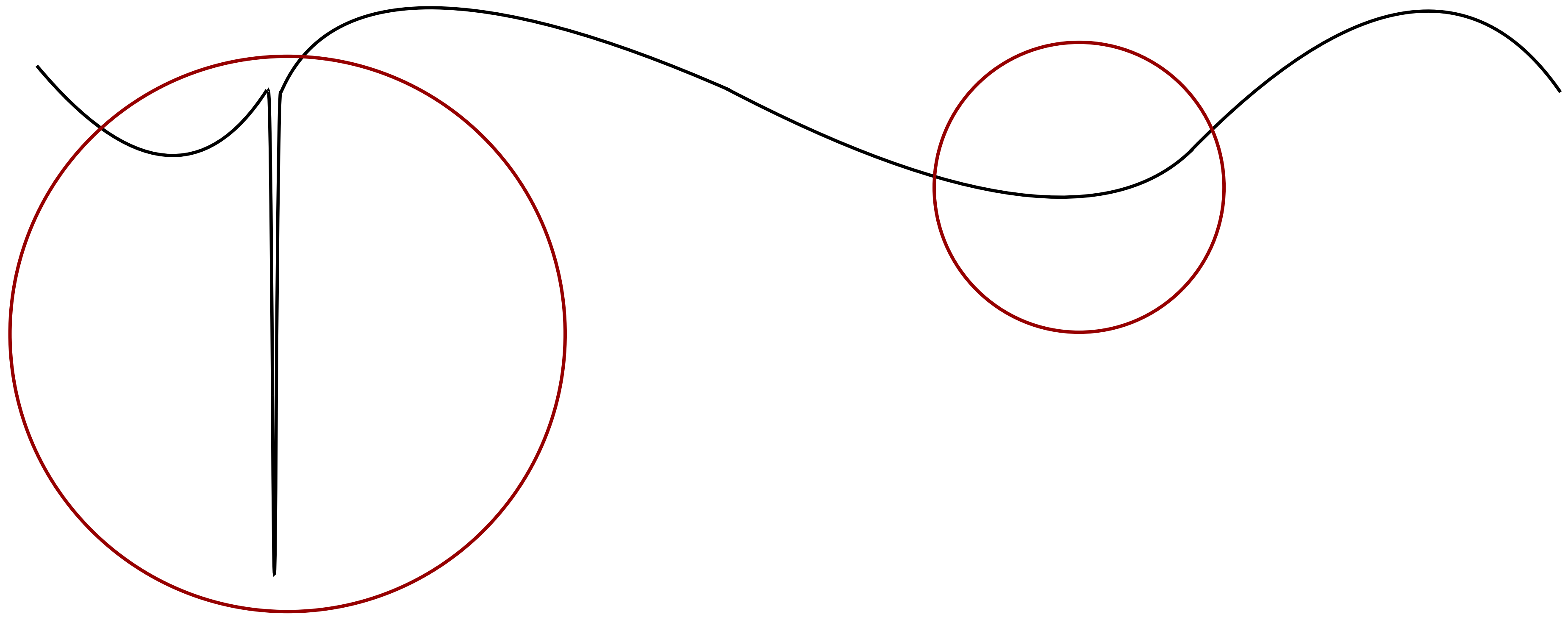
Author's motivation and problem†

Resonances: irregularities in the scattering cross-section

Bell-shaped resonances



Non bell-shaped resonances



Author's motivation and problem†

Almost all methods are based on:

Each resonance corresponds to a pole of the S-matrix at complex energy

$$E = E_r - \frac{i}{2}\Gamma$$

There is a special interest in:

Parametrizing the S-matrix to fit the data

One detail to consider:

The functional form of the parametrization must be adequate

Some approaches to the problem†

Jost functions method

- a Jost functions $f_\ell^{(\mathrm{in})}(E) \qquad f_\ell^{(\mathrm{out})}(E)$
- b S-matrix $S(E) = f_\ell^{(\mathrm{out})}(E)\left[f_\ell^{(\mathrm{in})}(E)\right]^{-1}$

Why does this method work?

Almost all the factors in this functions are given explicitly and in an exact way

The remaining unknown factors are always single-valued and analytic functions of E

Why isn't it enough?

The number of fitting parameters is on the order of 50

Some approaches to the problem[†]

R-matrix method

- Phenomenological R-matrix

$$R_\ell(E, B_R) = \sum_{n=1}^{N} \frac{[\gamma_{n\ell}(B_R)]^2}{E_{n\ell} - E}$$

Why does this method work?

Few fitting parameters

Why isn't it enough?

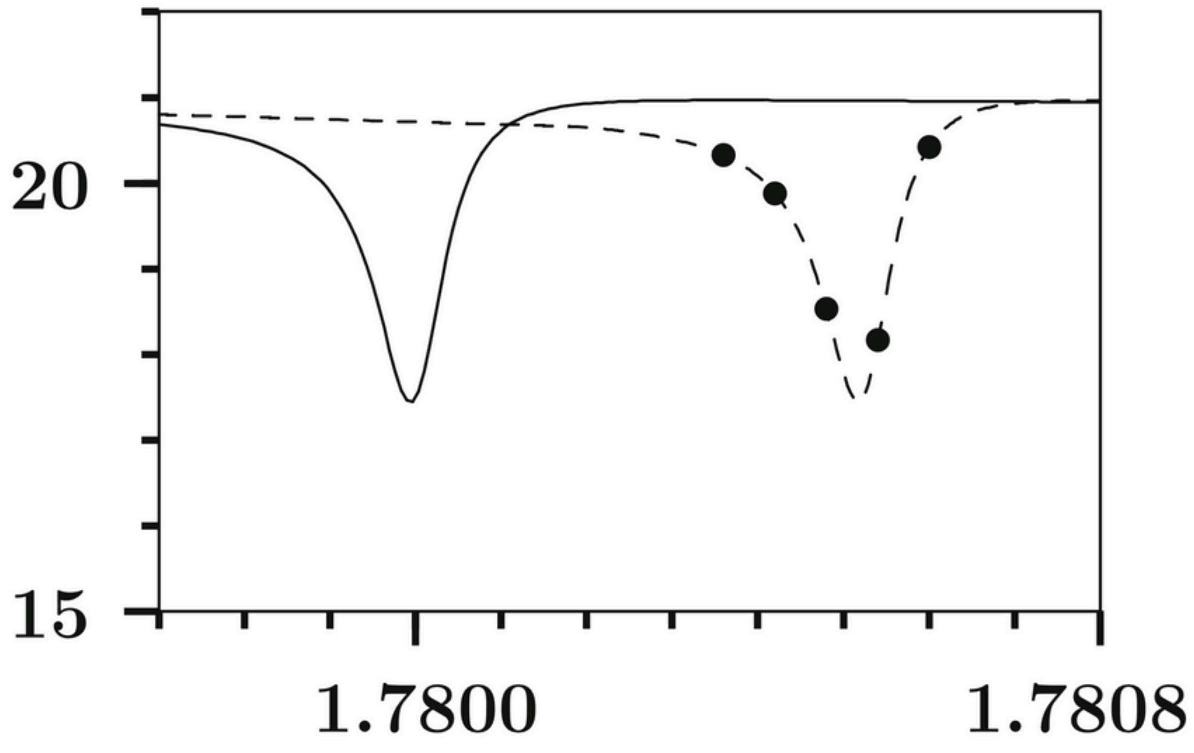
Arbitrary choice of the channel radius

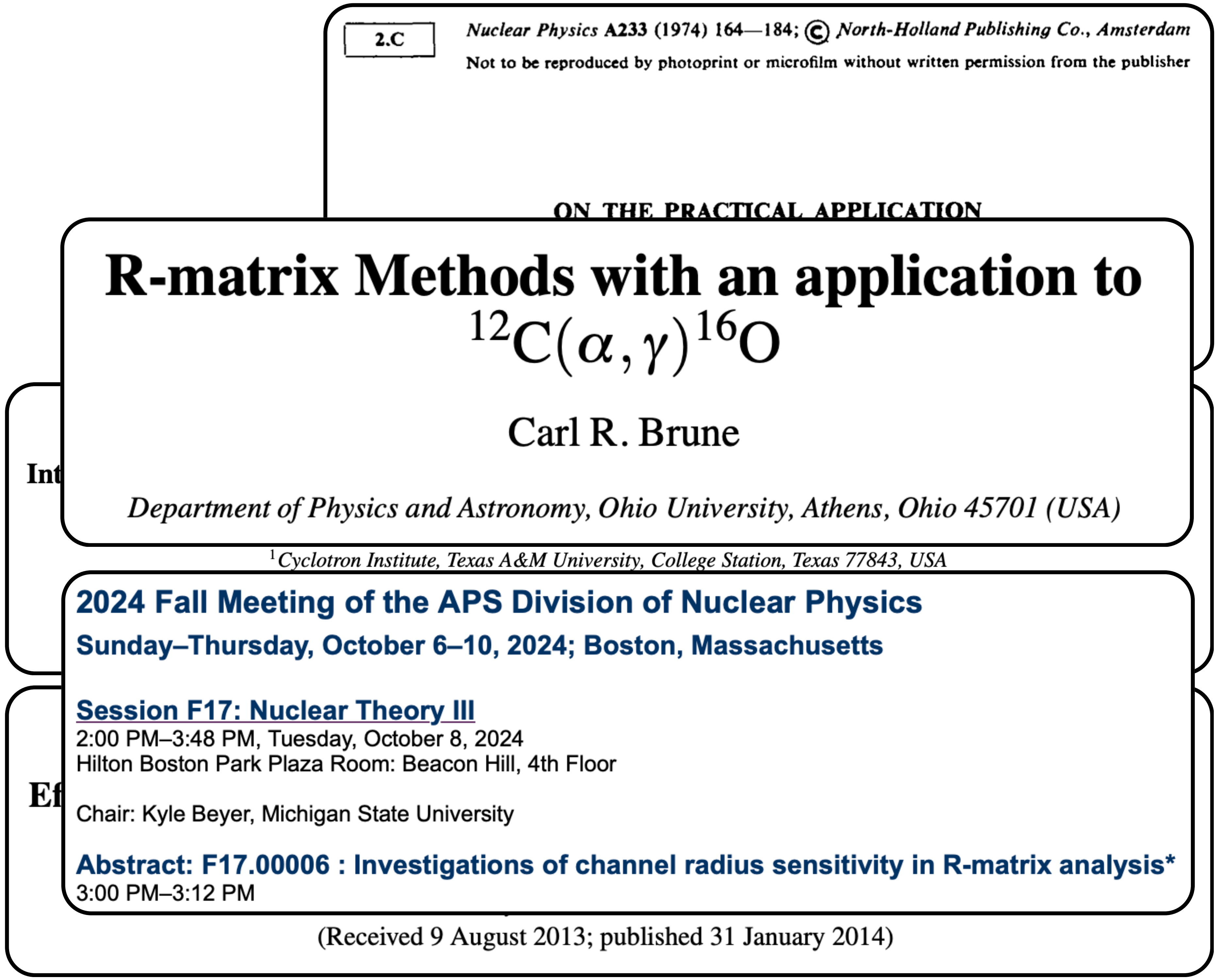
Problematic functional form of the S-matrix

Some approaches to the problem†

Why isn't it enough?

Arbitrary choice of the channel radius





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Nuclear Physics **A233** (1974) 164—184; © *North-Holland Publishing Co., Amsterdam*

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ON THE PRACTICAL APPLICATION

R-matrix Methods with an application to $^{12}C(\alpha,\gamma)^{16}O$

Carl R. Brune

Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701 (USA)

Int

[1]*Cyclotron Institute, Texas A&M University, College Station, Texas 77843, USA*

2024 Fall Meeting of the APS Division of Nuclear Physics

Sunday–Thursday, October 6–10, 2024; Boston, Massachusetts

Session F17: Nuclear Theory III

2:00 PM–3:48 PM, Tuesday, October 8, 2024

Hilton Boston Park Plaza Room: Beacon Hill, 4th Floor

Chair: Kyle Beyer, Michigan State University

Abstract: F17.00006 : Investigations of channel radius sensitivity in R-matrix analysis*

3:00 PM–3:12 PM

Ef

(Received 9 August 2013; published 31 January 2014)

Author's proposed approach†

Combine both methods!

Preliminary considerations

- ☑ Single-channel problem
- ☑ Artificial experimental data
- ☑ Noro-Taylor potential with a Coulomb tail

Reference list

† Vaandrager, P., Lekala, M. L., & Rakityansky, S. A. (2025). R-matrix type parametrization of the Jost function for extracting the resonance parameters from scattering data. European Physical Journal A, 61, 79.

* S.A. Rakityansky, Jost Functions in Quantum Mechanics: A Unified Approach to Scattering, Bound, and Resonant State Problems (Springer, Berlin, 2022)

‡ Canto, L. F., & Hussein, M. S. (2013). Scattering Theory of Molecules, Atoms and Nuclei. WORLD SCIENTIFIC. ISBN 978-9814329835

Theoretical background†‡*

Jost functions

Regular solution of the radial Schrödinger equation in the asymptotic limit

$$\Phi_\ell(k,r) \to \left[H_\ell^{(+)}(\eta,kr) f_\ell^{(\mathrm{in})}(\eta,k) + H_\ell^{(-)}(\eta,kr) f_\ell^{(\mathrm{out})}(\eta,k)\right]$$

Formal definition

Amplitudes of the incoming and outgoing Haenkel-Coulomb functions in the asymptotic behaviour of this solution

Theoretical background†‡*

How does the Jost function look?

$$f_\ell^{(\text{in/out})}(E) = e^{\mp i\delta_\ell^c} k^\ell \left\{ \frac{k}{D_\ell(\eta,k)} A_\ell(E) - [M(k) \pm i] D_\ell(\eta,k) B_\ell(E) \right\}$$

$$\delta_\ell^c(\eta) = \frac{1}{2i} \ln\left(\frac{\Gamma(\ell+1+i\eta)}{\Gamma(\ell+1-i\eta)} \right) \qquad D_\ell(\eta,k) = C_\ell(\eta) k^{\ell+1} \qquad M(k) = \frac{2\eta h(\eta)}{C_0^2(\eta)}$$

$$C_\ell(\eta) = \frac{e^{-\pi\eta/2}}{\Gamma(\ell+1)} \exp\left\{ \frac{1}{2} [\ln\Gamma(\ell+1+i\eta) + \ln\Gamma(\ell+1-i\eta)] \right\}$$

$$h(\eta) = \frac{1}{2}[\psi(1+i\eta) + \psi(1-i\eta)] - \ln\eta \qquad \psi(z) = \frac{\Gamma'(z)}{\Gamma(z)}$$

Theoretical background†‡*

How does the Jost function look?

$$f_\ell^{(\mathrm{in/out})}(E) = e^{\mp i\delta_\ell^c} k^\ell \left\{ \frac{k}{D_\ell(\eta,k)} A_\ell(E) - [M(k) \pm i] D_\ell(\eta,k) B_\ell(E) \right\}$$

$$A_\ell(E) \approx \sum_{n=0}^{N} a_n(\ell, E_0) \, (E - E_0)^n \qquad B_\ell(E) \approx \sum_{n=0}^{N} b_n(\ell, E_0) \, (E - E_0)^n$$

Fitting parameters!

Theoretical background[†,‡,*]

This gives us a clue about the proposed modification

$$\cancel{A_\ell(E) \approx \sum_{n=0}^{N} a_n(\ell, E_0)\,(E - E_0)^n} \qquad \cancel{B_\ell(E) \approx \sum_{n=0}^{N} b_n(\ell, E_0)\,(E - E_0)^n}$$

This Taylor series needs to be replaced!

The R-matrix is the solution

Theoretical background†‡*

Relation between the R-matrix and the Jost functions

$$f_\ell^{(\mathrm{in/out})}(E) = \frac{\pm i\, e^{\pm i\delta_\ell}\, k^\ell}{Q_\ell(E,B_R)} \left\{ H_\ell^{(\pm)}(\eta,ka) - \left[a\frac{d}{dr}H_\ell^{(\pm)}(\eta,kr)\Big|_{r=a} - B_R\, H_\ell^{(\pm)}(\eta,ka) \right] R_\ell(E,B_R) \right\}$$

$$Q_\ell(E,\boldsymbol{B}_R) = \sum_{n=1}^{N} \frac{\lambda_{n\ell}(\boldsymbol{B}_R)\gamma_{n\ell}(\boldsymbol{B}_R)}{E_{n\ell}-E}$$

Let’s remember our objective

$$f_\ell^{(\mathrm{in/out})}(E) = e^{\mp i\delta_\ell^c} k^\ell \left\{ \frac{k}{D_\ell(\eta,k)} A_\ell(E) - [M(k) \pm i] D_\ell(\eta,k) B_\ell(E) \right\}$$

Theoretical background†‡*

Relation between the R-matrix and the Jost functions

- **a** Comparison of the terms in both expressions
- **b** Rewriting Q and the R-matrix as sums of polynomials
- **c** Replace those expressions in the coefficients

$$A_\ell(E) = \sum_{n=0}^{N} \alpha_{n\ell} \mathcal{P}_n(E) \qquad B_\ell(E) = \sum_{n=0}^{N} \beta_{n\ell} \mathcal{P}_n(E)$$

$$\mathcal{P}_n(E) = \frac{\mathcal{P}_0(E)}{E_{n\ell} - E} \qquad \mathcal{P}_0(E) = \prod_{n=1}^{N} (E_{n\ell} - E)$$

New fitting parameters!

Understanding the method †

In a typical scenario

$$\sigma_{\text{total}}(E_i) \pm \Delta_i$$

$$i = 1, 2, \ldots, N^{(\text{data})}$$

The steps of the method are

- a Parametrize the functions

$$A_\ell(E) = \sum_{n=0}^{N} \alpha_{n\ell} \mathcal{P}_n(E) \qquad B_\ell(E) = \sum_{n=0}^{N} \beta_{n\ell} \mathcal{P}_n(E)$$

Understanding the method †

b Substituing them in the S-matrix

$$S_\ell(E) = e^{2i\delta_\ell^c} \frac{kA_\ell(E) - [M(k) - i]D_\ell^2(\eta, k)B_\ell(E)}{kA_\ell(E) - [M(k) + i]D_\ell^2(\eta, k)B_\ell(E)}$$

c Obtain the total cross-section by summing over several partial cross-sections

$$\sigma_{\text{total}}(E) = \sum_{\ell=0}^{\ell_{\max}} \sigma_\ell(E) \qquad \sigma_\ell(E) = \frac{\pi}{k^2}(2\ell+1)\left|S_\ell(E) - 1\right|^2$$

Understanding the method †

Little recap

What do we want?

Fitting the total cross-section experimental data to extract resonance parameters

How are we going to do it?

By fitting the parameters in the S-matrix

$$A_\ell(E) = \sum_{n=0}^{N} \alpha_{n\ell} \mathcal{P}_n(E) \qquad B_\ell(E) = \sum_{n=0}^{N} \beta_{n\ell} \mathcal{P}_n(E) \qquad \mathcal{P}_n(E) = \frac{\mathcal{P}_0(E)}{E_{n\ell} - E}$$

Reference list

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S.A. Sofianos, S.A. Rakityansky, Exact method for locating potential resonances and Regge trajectories. J. Phys. A: Math. Gen. 30, 3725–3737 (1997)

Understanding the method †

Let's talk about the implementation

Artificial experimental data

- Exact total cross-section using a given potential

$$V(r) = \frac{\hbar^2}{2\mu}\left(7.5r^2e^{-r} + \frac{2k\eta}{r}\right)$$

Understanding the method †#

Let's talk about the implementation

Artificial experimental data

Partial cross-section can be calculated using any of the many known methods for solving a two-body scattering problem

Direct calculation of the Jost functions

Complex coordinate method to solve the Schrödinger equation

Advantajes

No need of approximations, expansions or variational procedures

Understanding the method †#

Direct calculation of the Jost functions

$$r \in [0, 1]$$

$$r \in [1, 30]$$

a. Complex continuation of the radial coordinate

b. We look for a solution near r=0 in the form

$$\Phi_\ell(k, r) = F_\ell(\eta, kr) A_\ell(\eta, k, x, \theta) + G_\ell(\eta, kr) B_\ell(\eta, k, x, \theta)$$

c. We look for a solution for large r in the form

$$\Phi_\ell(k, r) = \frac{1}{2}\left[H_\ell^{(+)}(\eta, kr)\mathcal{F}_\ell^{(+)}(k, x, \theta) + H_\ell^{(-)}(\eta, kr)\mathcal{F}_\ell^{(-)}(k, x, \theta)\right]$$

Understanding the method †#

Direct calculation of the Jost functions

- We need to solve this first–order coupled differential equations for each solution

$$\partial_x \mathcal{F}_\ell^{(+)}(k,x,\theta) = -\frac{e^{i\theta}}{2ik} H_\ell^{(+)}(\eta,kr)V(r)\left[H_\ell^{(+)}(\eta,kr)\mathcal{F}_\ell^{(+)}(k,x,\theta) + H_\ell^{(-)}(\eta,kr)\mathcal{F}_\ell^{(-)}(k,x,\theta)\right]$$

$$\partial_x \mathcal{F}_\ell^{(+)}(k,x,\theta) = \frac{e^{i\theta}}{2ik} H_\ell^{(-)}(\eta,kr)V(r)\left[H_\ell^{(+)}(\eta,kr)\mathcal{F}_\ell^{(+)}(k,x,\theta) + H_\ell^{(-)}(\eta,kr)\mathcal{F}_\ell^{(-)}(k,x,\theta)\right]$$

$$\partial_x A_\ell(\eta,k,x,\theta) = \frac{e^{i\theta}}{k} G_\ell(\eta,kr)V(r)[F_\ell(\eta,kr)A_\ell(\eta,k,x,\theta) + G_\ell(\eta,kr)B_\ell(\eta,k,x,\theta)]$$

$$\partial_x B_\ell(\eta,k,x,\theta) = -\frac{e^{i\theta}}{k} F_\ell(\eta,kr)V(r) \quad \boxed{A_\ell(\eta,k,0,\theta) = 1\,, \qquad B_\ell(\eta,k,0,\theta) = 0}$$

Understanding the method

Comments on the reproduction of the exact curve

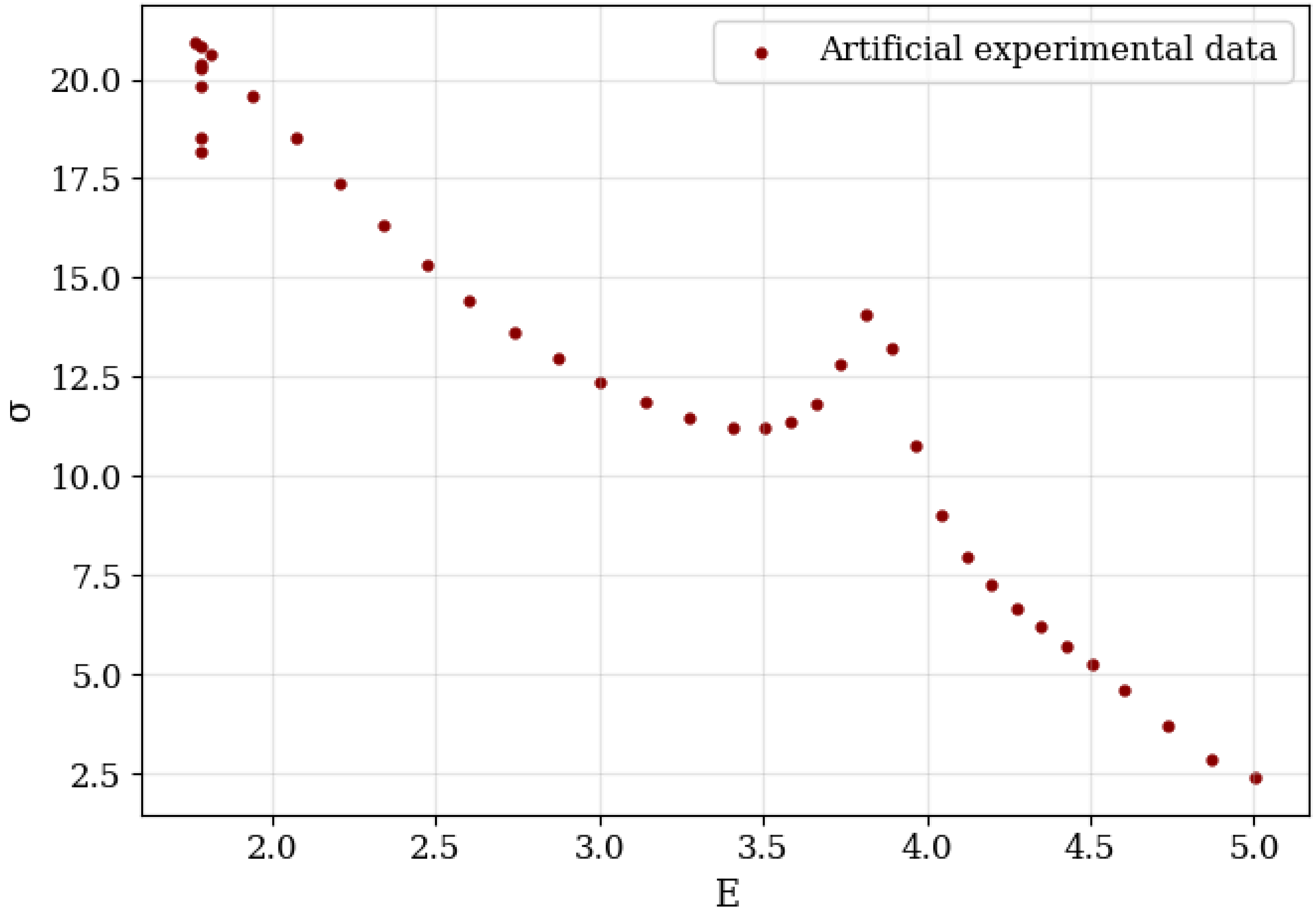
a Coupling of two differential equation systems in Python

b Problems with Coulomb wave functions in cmath library

c Number of points to get significant results

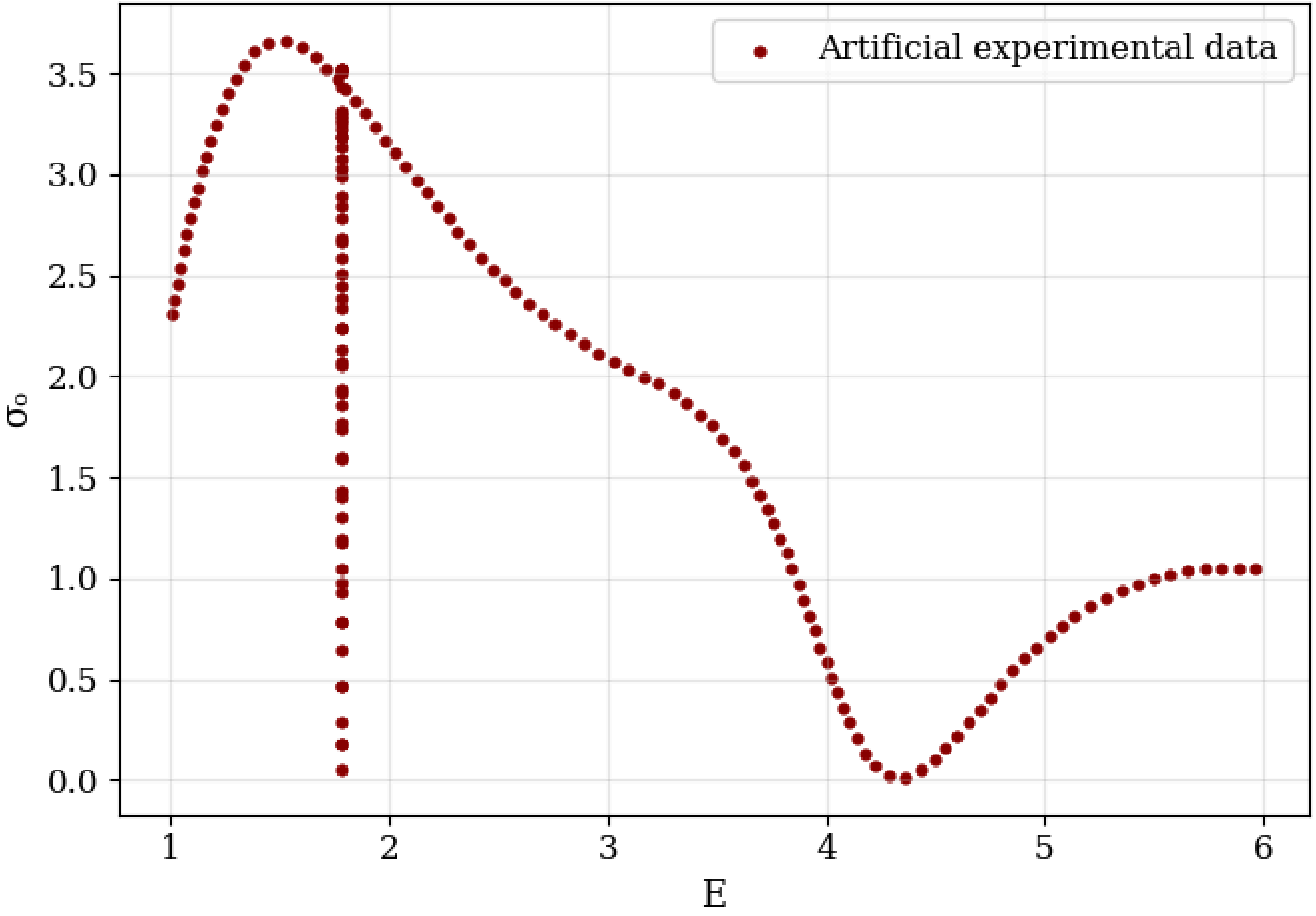
Understanding the method

Exact total cross-section curve



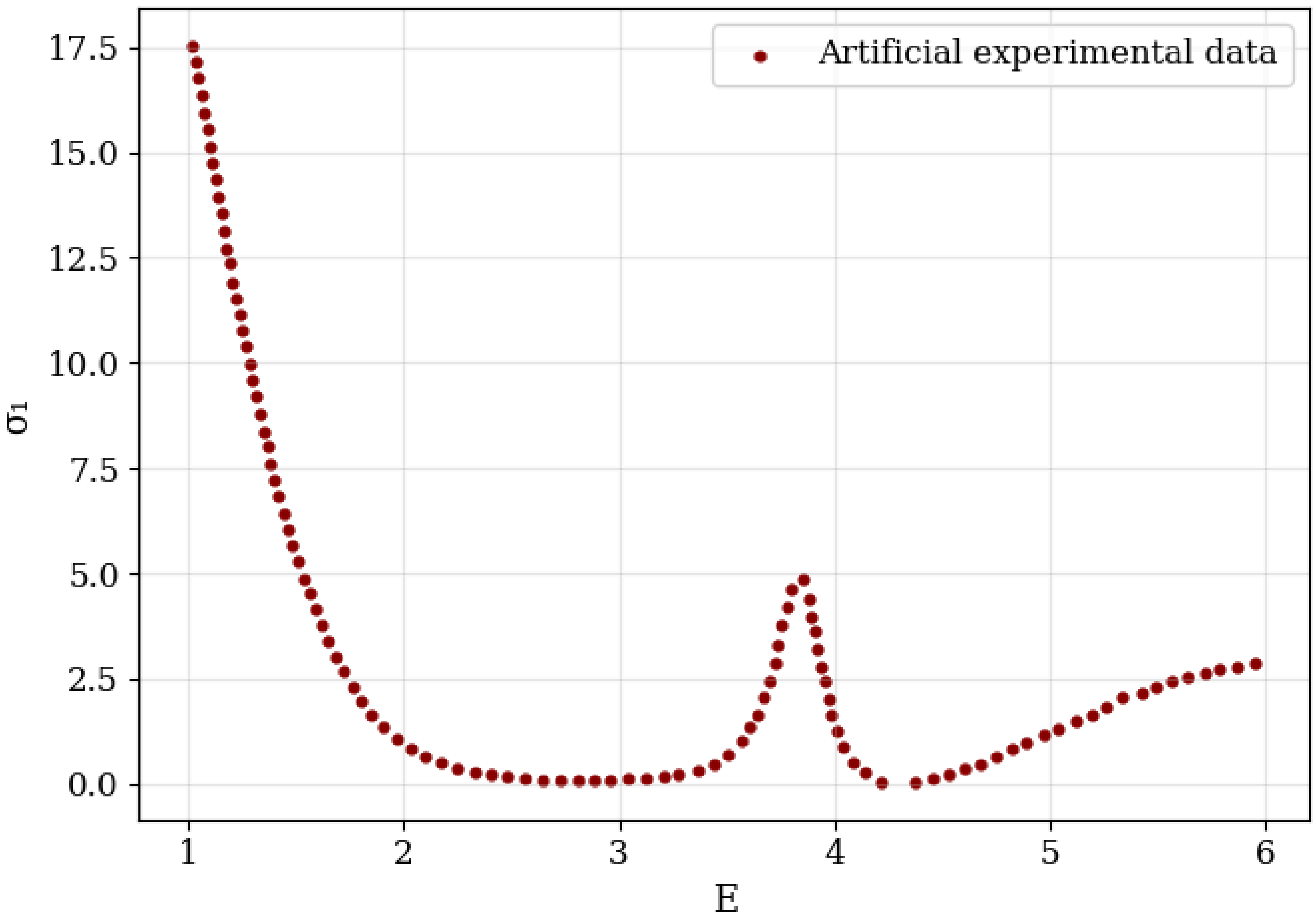
Understanding the method

Exact partial cross-section curves



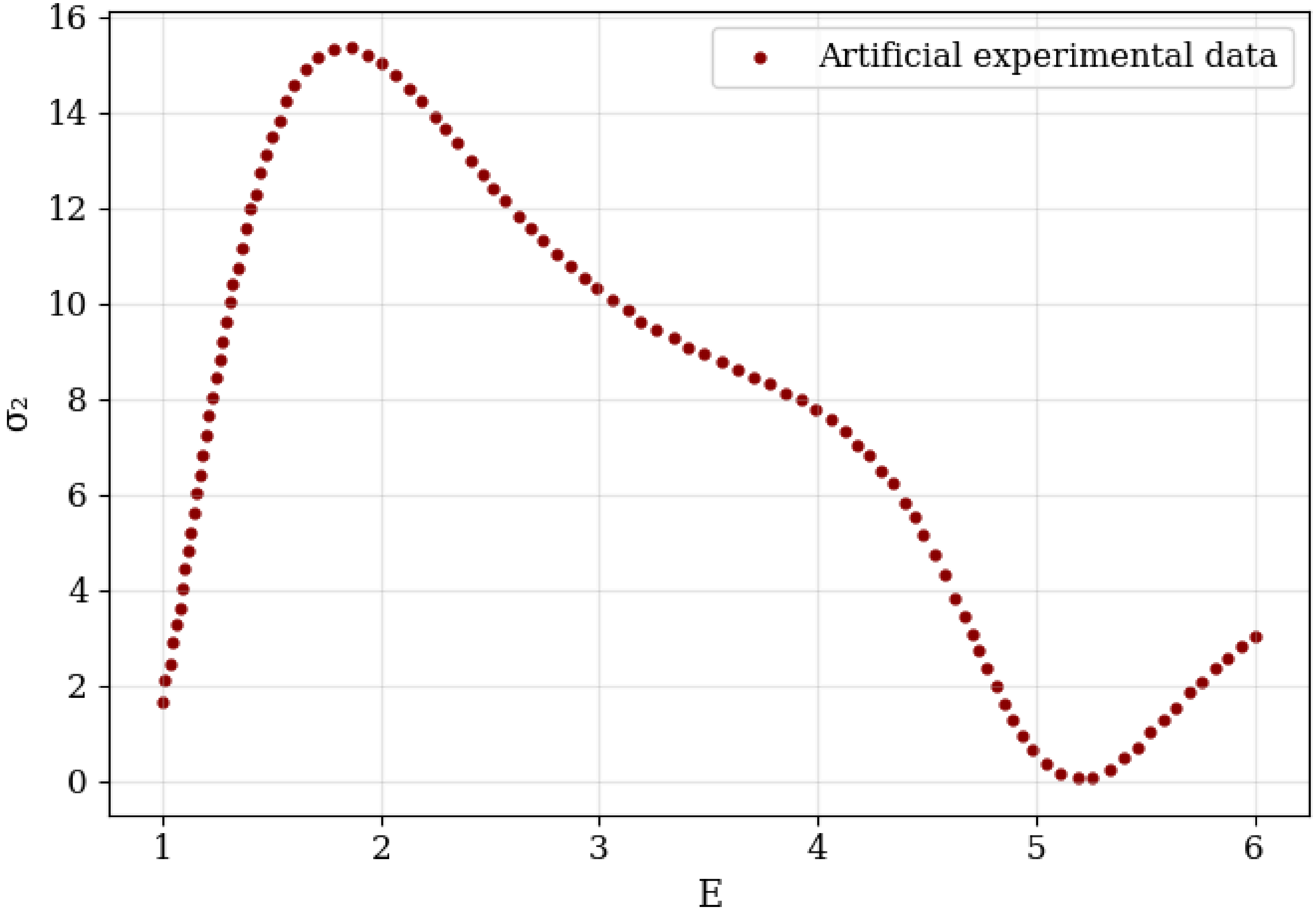
Understanding the method

Exact partial cross-section curves



Understanding the method

Exact partial cross-section curves



Understanding the method $^{\dagger\#}$

Fitting procedure

a. 40 energy data points between 1.7-5 to fit

b. Minimization routine MINUIT

   i. Find optimal values by minimizing

$$\chi^2 = \sum_{i=1}^{N^{(\mathrm{data})}} \left[\frac{\sigma_{\mathrm{total}}(E_i) - \sigma_{\mathrm{fit}}(E_i)}{\Delta_i} \right]^2$$

c. Find the zeros of the Jost functions

d. Extract resonance parameters

Understanding the method

Comments on the reproduction of the fitting curve

a We tested all the functions required for the fitting

b The Coulomb barrier factor was wrong

$$C_\ell(\eta) = \frac{e^{-\pi\eta/2}}{\Gamma(\ell+1)} \exp\left\{\frac{1}{2}\left[\ln\Gamma(\ell+1+i\eta) + \ln\Gamma(\ell+1-i\eta)\right]\right\} \frac{1}{(2\ell+1)!!}$$

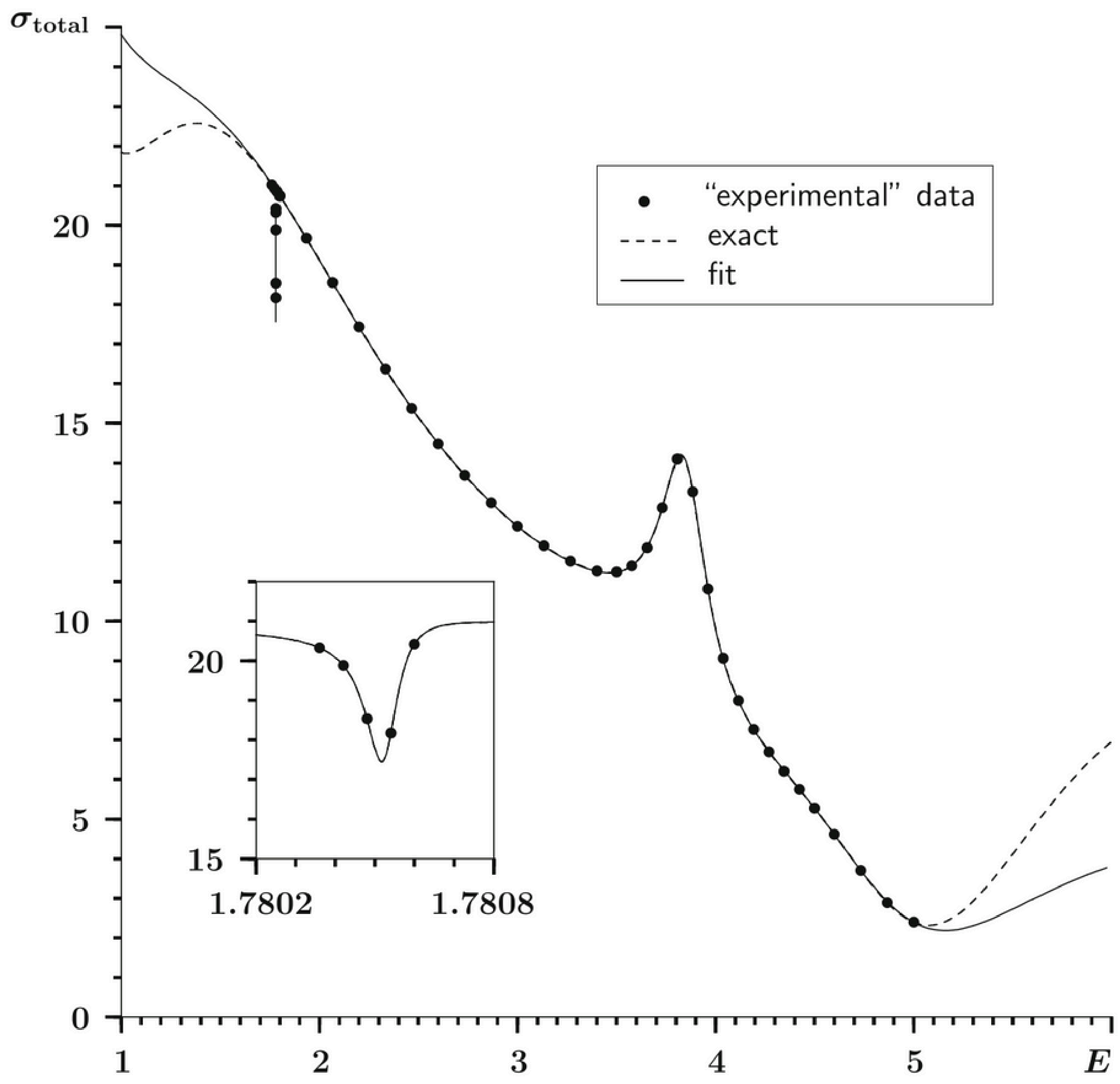
$$C_\ell(\eta) = \frac{2^\ell e^{-\pi\eta/2}}{\Gamma(2\ell+2)} |\Gamma(\ell+1 \pm i\eta)|$$

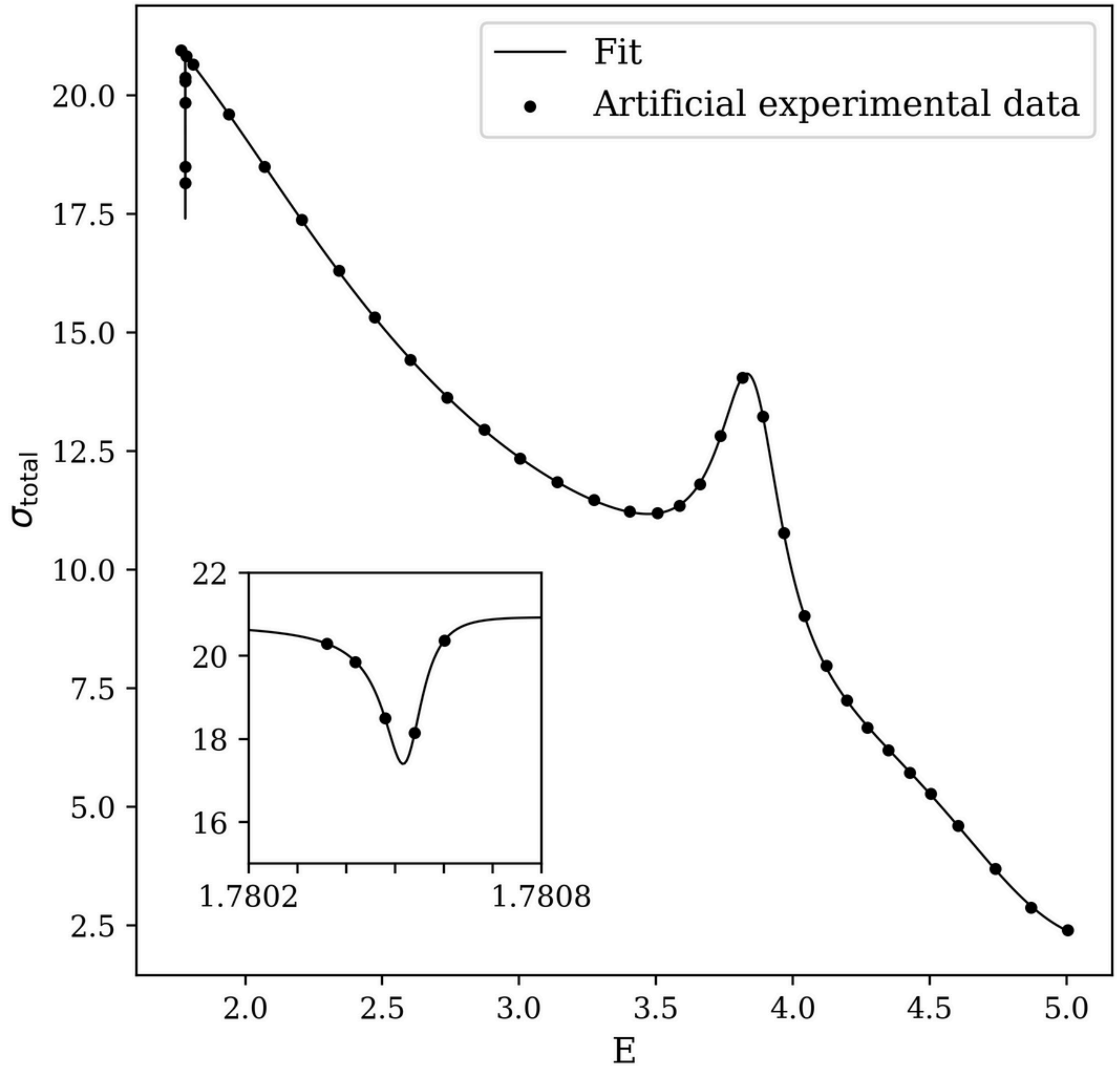
c η was incorrectly defined

$$\eta = -\frac{1}{2k} \qquad \eta = -\frac{1}{k}$$

Results

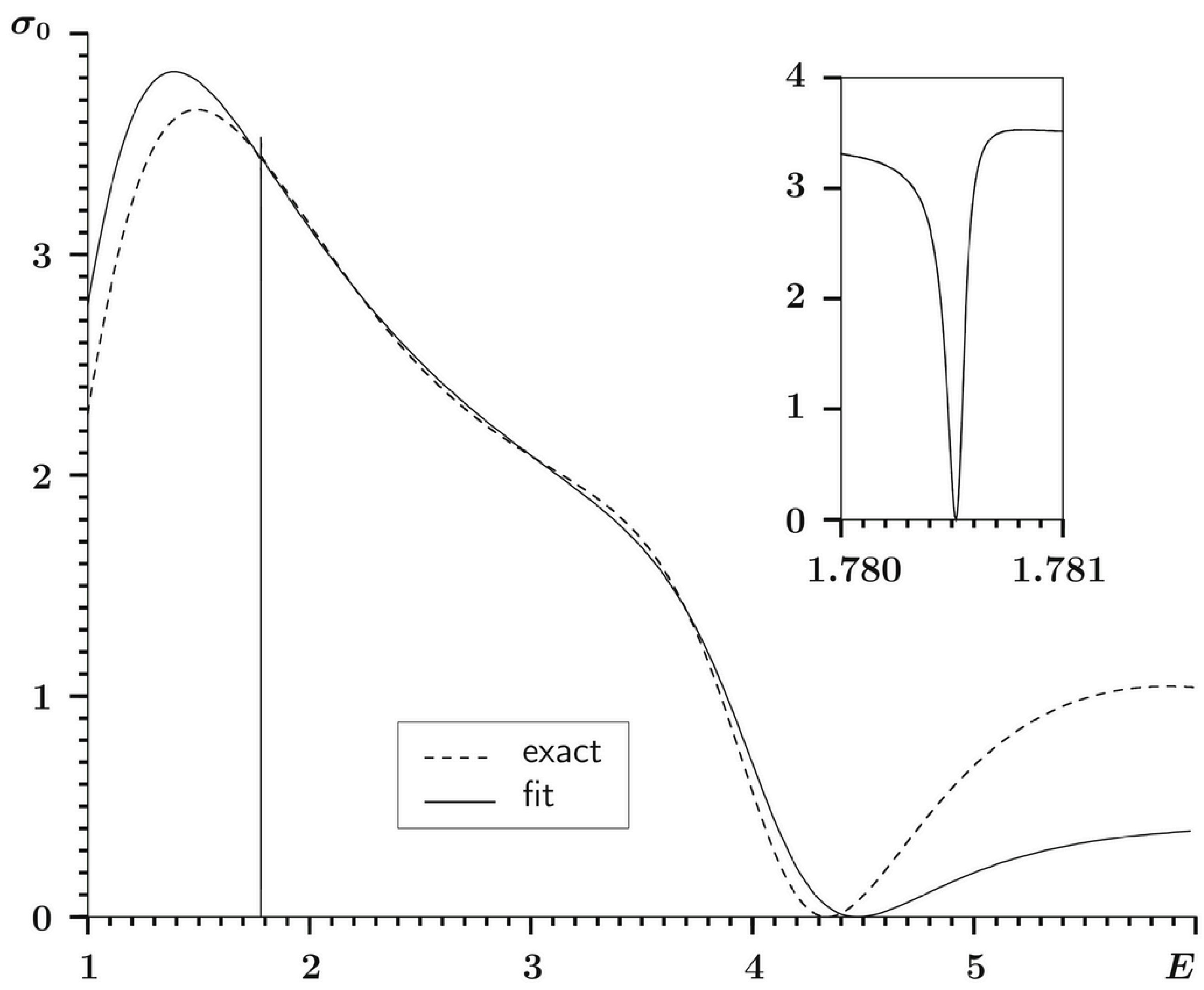
Total cross-section

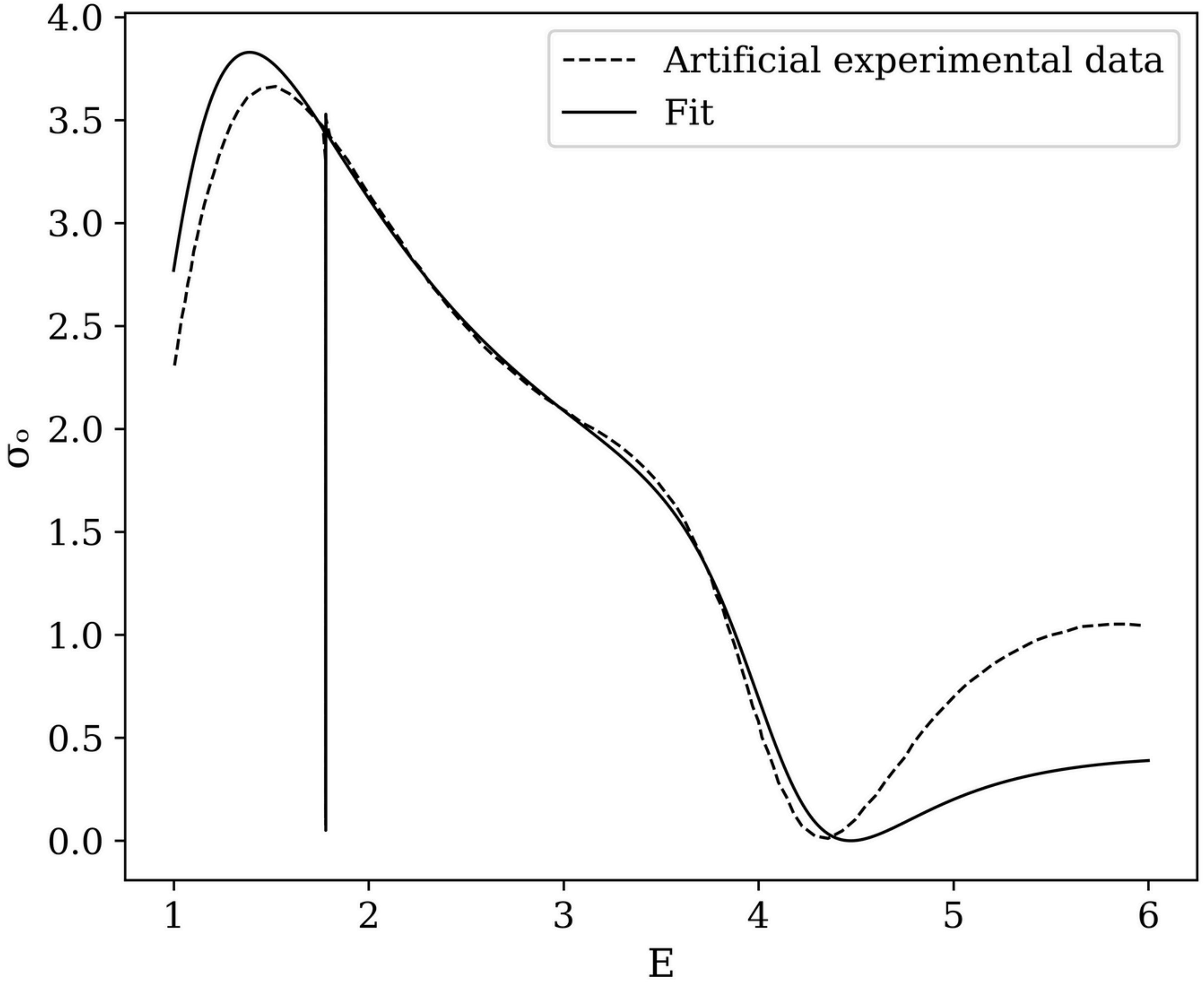




Results

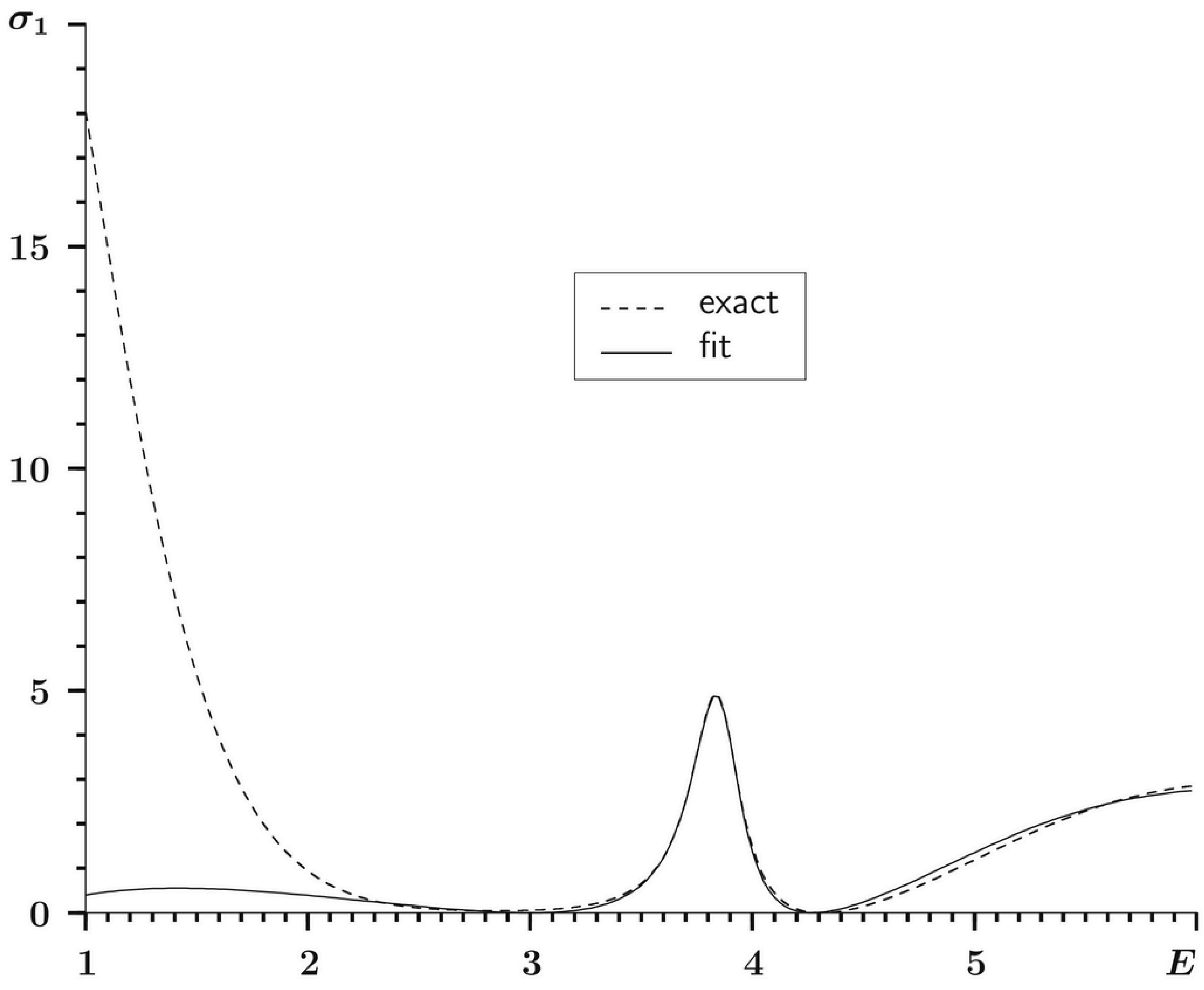
Partial cross-sections

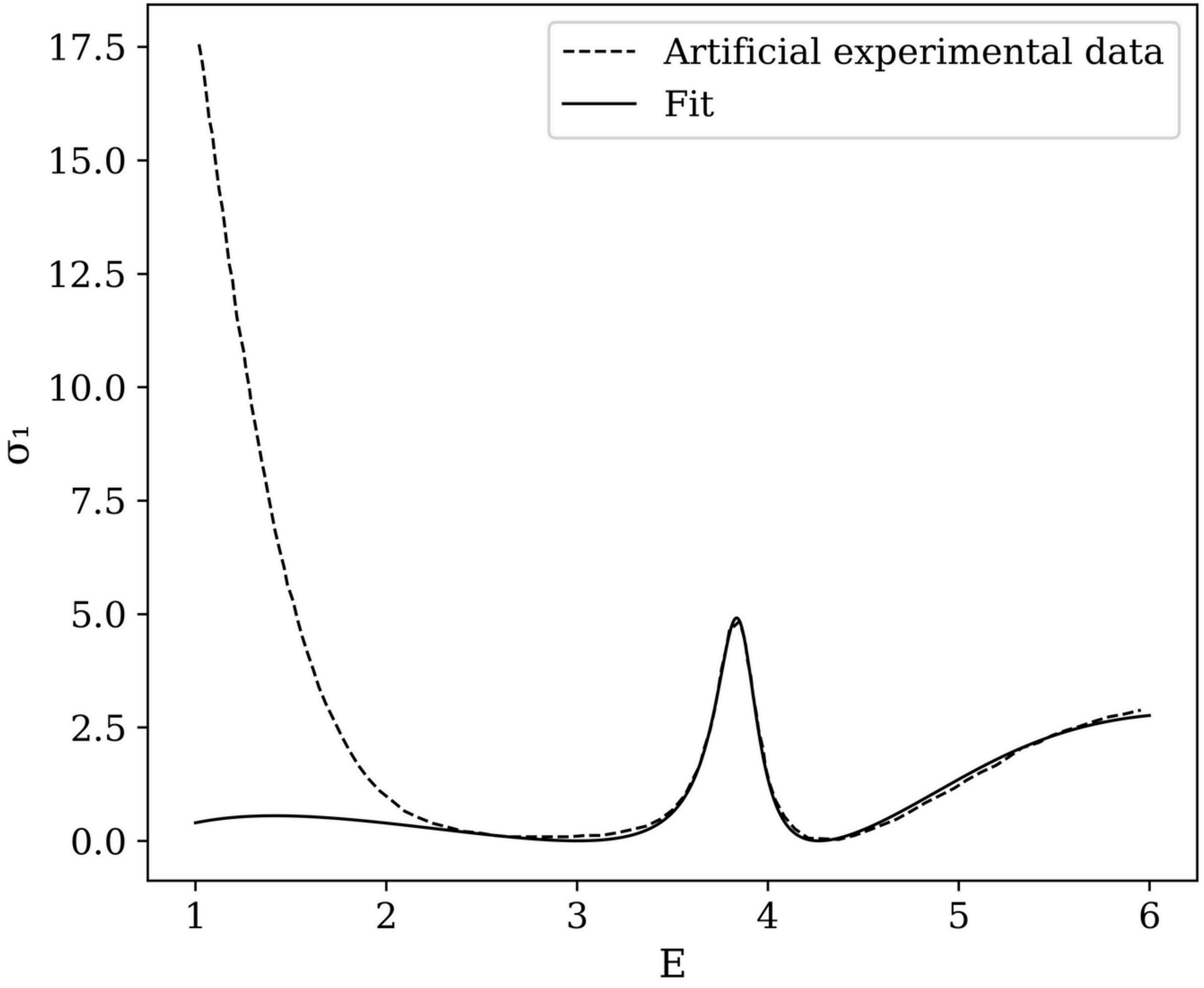




Results

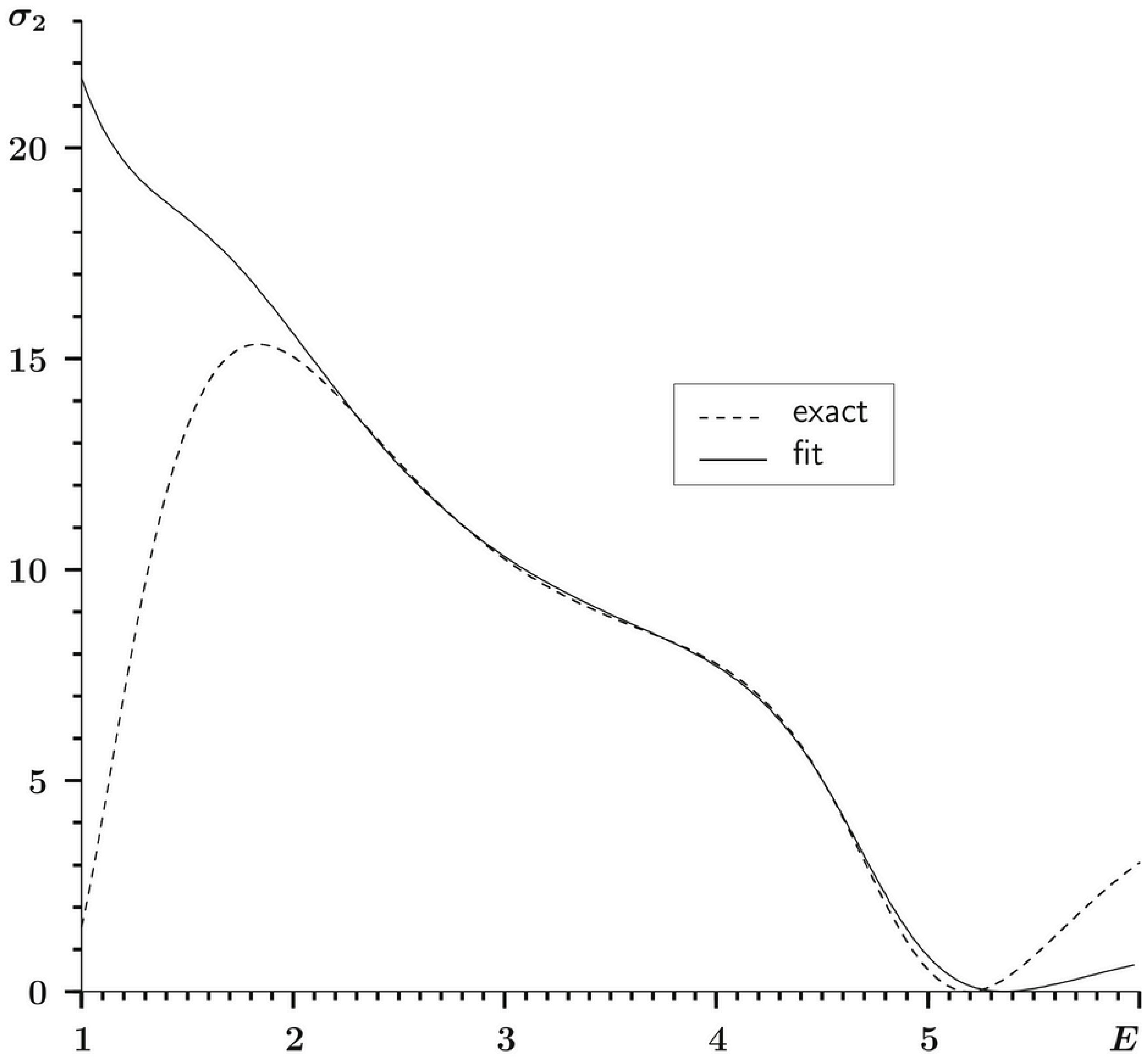
Partial cross-sections

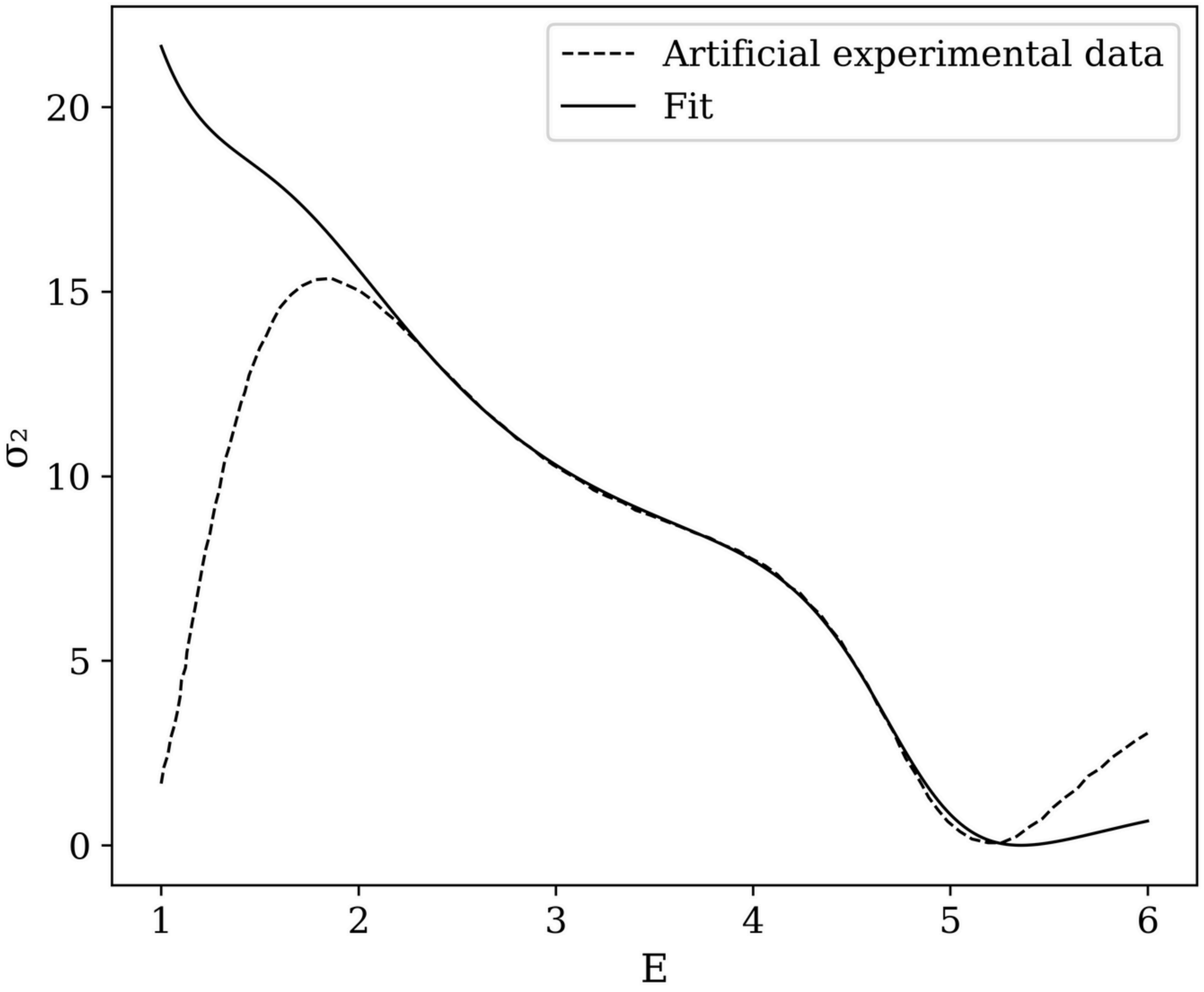




Results

Partial cross-sections





Results

Resonance parameters

ℓ	Exact		Paper fit		Our fit	
	E_r	Γ	E_r	Γ	E_r	Γ
0	1.7805	9.5719×10^{-5}	1.7805	9.6022×10^{-5}	1.7805	9.6022×10^{-5}
	4.1015	1.1563	4.1001	1.1265	4.0918	1.1242
1	3.8480	0.2754	3.8541	0.2724	3.8542	0.2736
2	4.9005	1.5675	4.8029	1.4238	4.7940	1.4365

Results

Resonance parameters

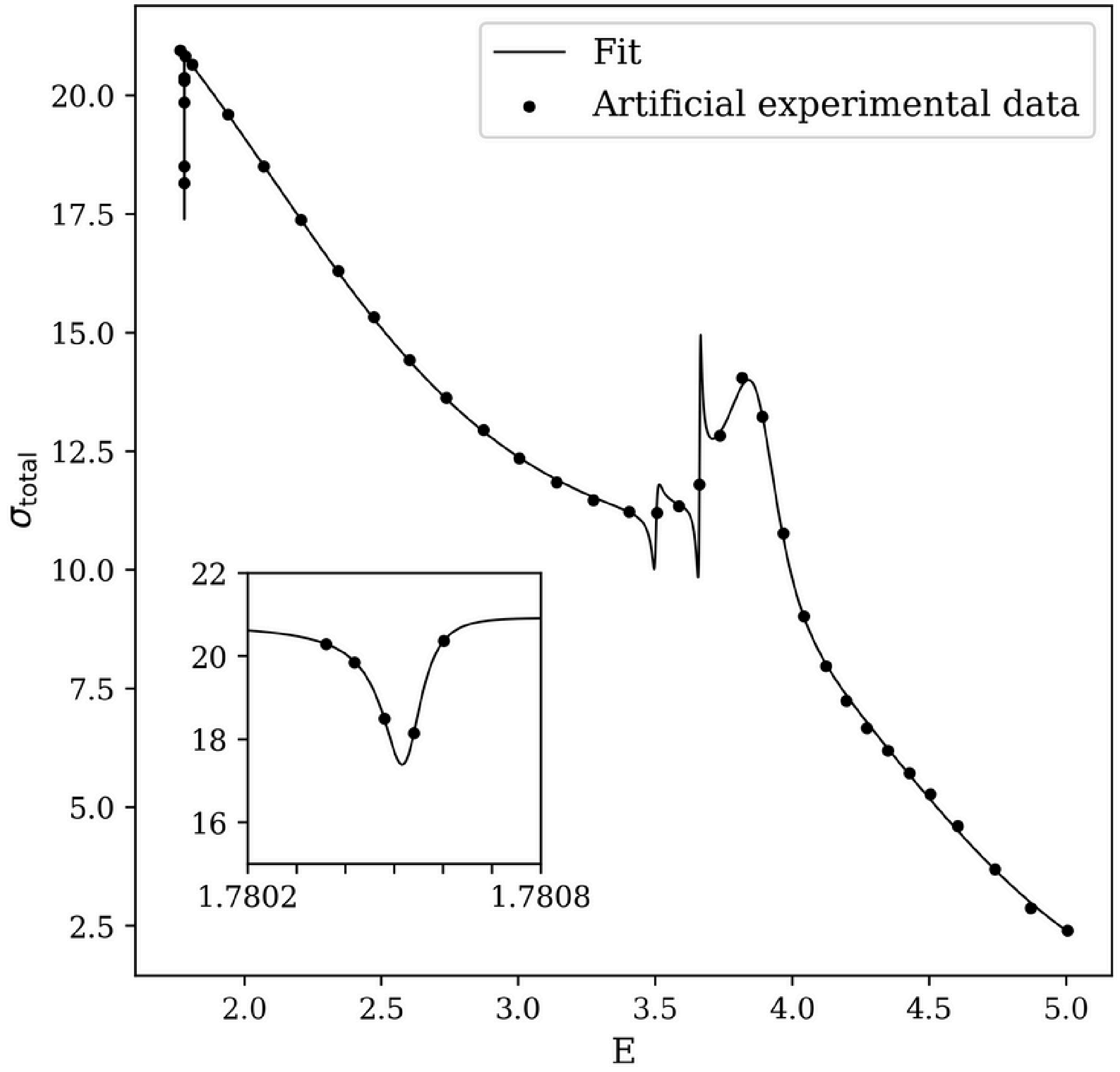
	Reported errors (%)			
	Paper fit		Our fit	
ℓ	E_r	Γ	E_r	Γ
0	6.5×10^{-6}	0.32	6.5×10^{-6}	0.32
	0.03	2.66	0.24	2.86
1	0.16	1.08	0.16	0.64
2	1.99	9.18	2.17	8.36

Conclusions

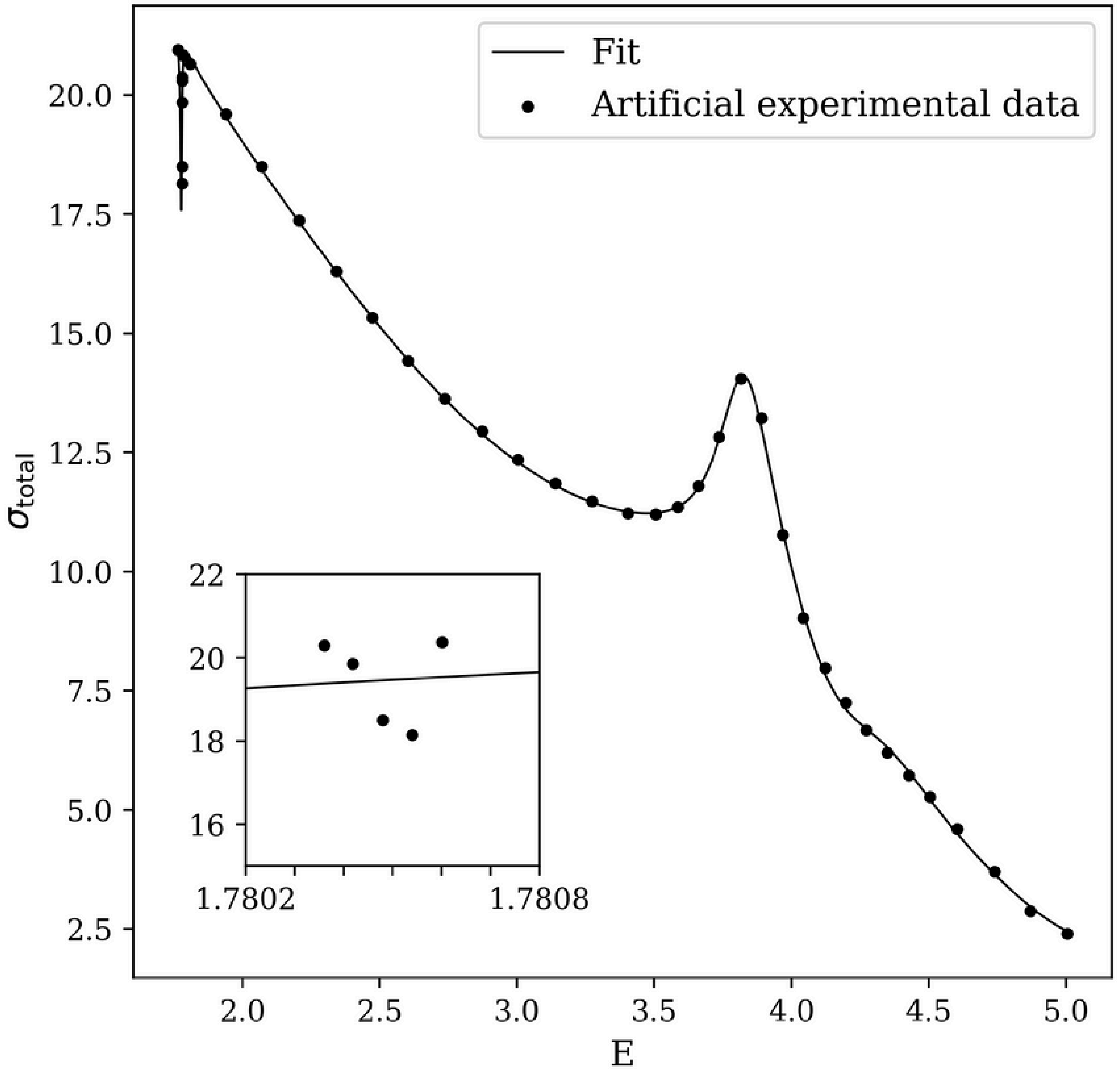
- We successfully reproduced the method described in the article, as well as the associated **fitting curves** and **resonance parameters**
  - MINUIT was actually pretty efficient at fitting many parameters
- The theoretical curve was not successfully reproduced, mainly due to **computational limitations** during the implementation
- The method has been shown to **outperform the original approaches**. However, its performance is still limited by the **high number of fitting parameters** and its **sensitivity** to specific parameter choices

Some interesting result

Changing β_{10} from 10 to 15



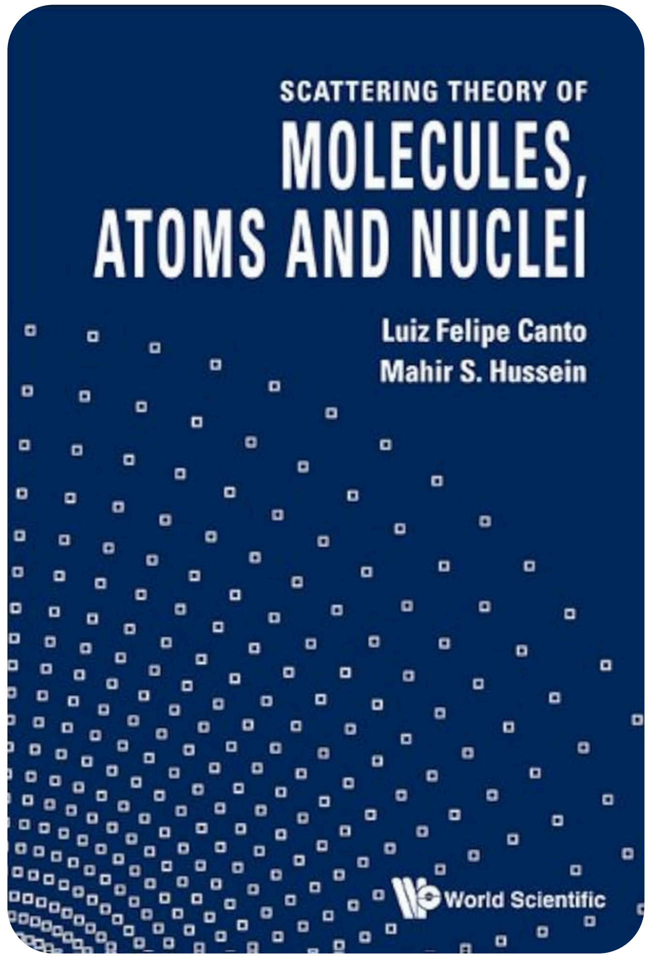
Changing E_{10} from 1.78 to 1.7



Undiscussed statements

The poles of the S-matrix contain the information about the resonance

Section 8.1.4



The S-matrix may fail to produce physical resonances when it is obtained from models based on polynomial sums

New Journal of Physics
The open access journal at the forefront of physics

PAPER • OPEN ACCESS

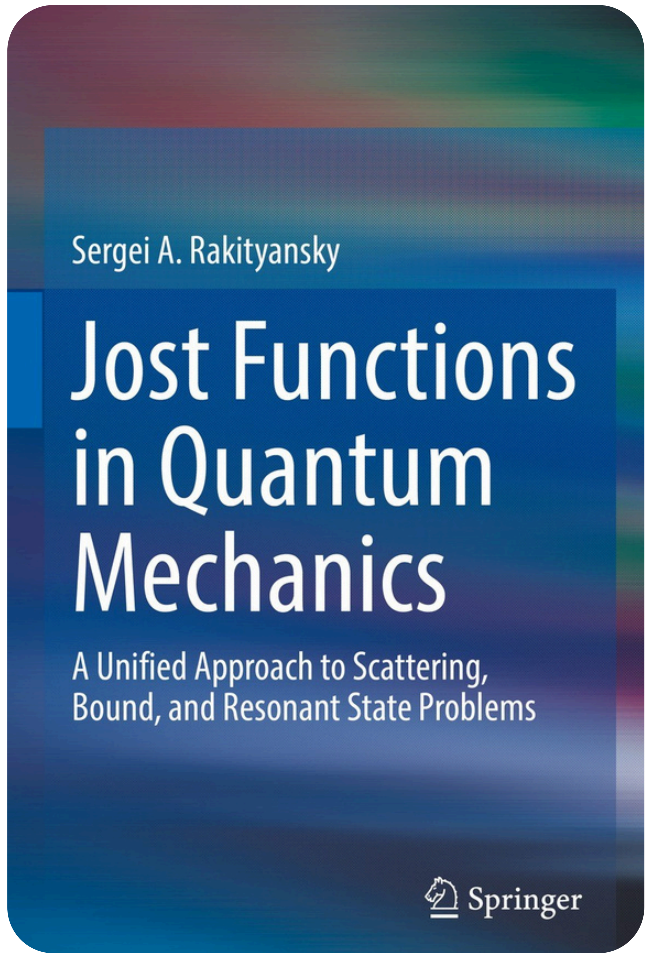
On beautiful analytic structure of the *S*-matrix

Alexander Moroz and Andrey E Miroshnichenko

Undiscussed statements

The S-matrix is the ratio of Jost functions

Section 4.6



The Jost functions can be expressed in terms of the R-matrix

The Jost function and Siegert pseudostates from R-matrix calculations at complex wavenumbers

P. Vaandrager, J. Dohet-Eraly and J-M. Sparenberg

Nuclear Physics and Quantum Physics, C.P. 229,
Université libre de Bruxelles (ULB), B 1050 Brussels, Belgium

June 22, 2023

Undiscussed statements

The boundary parameter can be set to zero

Section 3.4

IOP PUBLISHING REPORTS ON PROGRESS IN PHYSICS

Rep. Prog. Phys. **73** (2010) 036301 (44pp) doi:10.1088/0034-4885/73/3/036301

The *R*-matrix theory

P Descouvemont[1] and D Baye[1,2]

[1] Physique Nucléaire Théorique et Physique Mathématique, C.P. 229, Université Libre de Bruxelles (ULB), B 1050 Brussels, Belgium
[2] Physique Quantique, C.P. 165/82, Université Libre de Bruxelles (ULB), B 1050 Brussels, Belgium

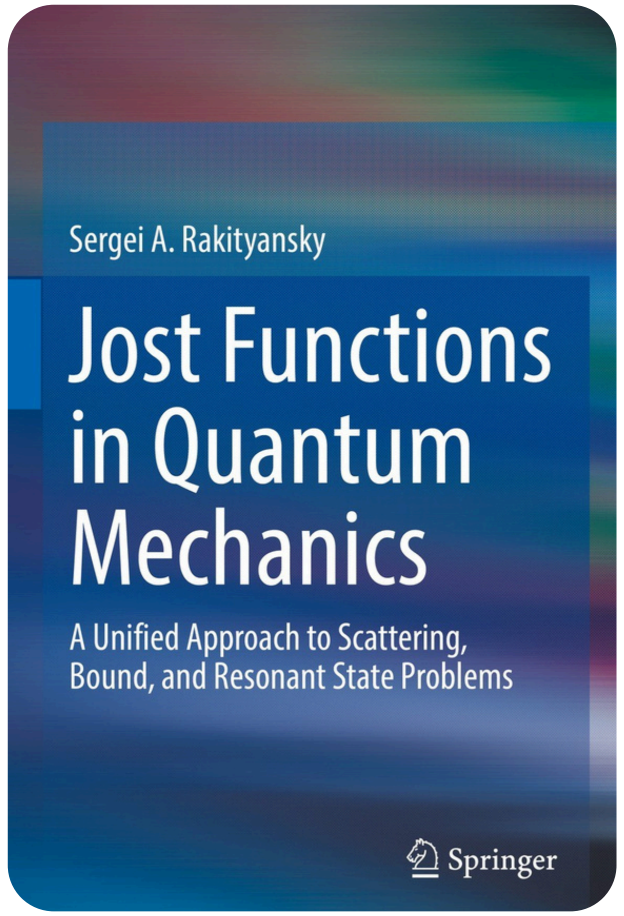
Final comment

Poles of the S-matrix related to resonance parameters

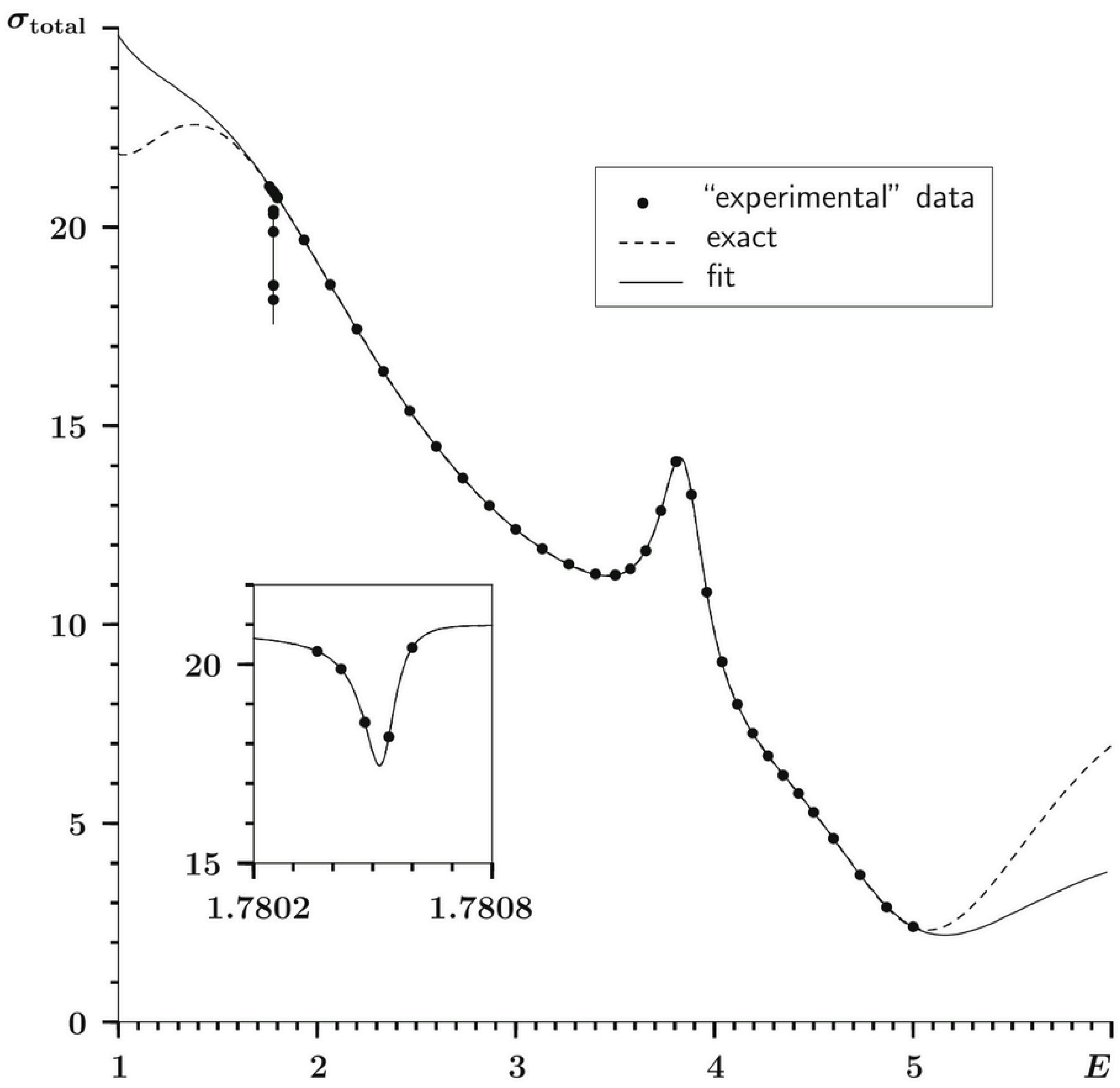
↓

Complex calculus basis

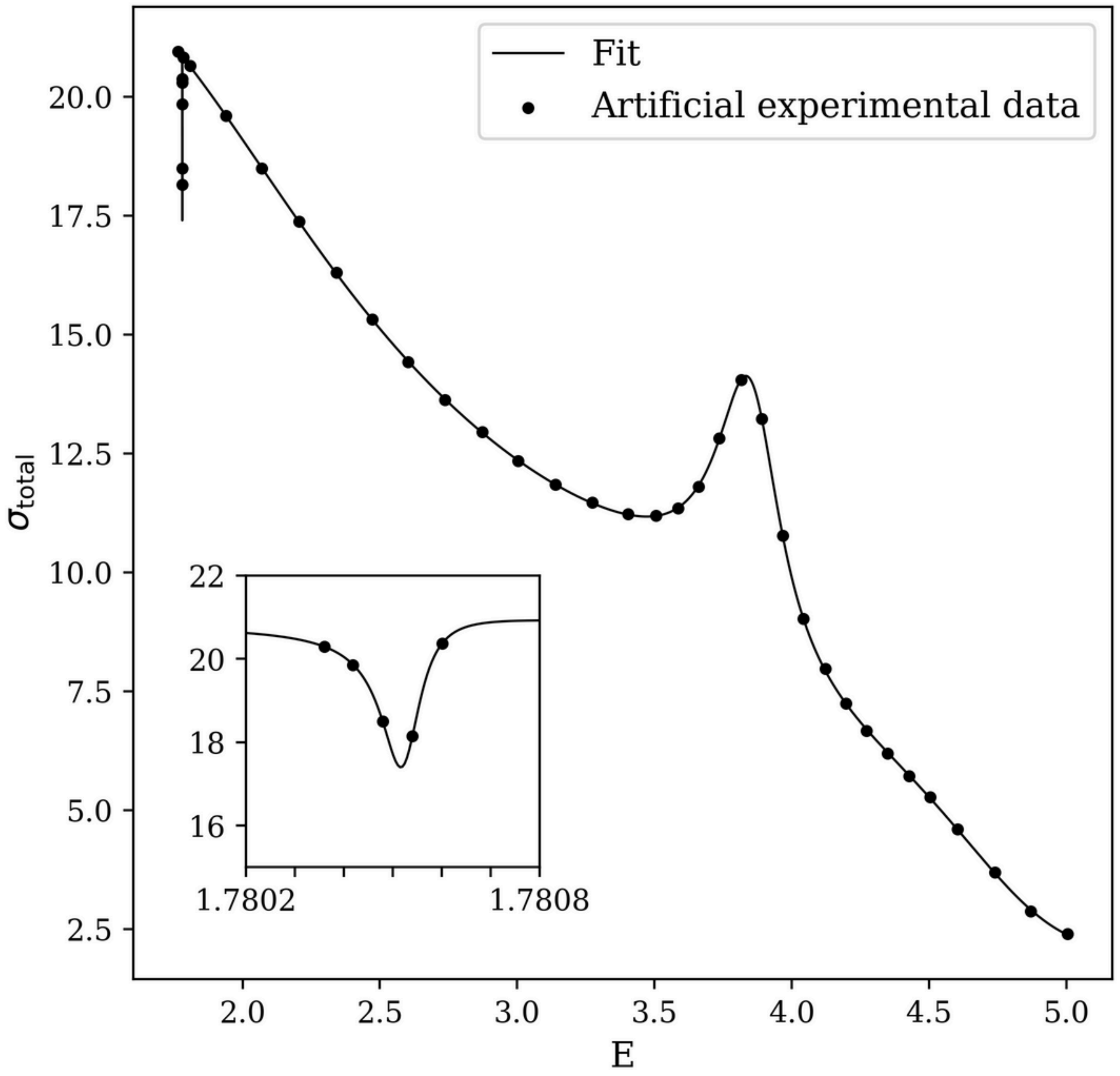
Chapter 4



Thank you!



$\sigma_{\rm total}$
"experimental" data
exact
fit
E



Fit
Artificial experimental data
$\sigma_{\rm total}$
E