Connecting experimental data and the analytic S-matrix

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Connecting Bound States to the Continuum , FRIB/NSCL/MSU

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Outline

- Interplay between theory and experiment
- Phenomenological R-matrix method
- ^{16}O system
- Some future opportunities

Some comments on experimental data...

- Experiments measure:
  cross sections
  energy spectra
  energies of bound states
  lifetimes
  ...
- Derived quantities:
  widths and energies of unbound states
  phase shifts and ANCs
  scattering lengths
  ...
- Various assumptions and nuclear theory are needed for the latter category.
- Sometimes it is useful to boil things down to a single number.
- The continuum is complicated, but we need a simple story.

Phenomenology

- Provide "best" estimates and uncertainties for applications (astrophysics, reactors, other nuclear theory,...)
- Can take input from both theory and experiment
- Provides bridges between theory, experiment, and applications

Phenomenological R-Matrix

- Exact implementation of quantum-mechanical symmetries and conservation laws (Unitarity)
- Treats long-ranged Coulomb potential explicitly
- Wavefunctions are expanded in terms of unknown basis functions
- Energy eigenvalues and the matrix elements of basis functions are adjustable parameters, which are typically optimized via χ^2 minimization (Bayesian methods also used).
- A wide range of physical observables can be fitted (e.g. cross sections, E_x, Γ_x,...)
- The fit can then be used to determine unmeasured quantities.
- Major Approximations: truncation (levels / channels) – but does not destroy unitarity

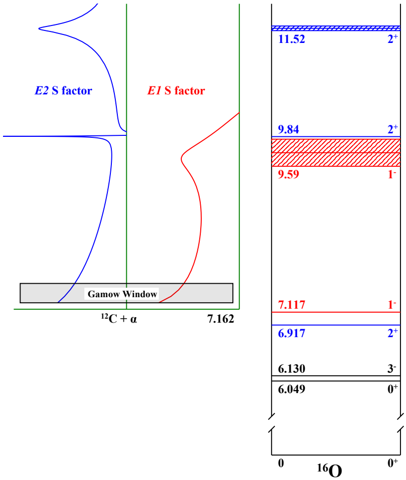
Phenomenological R-Matrix, Continued

- Inclusion of "background levels" is important.
- The channel radii are taken $\gtrsim$ nuclear surface (conclusions should be independent of radius)
- Equivalent to EFT in the zero-radius limit (Hale, Brown, Paris, Phys. Rev. C 89, 014623 (2014), for nuclear channels.

$^{12}C(\alpha,\gamma)^{16}O$: Important Energy Levels

Physics: Subthreshold resonances and interference

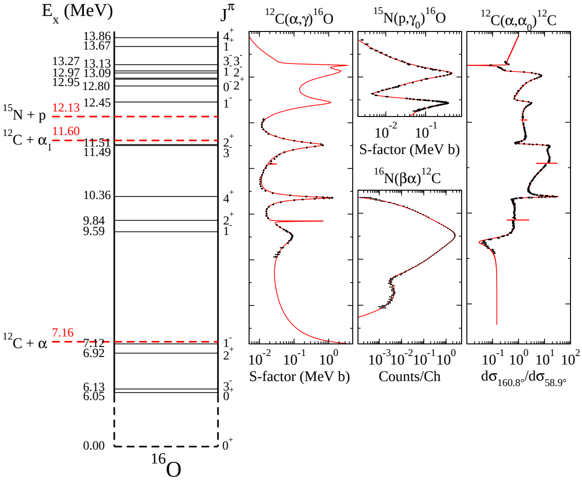
Note: Combination of experiment and theory required to obtain $S(300)$. Subthreshold resonances along with their interference must be considered in the theory.



A partial level diagram

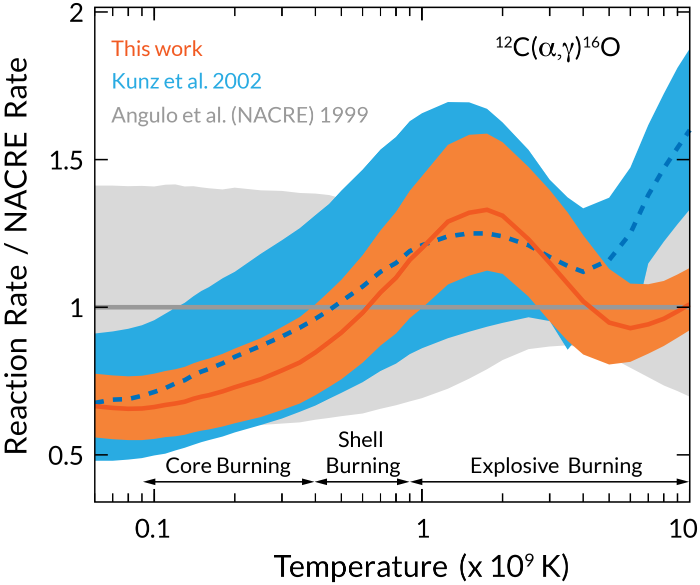
Global R-Matrix Analysis

Reviews of Modern Physics 89, 035007 (2017)



- James deBoer, R.E. Azuma, A. Best, C.R. Brune, C. E. Fields, J. Görres, S. Jones, M. Pignatari, D. Sayre, K. Smith, F. Timmes, E. Uberseder, M. Wiescher
- Over 15,000 data points fitted. 3 nuclear channels, 5 γ channels.
- Bound state information (E_x, Γ_γ, ANCs) also fitted or input.

Reaction Rate



R-Matrix Boundary Conditions

$$\rho = kr \qquad O = G_\ell + iF_\ell \qquad L = \rho\frac{O'}{O}\,|_{r=a}$$

- $\rho\dfrac{u'}{u}\,|_{r=a} = B$ real, energy-independent $\rightarrow$ real E_λ, γ_λ
  Wigner, Lane, Thomas,...
- $\rho\dfrac{u'}{u}\,|_{r=a} = \mathrm{Re}(L)\,|_{r=a}$ real, energy-dependent $\rightarrow$ real E_λ, γ_λ
  Helps with interpretation of parameters, equivalent to above
- $\rho\dfrac{u'}{u}\,|_{r=a} = L\,|_{r=a}$ complex, energy-dependent $\rightarrow$
  complex E_λ, γ_λ
  Siegert (1939), Gamow / Siegert states, not a practical basis for fitting data

In all of the above, E_λ and γ_λ also define poles and residues of a matrix (R, R_S, or S).

S-Matrix

$I = G_\ell - iF_\ell$
$\boldsymbol{A} =$ "energy level matrix" (E_λ, γ_λ, Coulomb functions)
$S_{\lambda c} = \mathrm{Re}[L_c(E_\lambda)]$

- $S_{c'c} = 2i\rho_{c'}^{1/2} O_{c'}^{-1} \boldsymbol{\gamma}_{c'}^T \boldsymbol{A} \boldsymbol{\gamma}_c \rho_c^{1/2} O_c^{-1} + I_{c'} O_c^{-1}$
- poles: $\boldsymbol{\mathcal{E}} \boldsymbol{g}_i = \tilde{E}_i \boldsymbol{g}_i$, where

$$
\begin{aligned}
(\boldsymbol{\mathcal{E}})_{\lambda\mu} &= (\boldsymbol{A}^{-1})_{\lambda\mu} + \tilde{E}\delta_{\lambda\mu} \\
&= E_\lambda \delta_{\lambda\mu} - \sum_c \gamma_{\lambda c}\gamma_{\mu c} L_c(\tilde{E}) \\
&\quad + \sum_c \begin{cases} \gamma_{\lambda c}^2 S_{\lambda c} & \lambda = \mu \\ \gamma_{\lambda c}\gamma_{\mu c} \frac{S_{\lambda c}(\tilde{E}-E_\mu) - S_{\mu c}(\tilde{E}-E_\lambda)}{E_\lambda - E_\mu} & \lambda \neq \mu \end{cases}
\end{aligned}
$$

Finding S-Matrix Poles

- $\boldsymbol{\mathcal{E}}$ is complex, symmetric, and energy-dependent.
- Number of of levels (dimension of $\boldsymbol{\mathcal{E}}$) typically < 10.
- Choose $k = k_R + ik_I$ to be to the right of the line $ik_r = -k_I$.
- Use Rayleigh Quotient iteration, starting from an R-matrix pole:

$$(\boldsymbol{g}_i)_{n+1} = [(\boldsymbol{\mathcal{E}_i})_n - (\tilde{E}_i)_n \boldsymbol{I}]^{-1} (\boldsymbol{g}_i)_n$$

$$(\tilde{E}_i)_{n+1} = (\tilde{E}_i)_n + \frac{(\boldsymbol{g_i})^T_{n+1}[(\boldsymbol{\mathcal{E}_i})_n - (\tilde{E}_i)_n](\boldsymbol{g}_i)_{n+1}}{(\boldsymbol{g_i})^T_{n+1}[1 - (\frac{d\boldsymbol{\mathcal{E}}_i}{dE})_n](\boldsymbol{g}_i)_{n+1}}$$

  Factor in denominator is important!
- then $\tilde{\gamma}_{ic} \equiv \boldsymbol{g}_i^T \boldsymbol{\gamma}_c$ and near the pole at $\tilde{E}_i$

$$S_{c'c} \approx 2i \frac{\rho_{c'}^{1/2} O_{c'}^{-1} \tilde{\gamma}_{ic'} \tilde{\gamma}_{ic} O_c^{-1} \rho_c^{1/2}}{(\tilde{E}_i - E)[\boldsymbol{g}^T \boldsymbol{g} + \sum_c \tilde{\gamma}_{ic}^2 \frac{dL_c}{dE}(\tilde{E}_i)]}$$

  $\boldsymbol{g}^T \boldsymbol{g}$ can be zero (?)

Some comments on the normalization factor

$$N^{-1} = \boldsymbol{g}^T \boldsymbol{g} + \sum_c \tilde{\gamma}_{ic}^2 \frac{dL_c}{dE}(\tilde{E}_i)$$

- Changes the normalization volume from in side the channel radii to all space.
- $\frac{dL_c}{dE}$ "=" $\frac{2\mu a}{\hbar^2 O^2(a)} \int_a^\infty O^2(r)\,dr$
- "=" $\rightarrow$ contour deformation or convergence factor required...
- This can be conveniently calculated via a continued fraction method.

Example: $^{12}\mathrm{C} + \alpha$ scattering

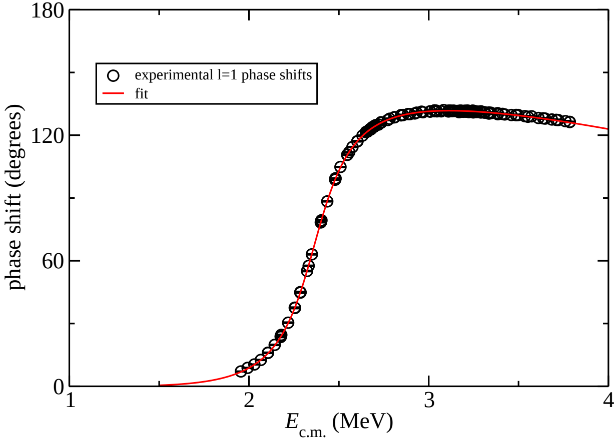
- Specifically, 170 $\ell = 1$ phase shift data points from Tishhauser *et al.* (2009).
- 3-level R-matrix fit: subthreshold resonance (-0.045 MeV), $\approx$ 2.4-MeV resonance, and a background pole.
- Only include $^{12}\mathrm{C} + \alpha$ channel.
- Fix ANC of subthreshold state to value determined using using transfer reactions.
- $\rightarrow$ 4 free parameters: E_λ and γ_λ for λ=2,3.
- Consider channel radii between 4.5 and 8.0 fm.
- Extract Γ using a Breit-Wigner on the real axis:

$$\Gamma_{\lambda c} = \frac{2\gamma_{\lambda c}^2 P_{\lambda c}}{1 + \sum_c \gamma_{\lambda c}^2 \frac{dS_c}{dE}(E_\lambda)}$$

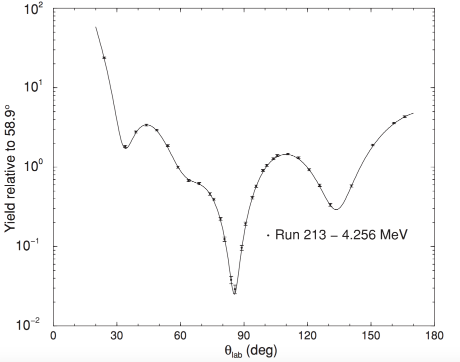
$$P_{\lambda c} = \mathrm{Im}[L_c(E_\lambda)]$$

- Extract S-matrix pole parameters.

Fit to Phase Shift Data

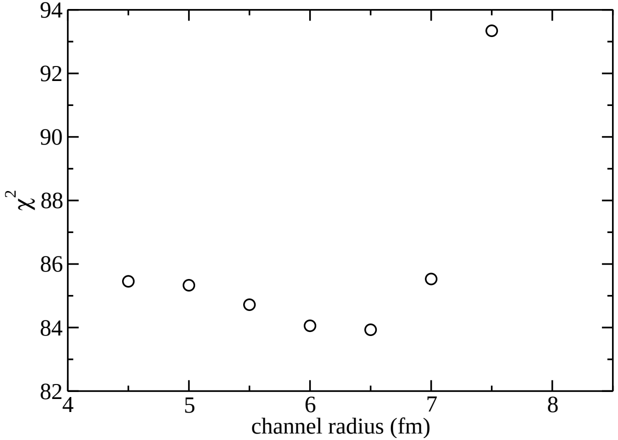


Fitting Cross Section Data is Better But...

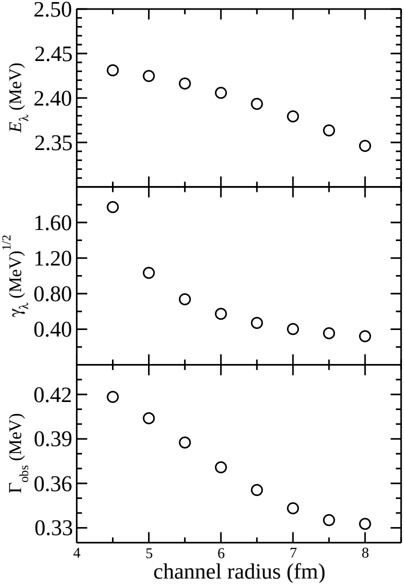


- Then you must model all partial waves.
- And average over energy of the measurement.
- This WAS done for the analysis in the RMP article.

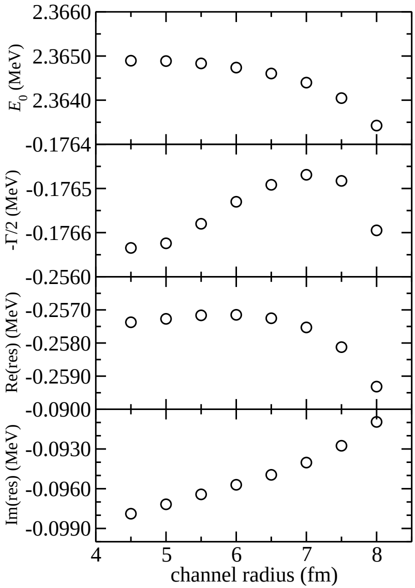
χ^2 Versus Channel Radius



Real Axis Parameters



S-Matrix Pole Parameters

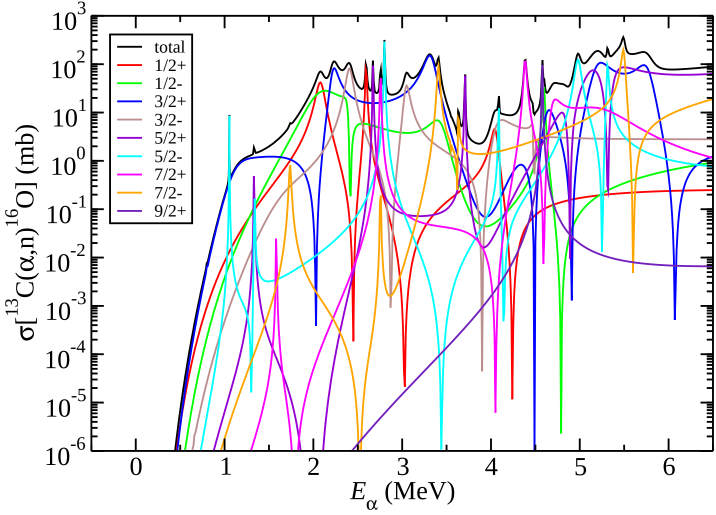


Some Comments on Alternatives

- Alternatives include:
  - Effective Range Theory
  - K-Matrix
- The approaches do not have a radius parameter.
- But there are downsides:
  - Effective Range Theory is not a natural tool for resonances.
  - The functional form of the "background" is unclear.
- The fact that R-matrix parameters correspond to a basis is an advantage.
- There are several computer codes available for R-matrix analysis, e.g. AZURE2 (`http:azure.nd.edu`)
- There have been a number of simple Effective Range style analyses for $^{12}C + \alpha$ recently:
  - Ramírez Suárez and Sparenberg, Phys. Rev. C **96**, 034601 (2017).
  - Ando, Phys. Rev C **97**, 014604 (2018).
  - Blokhintsev *et al.*, Phys. Rev C **97**, 024602 (2018).

R-matrix can handle quite complicated problems

ENDF/B-VII: G.M. Hale and M.W. Paris (LANL) R-Matrix Evaluation



Future Opportunities

- $^3\mathrm{He} + \alpha$, $^7\mathrm{Be} + p$, $^{12}\mathrm{C} + \alpha$
- $^{18}\mathrm{Ne}$ ($^{17}\mathrm{F} + p$), $^{19}\mathrm{Ne}$ ($^{15}\mathrm{O} + \alpha$),...
- $p+$ proton-rich beams (e.g. $^{11}\mathrm{C} + p$)
- α optical potential [e.g. $^{34}\mathrm{Ar}(\alpha, p)$]
- transfer reactions, including charge-exchange
- (> 2)-particle final states, e.g. $^{26}\mathrm{O}$, di-neutron, tetra-neutron

Thank you for your attention.