Determining resonances and other relevant scattering parameters from experimental cross-sections for non-relativistic two-body Coulomb scattering.

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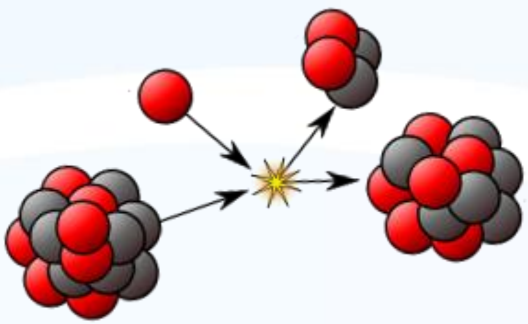
Outline of Presentation:

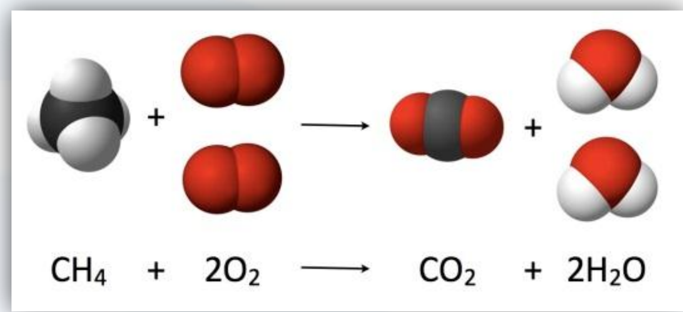
1. Resonances in quantum mechanics
   - Definition, intuitive understanding, importance
2. Resonances from Scattering data
   - Difficulty in determining parameters, methods
3. Jost matrices
   - Definition, properties
4. Jost functions for a given potential
   - Calculating from Schrodinger's equation
5. Semi-Analytic Jost matrices
   - Factorising branching dependence

6. Fitting Parameters
    - Construction of *S*-matrix (cross sections) from fitting parameters
7. Model potential
    - Description, “noise”, resonances, results from fitting, prediction, resonances from fitting
8. New study: $^{12}C + \alpha$ scattering :
    - Fitting of data, S-matrix residues & ANC values, preliminary results
9. Conclusion & Summary:
    - Discussion, future work

1. Resonances in Quantum Mechanics

- Resonances are **complex energy poles**, E_n, of the **Scattering matrix**.





$$|\psi_{out}\rangle = S|\psi_{in}\rangle$$

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

$$\sigma_{mn}(E) = \frac{\pi}{k_m^2}(2\ell_m + 1)\,|S_{nm}(E) - \delta_{mn}|^2$$

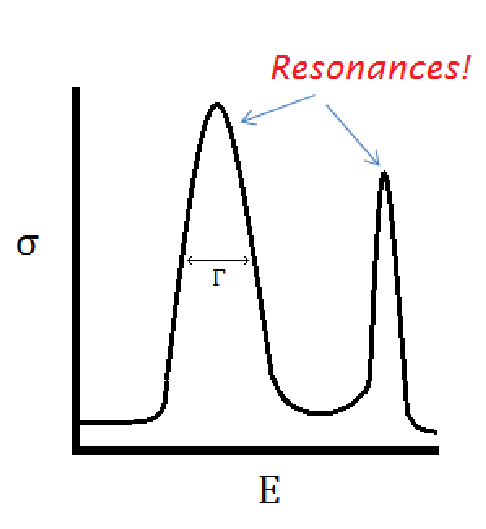
$$T_{1/2} = \frac{\hbar \ln 2}{\Gamma}$$

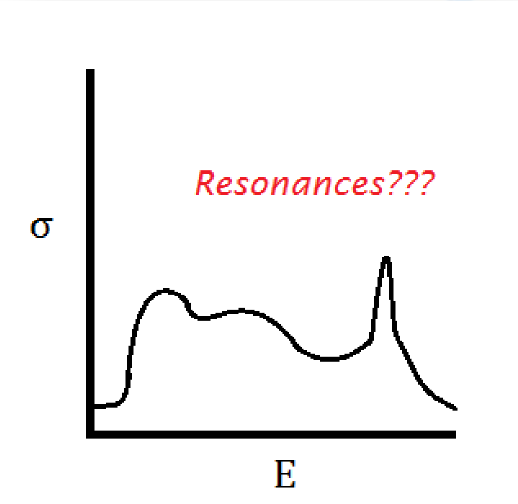
2. Resonances from Scattering data

$$T_{1/2} = \frac{\hbar \ln 2}{\Gamma}$$

$$E_{\text{res}} = E_{\text{r}} - i\frac{\Gamma}{2}$$

- **Breit-Wigner model** often **initially** used: reasonable approximation for **sharp resonances** with no interference between resonances.





- In most **physical scattering problems** there is much **overlap and averaging of peak structures** due to complicated partial-wave contributions as well as the contributions by the different channels.

- **Various data-fitting methods** are in existence. These methods roughly fall into **2 categories**:
  1. Using $\boldsymbol{E_r}$ **and** $\boldsymbol{\Gamma}$ **as fitting parameters**, like Breit-Wigner parameterization. **Number of resonances are fixed** at the outset for such methods.
  2. Using **arbitrary fitting parameters to construct** $\boldsymbol{S}$**-matrix on appropriate Riemann energy sheet**. Padé approximation a typical example.

- Our method, involving the **Jost functions**, falls within the second category.

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3. Jost Matrices

- The ***S*-matrix** can be written as the "**ratio**" of the incoming and outgoing **Jost matrices**.

$$S(E) = f^{(\mathrm{out})}(E)[f^{(\mathrm{in})}(E)]^{-1}$$

- The Jost *functions* (Single-channel Jost matrices) are defined as the **energy-dependent amplitudes** of the **incoming and outgoing spherical waves** in the **asymptotic limit** of the **regular solution** to the radial Schrödinger equation. The Jost matrices are the multi-channel analog.

$$\psi_a(\mathbf{r}) = \frac{u_a(r)}{r} Y_{\ell m}(\theta, \varphi)$$

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2} - V(r)\right] u_a(r) = 0$$

$$u_a(r) \xrightarrow[r\to\infty]{} f_\ell^{(in)}(E) h_\ell^{(-)}(kr) + f_\ell^{(out)}(E) h_\ell^{(+)}(kr)$$

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$$u_a(r) \xrightarrow[r\to\infty]{} f_\ell^{(in)}(E)h_\ell^{(-)}(kr) + f_\ell^{(out)}(E)h_\ell^{(+)}(kr)$$

- Resonances are complex energies, $\mathcal{E}$, which result in a zero determinant for the incoming Jost matrix.

$$\det f^{(\mathrm{in})}(\mathcal{E}) = 0$$

($f_\ell^{(in)}(\varepsilon) = 0$: single channel)

$$S(E) = f^{(\mathrm{out})}(E)[f^{(\mathrm{in})}(E)]^{-1}$$

- Jost functions are **energy dependent via the channel momenta, $\boldsymbol{k_n}$**, each of which has a **two-sheeted branching point at the threshold** energy E_n.

$$\det f^{(\text{in})}(\mathcal{E}) = 0$$

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

- The **energies corresponding with $\boldsymbol{k_n}$** values on the ***physical*** sheet **($\boldsymbol{Im(k_n) > 0}$)** which give zero determinant for $f^{(in)}(\varepsilon)$ are **resonances**.

- If the Jost matrices are constructed in such a way that they depend on energies not **explicitly on the physical sheet**, errors will arise in the resulting resonance parameters.

- This is **not a problem** if the Jost matrices are **mathematically determined from Schrödinger's equation** for a specific model potential, but **it is a problem when the Jost matrices are fitted to scattering data**.

4. Jost functions for a given potential (single channel)

Radial Coulomb Schrödinger equation

$$\left[\frac{d^2}{dr^2}+k^2-\frac{\ell(\ell+1)}{r^2}-V_S-\frac{2k\eta}{r}\right]u_a(r)=0$$

Regular Coulomb Solution

Irregular Coulomb Solution

$$u_\ell(E,r)=F_\ell(\eta,kr)A_\ell(E,r)+G_\ell(\eta,kr)B_\ell(E,r)$$

Variation of parameters method!

$$\begin{aligned}\partial_r A_\ell &= \frac{1}{k}G_\ell V_S(F_\ell A_\ell+G_\ell B_\ell)\\ \partial_r B_\ell &= -\frac{1}{k}F_\ell V_S(F_\ell A_\ell+G_\ell B_\ell)\end{aligned}$$

$$\mathscr{F}_\ell^{(in/out)}(E,r)=\frac{1}{2}\left[A_\ell(E,r)\mp iB_\ell(E,r)\right]$$

$$f_\ell^{(in/out)}(E)=\frac{e^{\mp i\sigma_\ell}}{C_\ell(\eta)(2\ell+1)!!}\lim_{r\to\infty}\mathscr{F}_\ell^{(in/out)}(E,r)$$

$$\sigma_\ell=\arg\Gamma(\ell+1+i\eta)$$

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

5. Semi-analytic Jost matrices

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

$$\eta = \frac{\mu e^2 Z_1 Z_2}{k\hbar^2}$$

- Now assume no model potential known (or necessary): only experimental scattering cross sections at specific energies are available.
- Fitting cannot be done directly: The Jost matrices are energy dependent via the channel momentum, k_n, which is responsible for the branching of the energy Riemann surface at each channel threshold energy, E_n.
- Factors with k-dependence are isolated in the Jost functions so that they are written in terms of functions entire in E.

Factorized Coulomb Functions

$$F_\ell(\eta, kr) = D_\ell(\eta, k)\tilde{F}_\ell(E, r)$$

$$G_\ell(\eta, kr)) = M(\eta)D_\ell(\eta, k)\tilde{F}_\ell(E, r) + \frac{k}{D_\ell(\eta, k)}\tilde{G}_\ell(E, r)$$

*

* E. Lambert, "Fonction de portée effective et déplacement en énergie des états liés en présence d'un potentiel coulombien modifié," *Helv. Phys. Acta*, no. 42, pp. 667–677, 1969.

- The Jost matrices for Coulomb scattering are parameterized to factorize the problematic k_n and $\eta(k)$ dependence:

$$f_{mn}^{(\mathrm{in/out})}(E) = \frac{e^{\pi\eta_m/2}\ell_m!}{2\Gamma(\ell_m+1\pm i\eta_m)}\left\{\frac{C_{\ell_n}(\eta_n)k_n^{\ell_n+1}}{C_{\ell_m}(\eta_m)k_m^{\ell_m+1}}A_{mn}(E) - \left[\frac{2\eta_m h(\eta_m)}{C_0^2(\eta_m)}\pm i\right]C_{\ell_m}(\eta_m)C_{\ell_n}(\eta_n)k_m^{\ell_m}k_n^{\ell_n+1}B_{mn}(E)\right\}$$ *

$$h(\eta) = \frac{1}{2}\left[\psi(i\eta)+\psi(-i\eta)\right] - \ln\hat{\eta},$$

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

$$\psi(z) = \frac{\Gamma'(z)}{\Gamma(z)},$$

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

$$\eta = \frac{\mu e^2 Z_1 Z_2}{k\hbar^2}$$

* S. A. Rakityansky and N. Elander, *J. Math. Phys.* **54** (2013) 122112.

6. Fitting Parameters

- The remaining unknown matrices $A(E)$ and $B(E)$ are shown to be single-valued and holomorphic functions of the energy, defined on a simple energy plane without branching points.

$$A(E) \approx \sum_{i=0}^{M} a_i(E_0)(E - E_0)^i,$$

$$B(E) \approx \sum_{i=0}^{M} b_i(E_0)(E - E_0)^i,$$

- Since $A(E)$ and $B(E)$ are analytic, both can be expanded in the Taylor series around any point, E_0. $A(E)$ and $B(E)$ can thus be approximated by the first M terms in the series.

- The matrices a_i and b_i are the variable fitting parameters. Suitably adjusting them allows the total scattering cross-section to be fitted via the Jost matrices:

Jost matrices→ S matrix → Cross Section (experimental)

- The fitting is done with the MINUIT programme in Fortran.

Two-channel data:

$$\sigma_{1,1}\left(E_{i_1}^{(1,1)}\right) \pm \delta_{i_1}^{(1,1)}, \qquad i_1 = 1,2,3,\ldots,N^{(1,1)}$$

$$\sigma_{1,2}\left(E_{i_2}^{(1,2)}\right) \pm \delta_{i_2}^{(1,2)}, \qquad i_2 = 1,2,3,\ldots,N^{(1,2)}$$

$$\sigma_{2,1}\left(E_{i_3}^{(2,1)}\right) \pm \delta_{i_3}^{(2,1)}, \qquad i_3 = 1,2,3,\ldots,N^{(2,1)}$$

$$\sigma_{2,2}\left(E_{i_4}^{(2,2)}\right) \pm \delta_{i_4}^{(2,2)}, \qquad i_4 = 1,2,3,\ldots,N^{(2,2)}$$

$$\chi^2 = \sum_{i_1=1}^{N^{(1,1)}} \left[\frac{\sigma_{1,1}\left(E_{i_1}^{(1,1)}\right) - \sigma_{1,1}^{fit}\left(E_{i_1}^{(1,1)}\right)}{\delta_{i_1}^{(1,1)}}\right]^2 + \sum_{i_2=1}^{N^{(1,2)}} \left[\frac{\sigma_{1,2}\left(E_{i_2}^{(1,2)}\right) - \sigma_{1,2}^{fit}\left(E_{i_2}^{(1,2)}\right)}{\delta_{i_2}^{(1,2)}}\right]^2 + \sum_{i_3=1}^{N^{(2,1)}} \left[\frac{\sigma_{2,1}\left(E_{i_3}^{(2,1)}\right) - \sigma_{2,1}^{fit}\left(E_{i_3}^{(2,1)}\right)}{\delta_{i_3}^{(2,1)}}\right]^2 + \sum_{i_4=1}^{N^{(2,2)}} \left[\frac{\sigma_{2,2}\left(E_{i_4}^{(2,2)}\right) - \sigma_{2,2}^{fit}\left(E_{i_4}^{(2,2)}\right)}{\delta_{i_4}^{(2,2)}}\right]^2 + \sum_j |S_{1,2}(E_j) - S_{2,1}(E_j)|$$

$$\sigma_{mn}^{fit}(E) = \frac{\pi}{k_m^2}(2\ell_m + 1)\left|S_{nm}(E) - \delta_{mn}\right|^2$$

$$S(E) = f^{(out)}(E)\left[f^{(in)}(E)\right]^{-1}$$

$$A(E) \approx \sum_{i=0}^{M} a_i(E_0)(E - E_0)^i,$$

$$B(E) \approx \sum_{i=0}^{M} b_i(E_0)(E - E_0)^i,$$

Expansion coefficients are fitting parameters

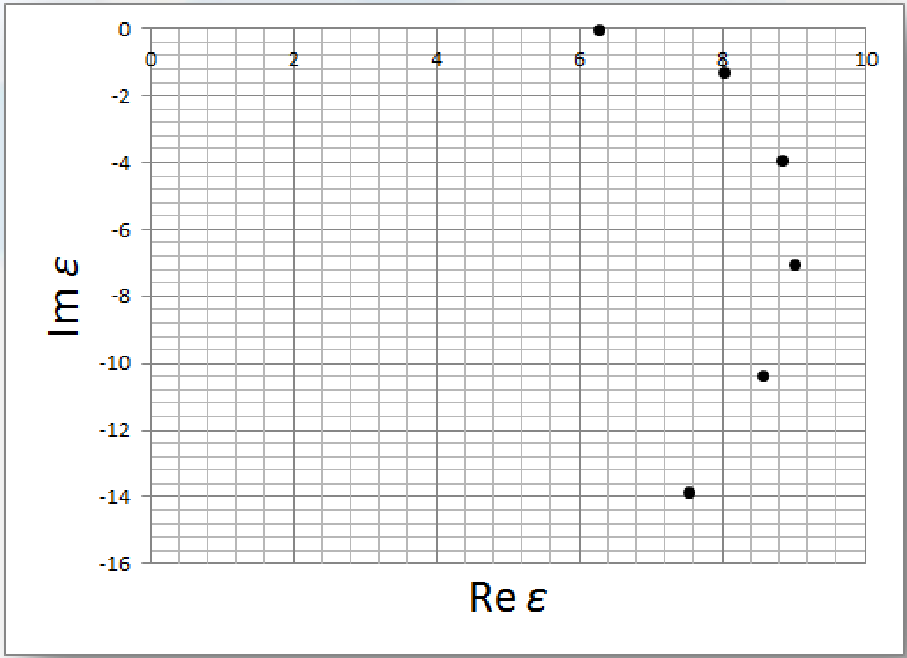
7. Model Potential

- A two-channel model potential for a two-body problem where the resonances are known is used to generate scattering data.

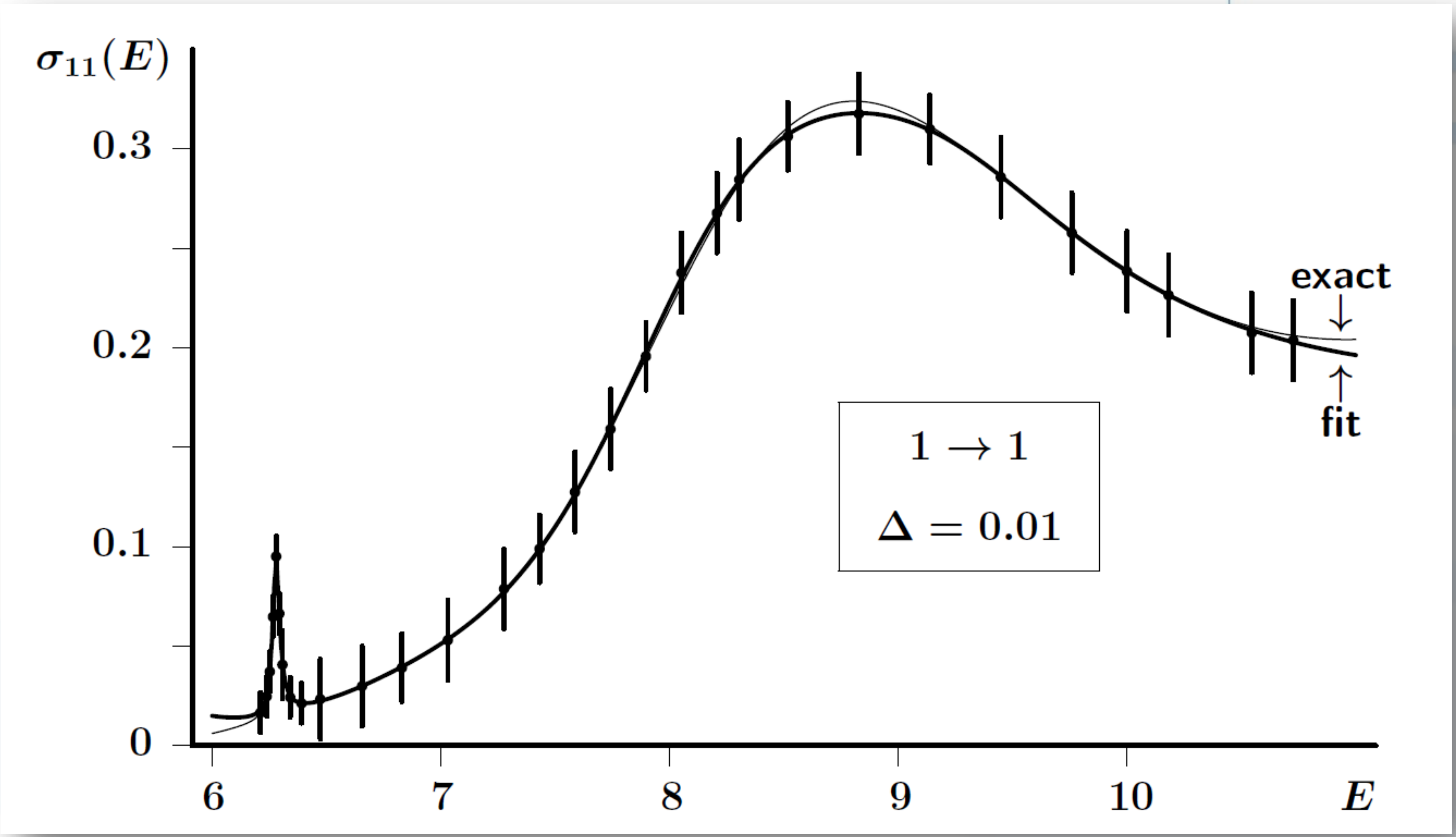
$$V(r) = \begin{pmatrix} -1.0 & -7.5 \\ -7.5 & 7.5 \end{pmatrix} r^2 e^{-r} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \frac{1}{r}$$

- Experimental "noise" is introduced in the data by shifting each generated data point up or down by a random normally-distributed percentage. The standard deviation, Δ of the normal distribution used then corresponds with the magnitude of the "noise".

- Resonances for the model potential:



7. Model Potential: Results - fit



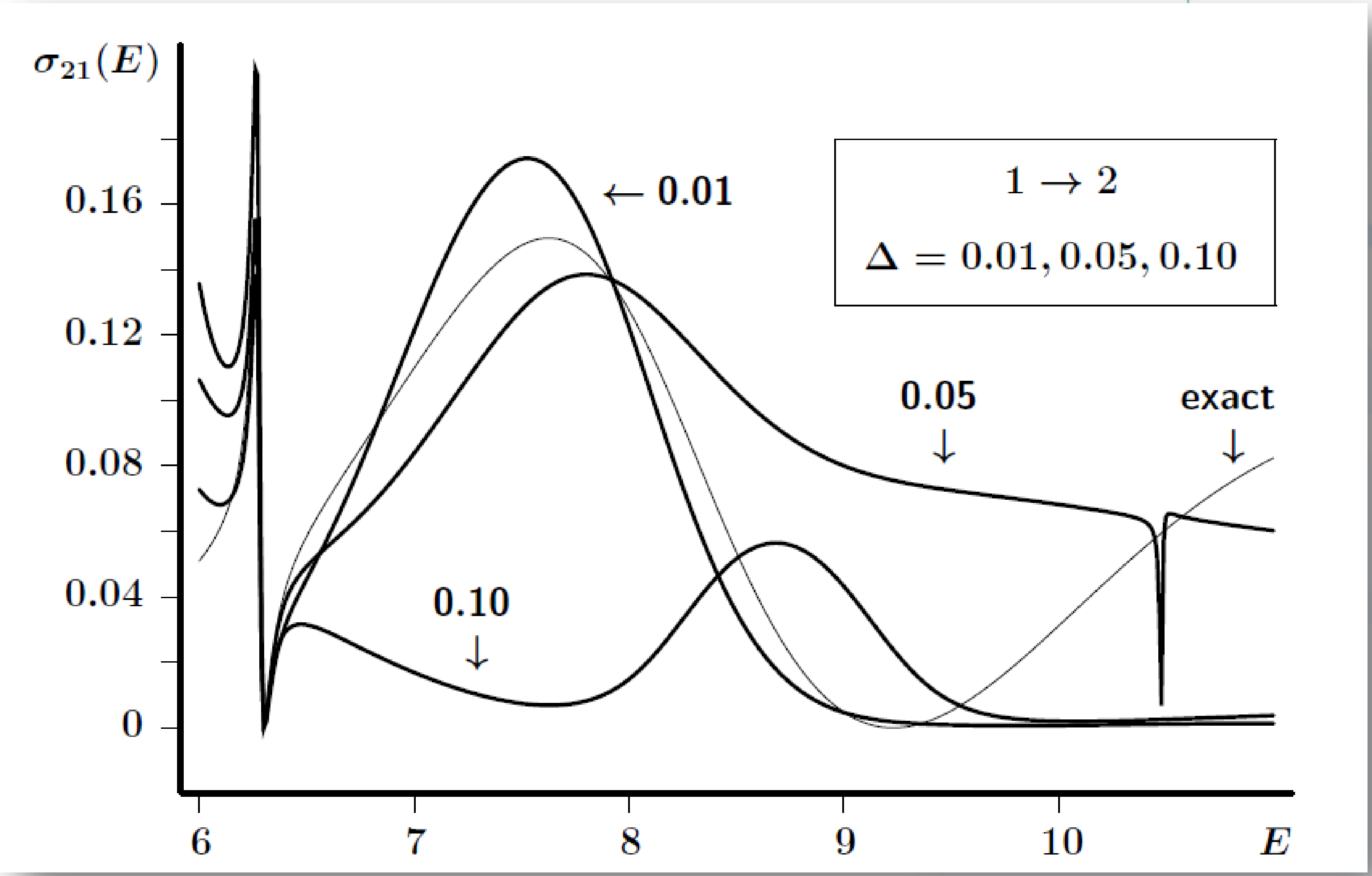
$\mu_1 = \mu_2 = 1 \qquad \hbar c = 1$

$\ell_1 = \ell_2 = 0 \qquad E_1 = 0$ and $E_2 = 0.1$

7. Model Potential: Results - resonances

Resonance	Δ	E_r	Γ	Γ_1	Γ_2
1	exact	6.278042552	0.036866729	0.006898807	0.029967922
	0.01	6.277997424	0.036731019	0.006721542	0.030009477
	0.05	6.278563562	0.035568397	0.006497720	0.029070677
	0.10	6.278669302	0.036236713	0.006638945	0.029597768
2	exact	8.038507867	2.563111275	0.617710684	1.945400591
	0.01	7.998939904	2.096675299	0.623726003	1.472949296
	0.05	7.676616089	2.502856671	0.792088450	1.710768220
	0.10	7.968634195	1.662113407	0.231505793	1.430607614
3	exact	8.861433400	7.883809114	1.949506410	5.934302704
	0.01	11.21325906	3.204531546	0.031776330	3.172755216
	0.05	9.188805831	2.549030291	0.364986606	2.184043685
	0.10	9.259323135	2.226793463	1.232709401	0.994084062

7. Model Potential: Results - prediction



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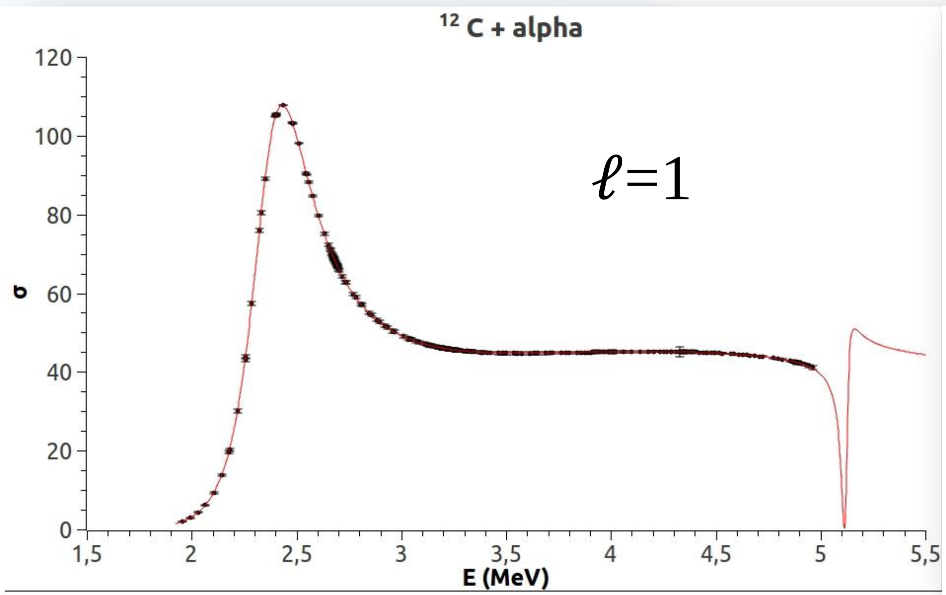
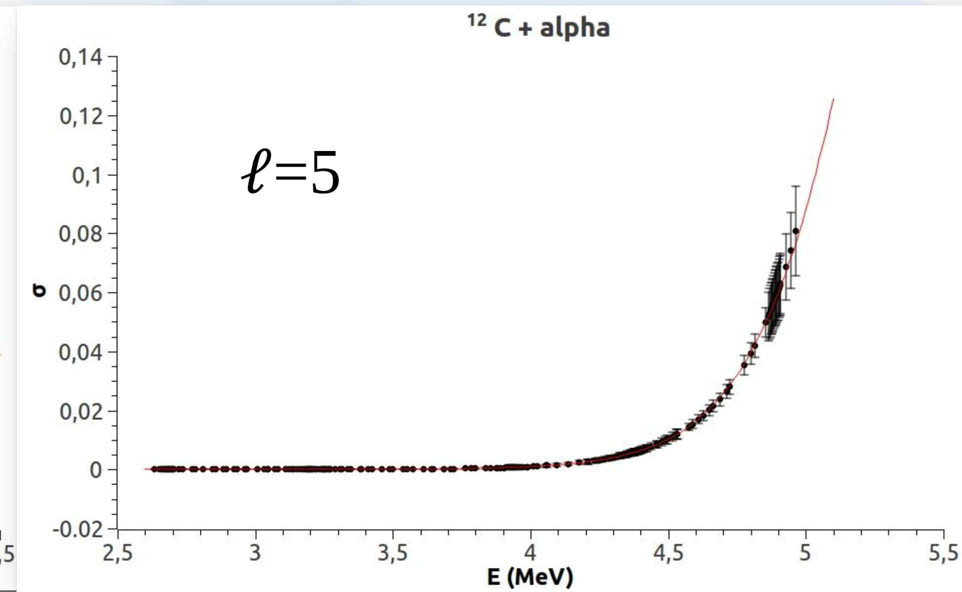
8. New study: $^{12}C + \alpha$ scattering (2 MeV – 7 MeV)

- Data from Notre Dame University & Los Alamos National lab, published by P. Tischhauser et al, 2009.
- Fitting the data duplicates resonances of previous studies very well. Our method is superior, as the fitted function is explicitly analytic.
- Possible new resonances have been found for states 5^- and 6^+.





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8. New study: $^{12}C + \alpha$ scattering (2 MeV – 7 MeV)

- S-matrix residues for specific resonance energies can also be calculated from Jost functions.

$$S_\ell(E) \approx \frac{R_\ell}{E - E_n}$$

$$\text{Res}\,[S_\ell(E_n)] = \frac{f_\ell^{(\text{out})}(E_n)}{\dot{f}_\ell^{(\text{in})}(E_n)}$$

- A relation between the S-matrix residues and the Asymptotic Normalization Coefficient (ANC) is derived, based on work by Irgaziev & Orlov*:

$$Res[S_\ell, k_R] = i\,(-1)^{\ell+1}\,\frac{\Gamma(\ell+1-i\eta)}{\Gamma(\ell+1+i\eta)}\;C_\ell^2 \;= i\,(-1)^{\ell+1}\,e^{-2i\sigma_\ell}\;C_\ell^2$$

- ANC values are related to lifetime of **stars** and is of huge importance in astrophysics.

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* B.F Irgaziev and Yu.V. Orlov, "Resonance properties including asymptotic normalization coefficients deduced from phase-shift data without the effective-range function", arXiv:1801.05933 [nucl-th], 2018

8. New study: $^{12}C + \alpha$ scattering (2 MeV – 7 MeV) Preliminary results:

J^{π}	Reference	Resonance ($^{16}O^*$)		|ANC|
		E_R (MeV)	Γ (MeV)	
0^+	**This paper**	**4.8885 ±0.0005**	**0.0014 ±0.00015**	**0.04027 ± 0.00199**
	Tischhauser	4.888 ±0.008	0.0015 ±0.0005	-
1^-	**This paper**	**2.3648 ±0.0006**	**0.355 ±0.005**	**0.1847 ± 0.0018**
	Tischhauser	2.493 ±0.011	0.420 ±0.020	-
	Orlov	**2.364**	**0.356**	**0.185**
3^-	**This paper**	**4.21606 ±0.00009**	**0.8253 ±0.0001**	**0.2359 ± 0.00004**
	Tischhauser	4.440 ±0.015	0.800 ±0.100	-
	Orlov	**4.214**	**0.812**	**0.234**
5^-	**This paper**	**3.9 ± 0.8**	**1.8 ± 0.4**	**0.016 ± 0.006**

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9. Conclusions & Summary

- Sufficiently accurate results obtained for single- and two-channel scattering model problem. This was made possible by the proper analytic structure used for the fitting.
- While often yielding reasonable results, other methods are not rigorous in nature and rely on a suitable guess for the behaviour of the *S*-Matrix. The method we used is rigorous and exact, and can be applied to any non-relativistic two-body scattering problem involving Coulomb interactions.
- Successfully determined resonances for elastic $^{12}C + \alpha$ scattering.
- Successfully derived equation relating *S*-Matrix residues to ANC values, related to star lifetime.
- Successfully calculated ANC values for resonances for $\ell=0$ to $\ell=6$.
- Future work: $d + \alpha$ scattering; 2-channel problem.

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Grazie!

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