preamble

Parametrization of the S-matrix as a way for locating bound and resonance states: multichannel case

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Outline

- Introduction
- Calculational methods
- Results
- Conclusions

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- Proper understanding of the properties of a quantum system is essential
- Prediction of the behaviour of such a system cannot be achieved without knowing its spectrum i.e. the energies of its bound, virtual, resonances and scattering states
- Different methods exist for locating these spectra points

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- Different methods exist for locating these spectra points

- We propose a universal method that is insensitive to the interaction potential.

The main idea behind this method is based on the coincidence principle:

Two analytic functions coinciding on a curve segment are identical everywhere in the complex plane

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- Given the complex-valued matrices $\mathbf{S}_\ell(E) \;\; \forall \; E \in [0, \infty)$

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- Such behaviour is provided by the matrix Padé approximant of order [N, N]

$$\tilde{\mathbf{S}}_\ell(E) = \mathbf{P}(E)[\mathbf{Q}(E)]^{-1} = \frac{\sum_{n=0}^{N} \mathbf{p}_n E^n}{\sum_{n=0}^{N} \mathbf{q}_n E^n} \qquad (1)$$

Fitting parameters

The exact S-matrix is given by

$$\mathbf{S}_\ell(E) = \mathbf{F}_\ell^{(\mathsf{out})}(E)[\mathbf{F}_\ell^{(\mathsf{in})}(E)]^{-1} \tag{2}$$

where $\mathbf{F}_\ell^{(\mathsf{in/out})}(E)$ are the Jost matrices. They are the amplitudes of the incoming and outgoing waves in the radial wavefunction,

$$\mathbf{\Phi}(E,r) = \mathbf{H}^{(\mathsf{in})}(E,r)\mathbf{F}^{(\mathsf{in})}(E) + \mathbf{H}^{(\mathsf{out})}(E,r)\mathbf{F}^{(\mathsf{out})}(E)$$
or
$$\mathbf{\Phi}(E,r) = \mathbf{J}(E,r)\mathbf{A}(E,r) - \mathbf{N}(E,r)\mathbf{B}(E,r)$$

$$F_{mn}^{(\mathsf{in})}(E,k_1,k_2,\dots) = \frac{1}{2}\left[\frac{k_n^{\ell_n+1}}{k_m^{\ell_m+1}}\,\widetilde{A}_{mn}(E) - i\,k_m^{\ell_m}\,k_n^{\ell_n+1}\,\widetilde{B}_{mn}(E)\right] \tag{3}$$

and by symmetry

$$F_{mn}^{(\mathsf{out})}(E,k_1,k_2,\dots) = (-1)^{\ell_m+\ell_n}\,F_{mn}^{(\mathsf{in})}(E,k_1,k_2,\dots) \tag{4}$$

$$k_n = \sqrt{\frac{2\mu_n}{\hbar^2}(E - E_n^{\mathsf{th}})} \tag{5}$$

Pade approximation

$$\widetilde{\mathbf{A}}(E) \approx \sum_{n=0}^{N} \boldsymbol{\alpha}^{(n)} E^n, \qquad \widetilde{\mathbf{B}}(E) \approx \sum_{n=0}^{N} \boldsymbol{\beta}^{(n)} E^n \tag{6}$$

We have to determine $2(N+1)$ unknown matrices $\boldsymbol{\alpha}^{(i)}$ and $\boldsymbol{\beta}^{(i)}$, $i = 0, 1, 2, \ldots, N$.
Suppose that the S-matrix is known at $2(N+1)$ points along the real energy axis: $E_1, E_2, \ldots, E_{2(N+1)}$. Then the unknown matrices $\boldsymbol{\alpha}^{(i)}, \boldsymbol{\beta}^{(i)}$ can be found from the system of equations

$$\mathbf{S}(E_i) = \mathbf{F}^{(\text{out})} \left[\mathbf{F}^{(\text{in})}\right]^{-1}, \qquad i = 1, 2, \ldots, 2(N+1) \tag{7}$$

Multiplying by $\mathbf{F}^{(\text{in})}$ from the right, we can re-write this as

$$\mathbf{F}^{(\text{out})}(k_1, k_2, E_i) = \mathbf{S}(E_i)\, \mathbf{F}^{(\text{in})}(k_1, k_2, E_i) \tag{8}$$

Substituting all the above formulae, we find that this is a linear system of equations for $\alpha_{mn}^{(i)}$ and $\beta_{mn}^{(i)}$.

Poles determination

The two procedures are:

- We determine the fitting paramaters $\alpha^{(i)}$ and $\beta^{(i)}$ by solving equation (8)
- We search for the roots of equation (3) in the complex energy plane for the positions of the spectral points

Result: Exactly solvable model potential

$$\mathbf{V}(r) = \begin{cases} \mathbf{U} & \text{for } 0 \leq r \leq 1 \\ \mathbf{0} & \text{otherwise} \end{cases} \qquad (9)$$

$$\mathbf{U} = -\begin{pmatrix} 2.0 & 0.5\lambda \\ 0.5\lambda & 2.0 \end{pmatrix}$$

where λ is the switching parameter.
The channel thresholds are $E_1 = 0$ and $E_2 = 2$

The units in this model are chosen in such a way that $\mu_1 = \mu_2 = \hbar c = 1$.

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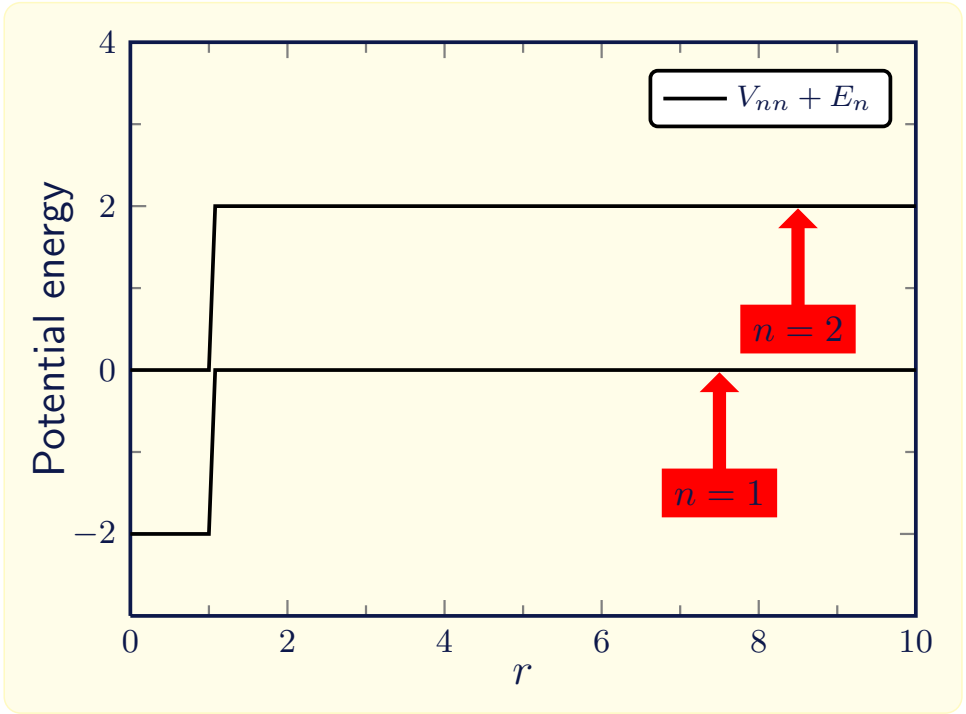

Figure 1. Square-well diagonal channel potentials of (9). The potentials are shifted by the threshold energies E_n.

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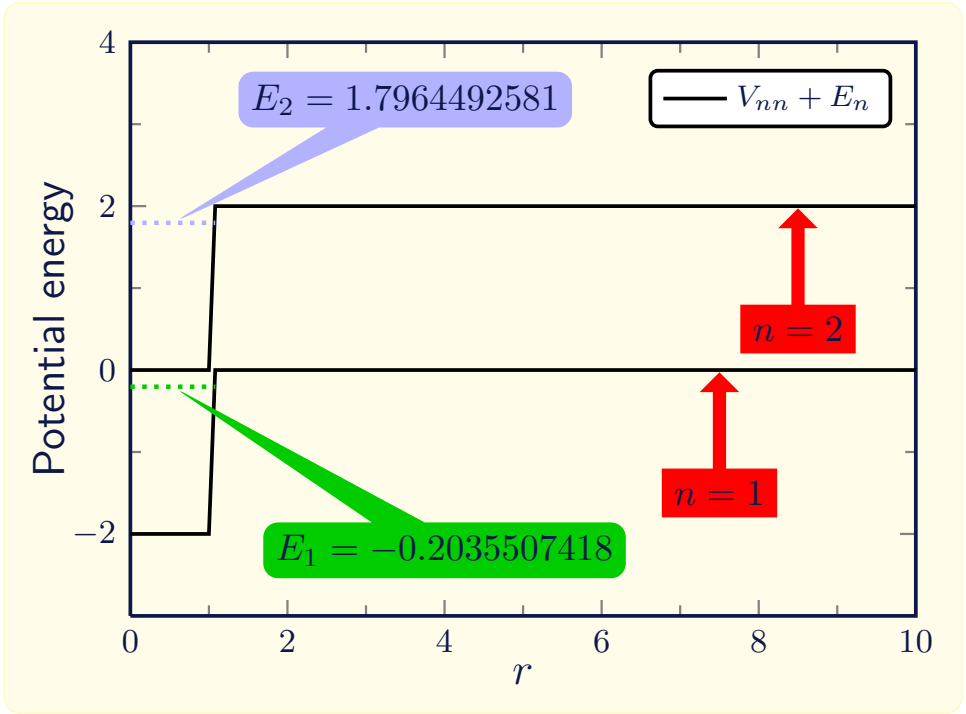

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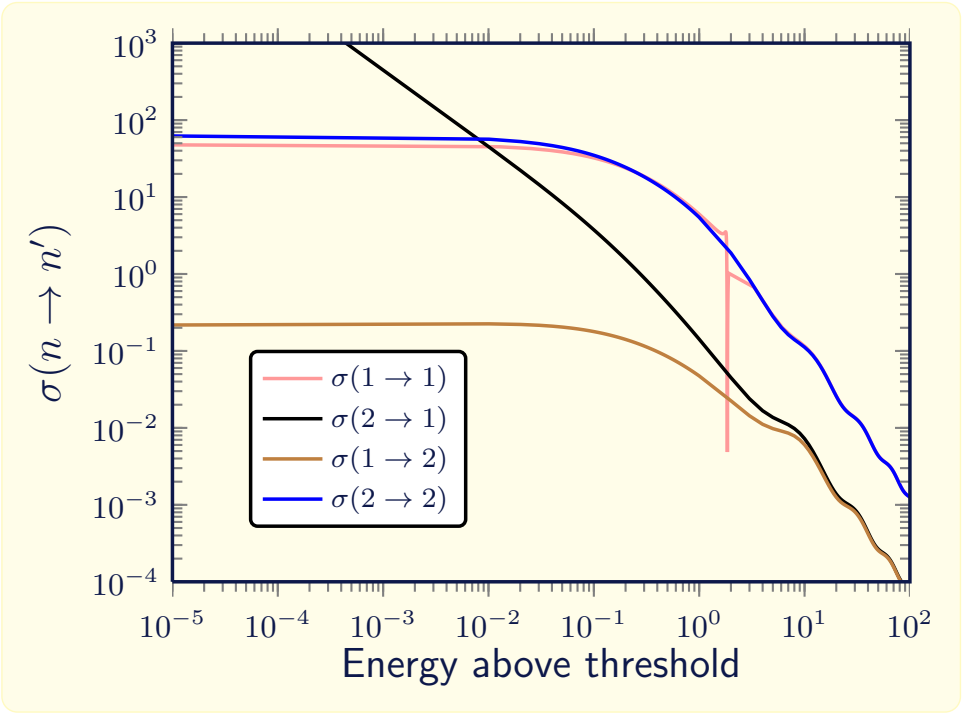

Figure 1. Exact cross sections. Horizontal axis corresponds to E in the case of $1 \to 1$ transitions and to $E - E_2$ in all other cases.

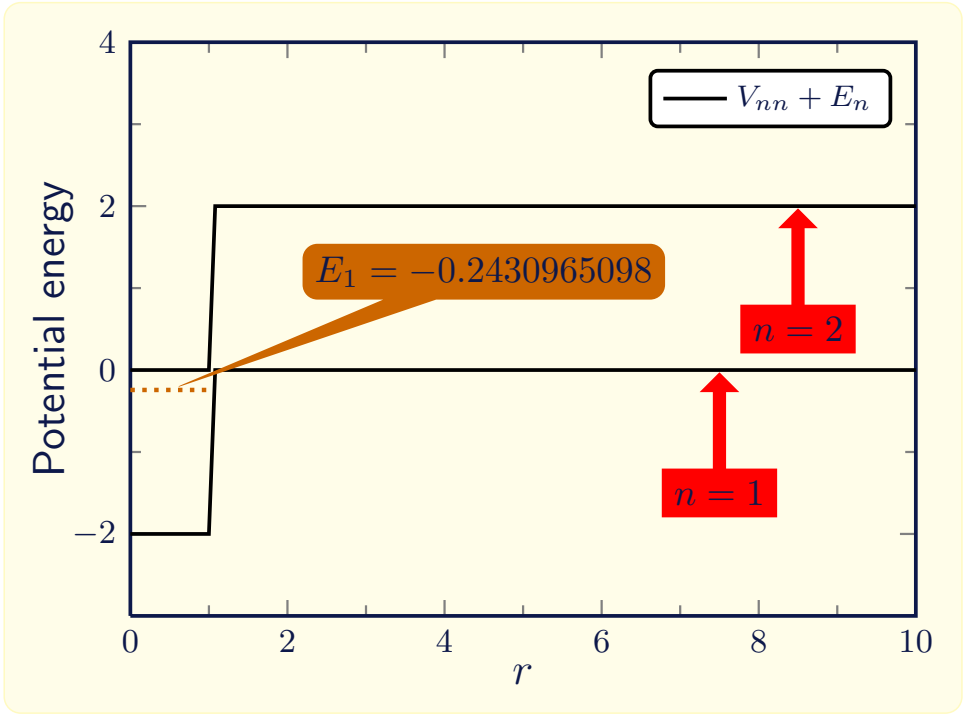

Figure 2. Square-well diagonal channel potentials of (9). The potentials are shifted by the threshold energies E_n.

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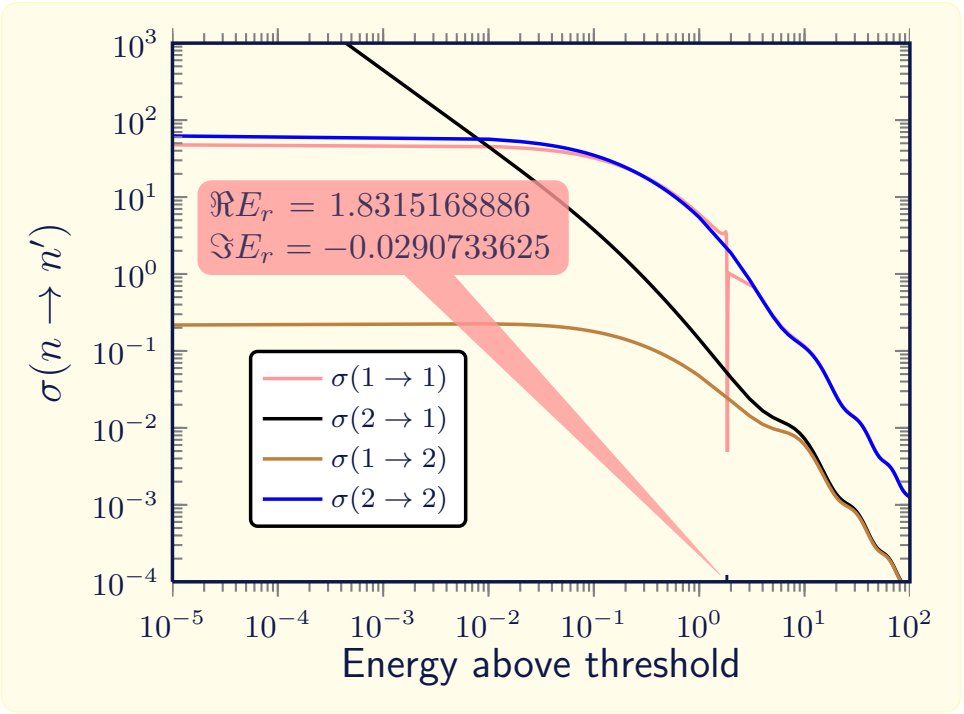

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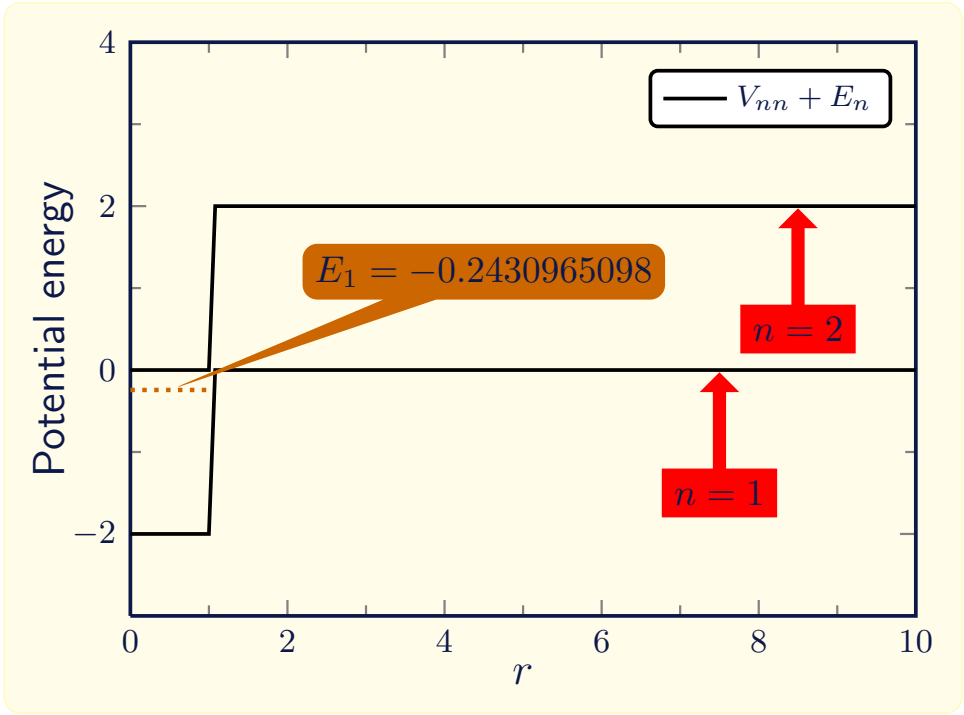

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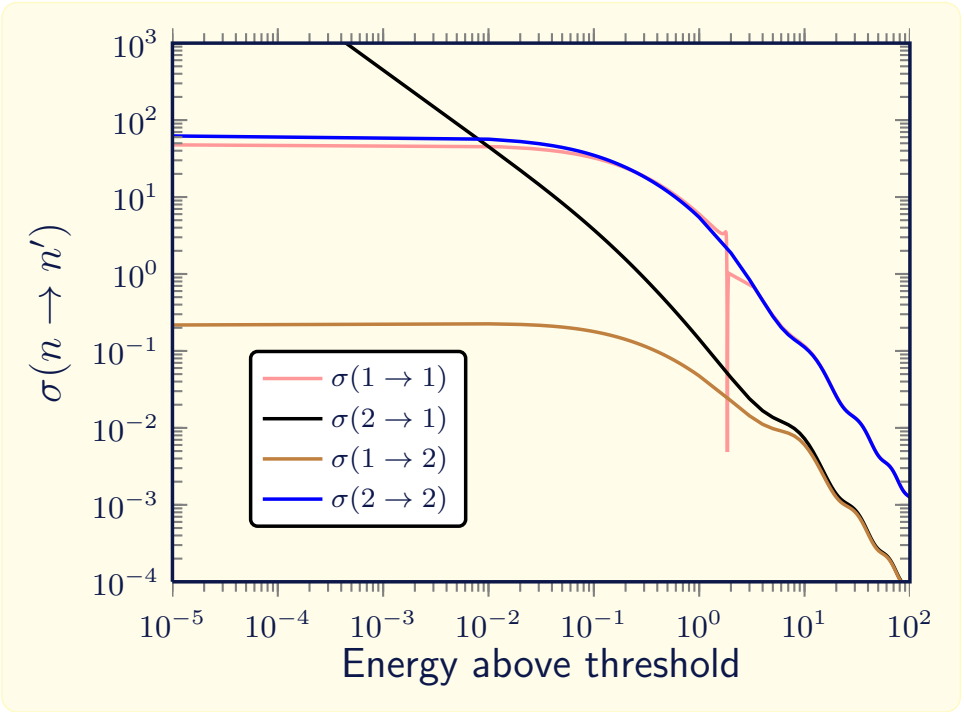

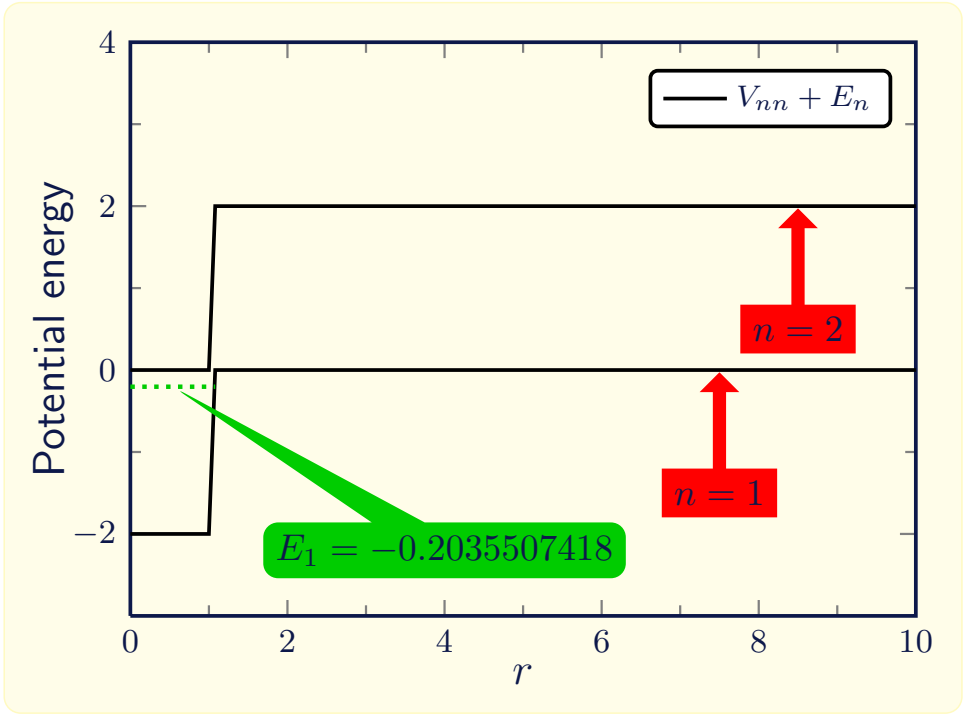

Table 1. Computed poles of the approximate function $\tilde{\mathbf{S}}(E)$ for the potential (9) with N fitting points evenly distributed over the interval $1\ \mathrm{MeV} \leqslant E \leqslant 10\ \mathrm{MeV}$.

ID	N	$\Re(E)$	$\Im(E)$		
$\lambda = 0$	2	0.9346579288	-0.2046585820	1.2144390251	6.71×10^{-16}
	5	-0.2020229243	-1.24×10^{-12}	1.7964492680	3.03×10^{-15}
	7	-0.2035497226	-1.46×10^{-11}	1.7964492581	-2.12×10^{-14}
	10	**-0.2035506639**	1.54×10^{-10}	**1.7964492581**	4.54×10^{-13}

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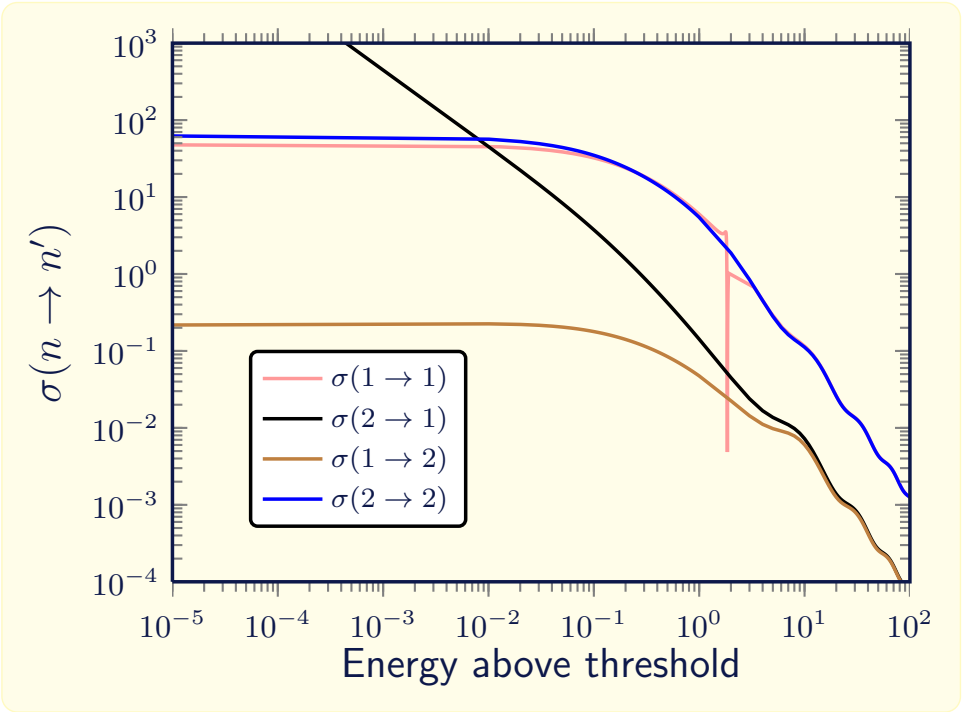

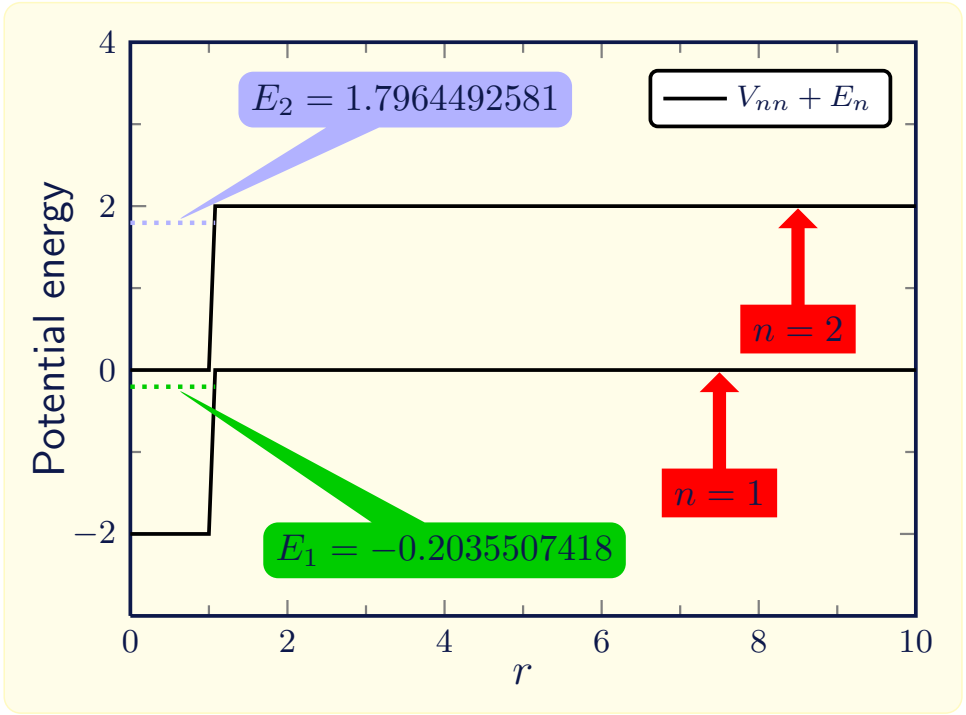

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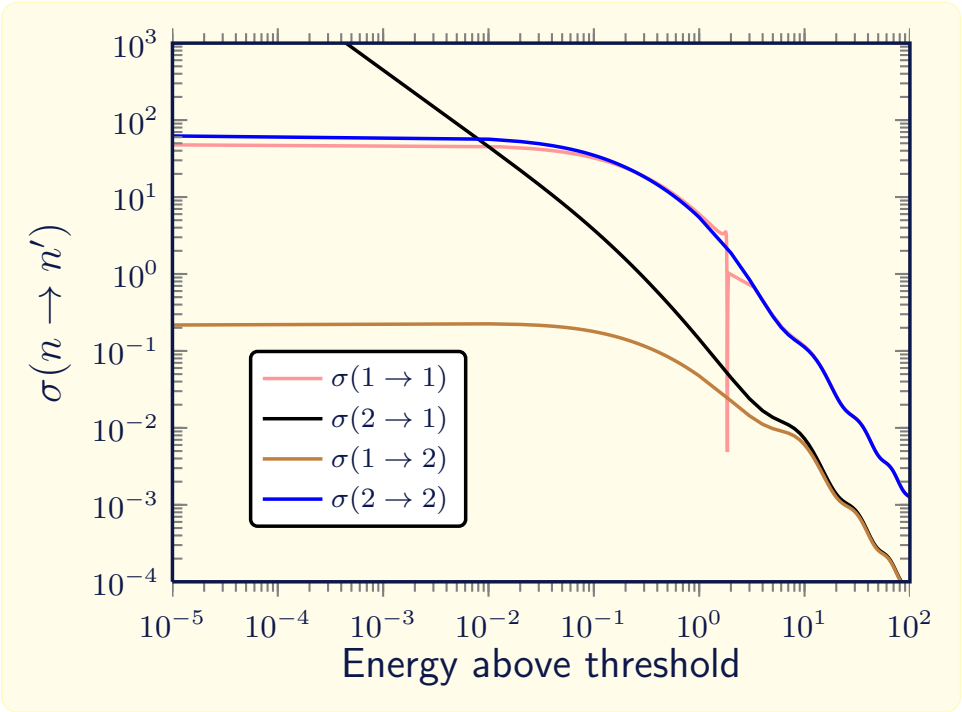

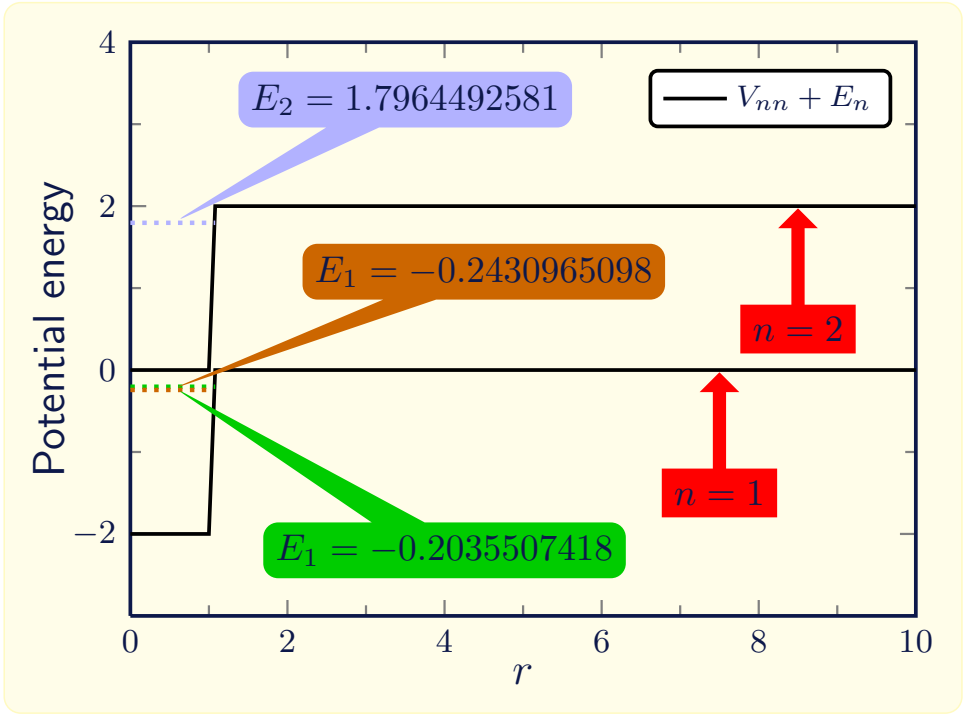

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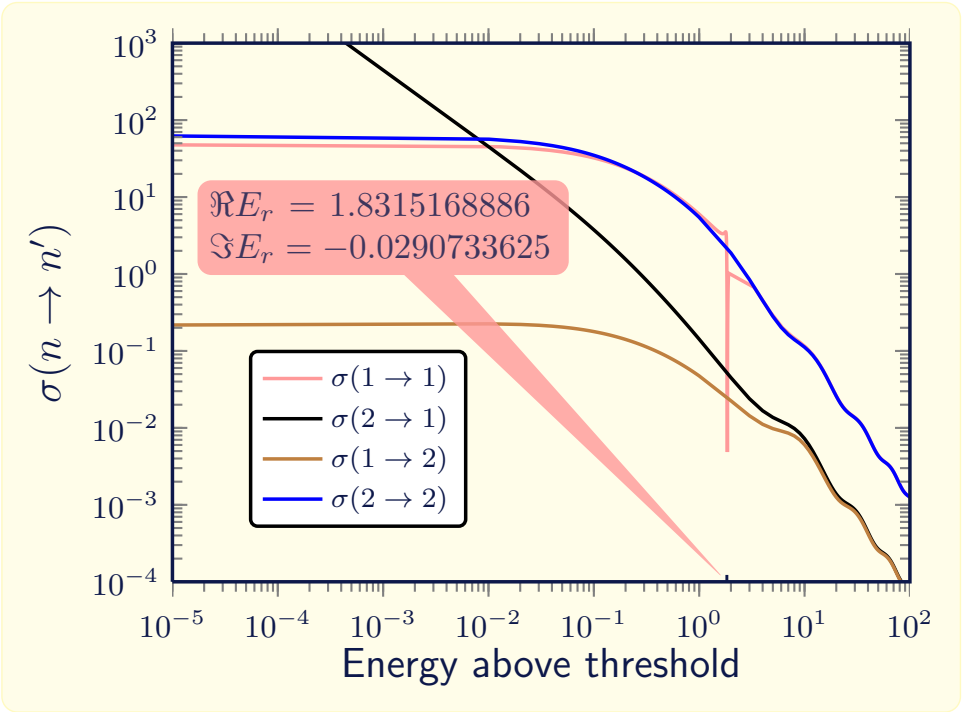

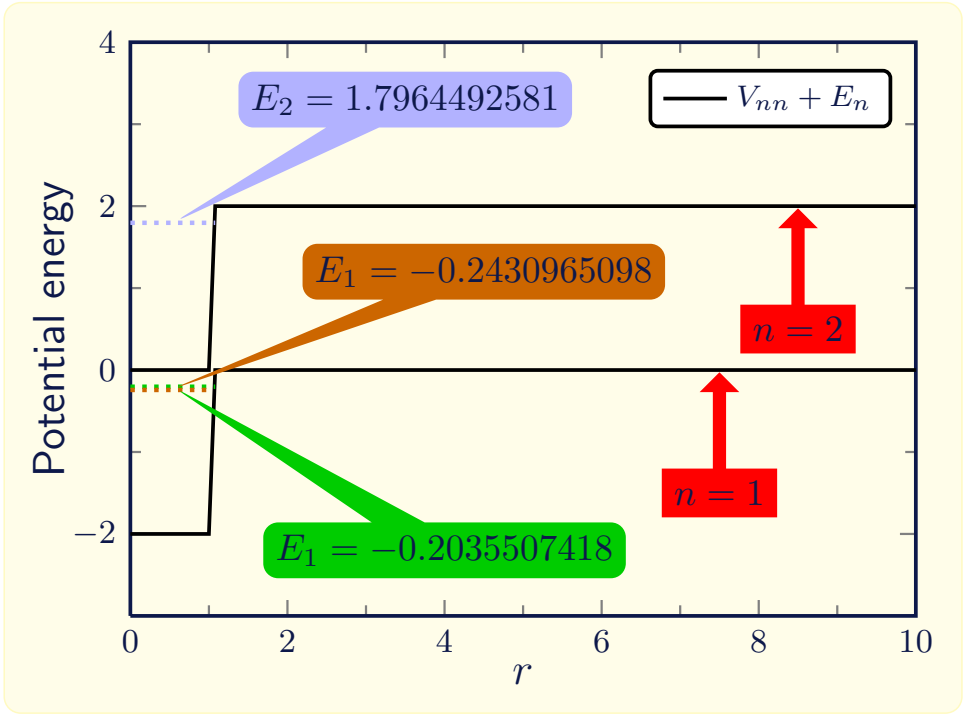

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Result: Noro–Taylor model potential

$$\mathbf{V}(r) = \begin{pmatrix} -1.0 & -7.5 \\ -7.5 & 7.5 \end{pmatrix} r^2\, e^{-r} \qquad (9)$$

The thresholds energies are $E_1 = 0$ and $E_2 = 0.1$

The units in this model are chosen in such a way that $\mu_1 = \mu_2 = \hbar c = 1$.

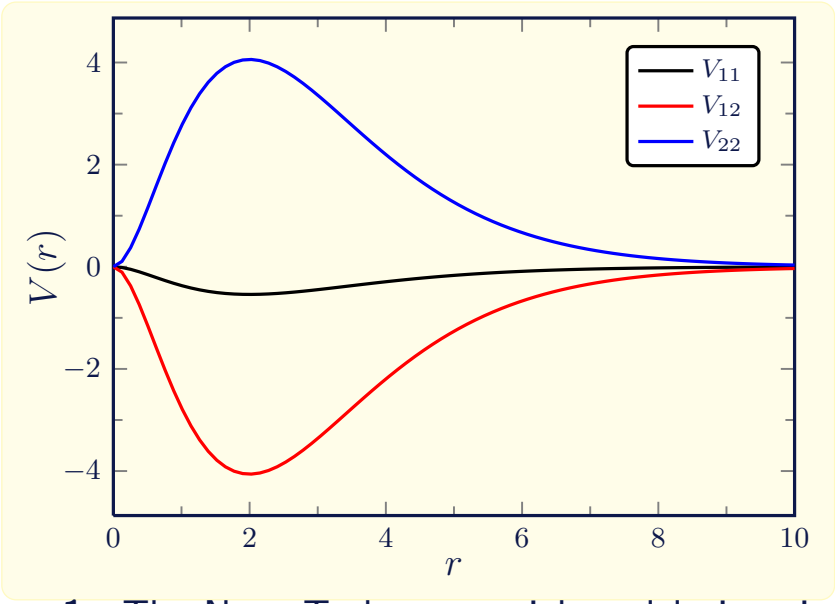

Figure 1. The Noro–Taylor potential model given in Equation (9).

[T. Noro and H. S. Taylor 1980 J. Phys. B: Atom. Molec. Phys., **13** L377]

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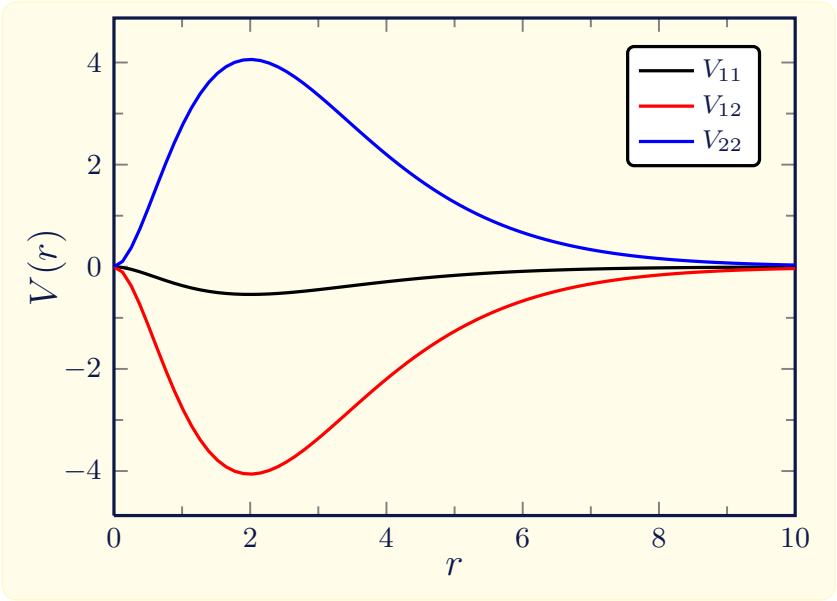

Table 2. The resonance energies obtained for the Noro–Taylor potential (9) for $\ell = 0, 1$. They were obtained using the rigorous Jost-function method described in Rakitianski and Elander.

	$\ell = 0$		$\ell = 1$	
no.	$\Re E$	$\Im E$	$\Re E$	$\Im E$
1	4.768197	−0.000710	6.703719	−0.125653
2	7.241200	−0.755956	8.012942	−1.920165
3	8.171217	−3.254166	8.595336	−4.718772
4	8.440526	−6.281492	8.511458	−7.887032
5	8.072643	−9.572815	7.824340	−11.256937
6	7.123813	−13.012669	6.584809	−14.741148

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Table 3. Comparison of the first five resonance points for the potential (9) for $\ell = 0, 1$.

ℓ	no.		$\Re E$	$\Im E$
0	1	Exact	4.768197	-0.000710
		Approx.	4.768197	-0.000710
	2	Exact	7.241200	-0.755956
		Approx.	7.241200	-0.755956
	3	Exact	8.171217	-3.254166
		Approx.	8.171199	-3.254177
	4	Exact	8.440526	-6.281492
		Approx.	8.431643	-6.261440
	5	Exact	8.072643	-9.572815
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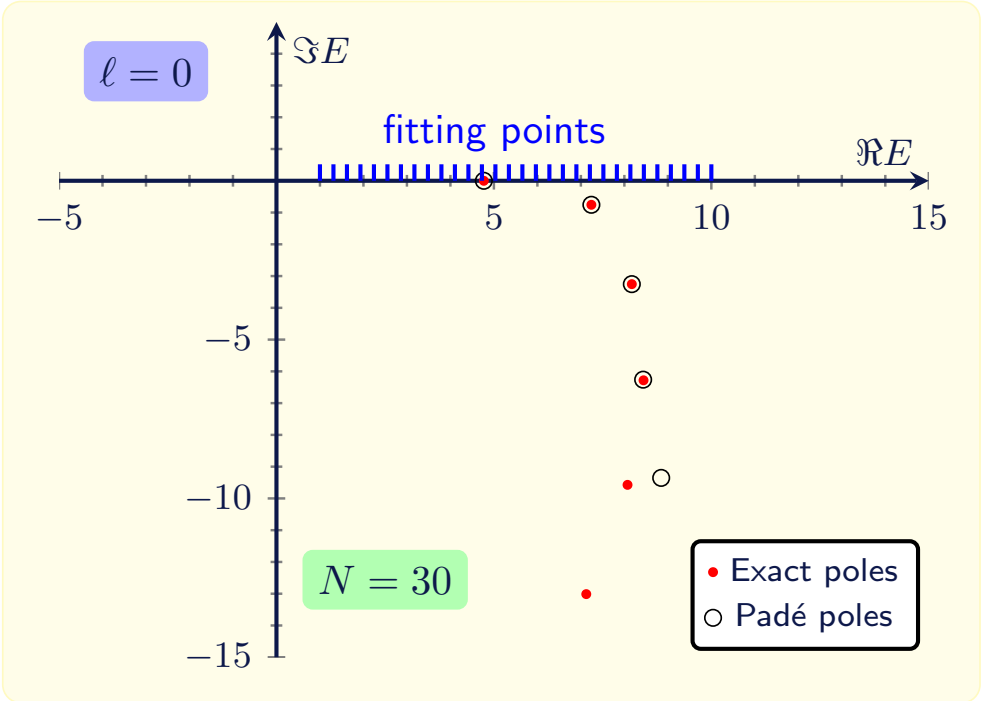

Figure 1. The exact positions of the S-wave resonance poles (red dots) on the complex energy plane for the potential (9), and the corresponding poles of the Padé approximation (open circles). The corresponding fitting points on the $\Re E$-axis are indicated by vertical bars.

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		Approx.	8.596118	−4.720121
	4	Exact	8.511458	−7.887032
		Approx.	8.383264	−7.5417706
	5	Exact	7.824340	−11.256937
		Approx.	6.925101	−15.401273

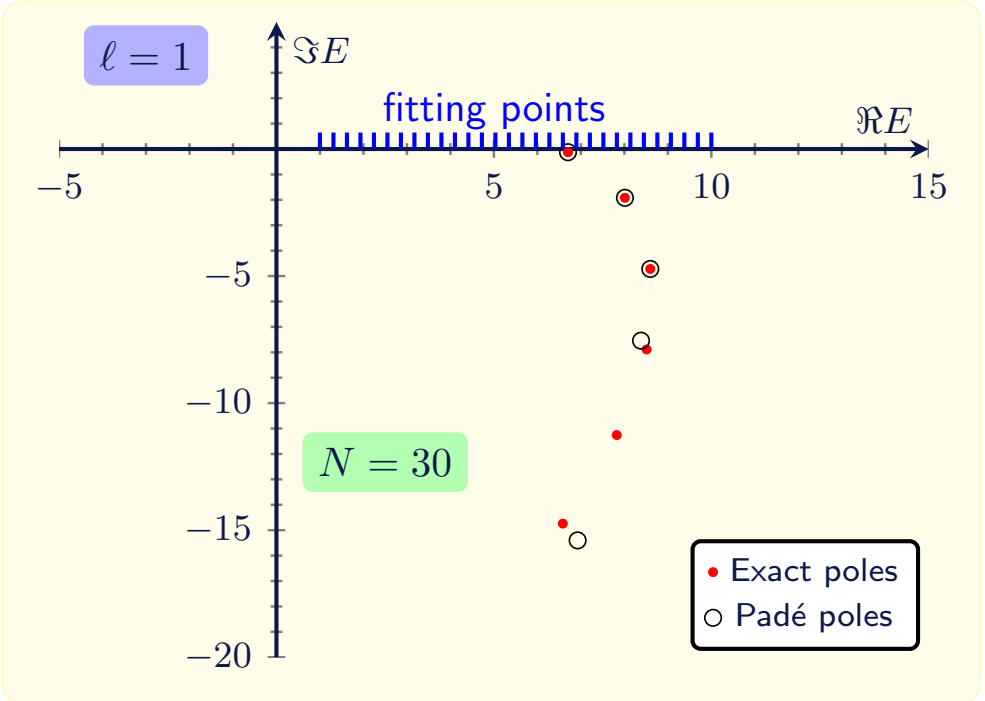

Figure 1. The exact positions of the P-wave resonance poles (red dots) on the complex energy plane for the potential (9), and the corresponding poles of the Padé approximation (open circles). The corresponding fitting points on the $\Re E$-axis are indicated by vertical bars.

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Conclusions

- The known value of the S-matrix has been analytically continued to the domains of complex energy
- The poles of the S-matrix corresponding to the spectral points have been successfully located
- The numerical examples show that the proposed method is stable and accurate
- The universality of the method has been confirmed

ONLOOK

- **Extend the method to include potentials with coulomb tail**
- **Combined with any phase-shift analysis procedure, the method would be able to do spectral analysis of the experimental cross-section data**

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