Additional Topics in Phenomenological R-Matrix

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Additional Topics in Phenomenological R-Matrix

- Level Matrix Representation
- Other Basis Choices
- How do you define a resonance?
- Photon Channels

The S Matrix in the Level Matrix Representation

- Recall that the R- and S-matrices can be defined in terms of *channel-space* matrices

$$\begin{aligned} R_{c'c} &= \sum_{\lambda} \frac{\gamma_{\lambda c'}\gamma_{\lambda c}}{E_\lambda - E} \\ \boldsymbol{S} &= \boldsymbol{\Omega}\left[\mathbf{1} + 2i\boldsymbol{P}^{1/2}[\mathbf{1} - \boldsymbol{R}(\boldsymbol{L} - \boldsymbol{B})]^{-1}\boldsymbol{R}\boldsymbol{P}^{1/2}\right]\boldsymbol{\Omega}. \end{aligned}$$

- Interestingly, the S matrix can also be written as

$$S_{c'c} = \Omega_{c'}\Omega_c\left[\delta_{c'c} + 2i(P_{c'}P_c)^{1/2}\boldsymbol{\gamma}_{c'}^T\boldsymbol{A}\boldsymbol{\gamma}_c\right],$$

where $\boldsymbol{\gamma}_c$ is a column vector in *level space* and the level matrix $\boldsymbol{A}$ is a square matrix in level space:

$$[\boldsymbol{A}^{-1}]_{\lambda\mu} = (E_\lambda - E)\delta_{\lambda\mu} - \sum_c \gamma_{\lambda c}\gamma_{\mu c}(S_c + iP_c - B_c).$$

- The equivalence of these two forms is proven in Lane and Thomas. Linear algebraists would call it an application of the Woodbury matrix identity.

Issue with the Boundary Condition

- $B_c(E_R) = S_c(E_R)$ can only be chosen for one level for each J^π.
- In a multi-level situation, $B_c(E_R) \neq S_c(E_R)$ causes the the resonance energy and partial widths of that level to depend on *all* of the R-matrix parameters.
- This makes fitting more difficult. For example, what do you do with $J^\pi = 2^+$ for $^{12}\mathrm{C}(\alpha, \gamma)^{16}\mathrm{O}$, where there is a bound state and a very narrow ($\Gamma_\alpha < 1$ keV) level at $E_R = 2.68$ MeV?

A Better Way to Manage the Boundary Conditions

- Redefine the parameters E_λ and $\gamma_{\lambda c}$ so that they correspond to $B_c(E_R) = S_c(E_R)$ for all levels. See CRB, Phy. C**66**, 044611 (2002).
- This leads to

$$S_{c'c} = \Omega_{c'}\Omega_c \left[\delta_{c'c} + 2i(P_{c'}P_c)^{1/2}\boldsymbol{\gamma}_{c'}^T \boldsymbol{A}\boldsymbol{\gamma}_c\right], \quad \text{and}$$

$$[\boldsymbol{A}^{-1}]_{\lambda\mu} = (E_\lambda - E)\delta_{\lambda\mu} - \sum_c \gamma_{\lambda c}\gamma_{\mu c}(S_c + iP_c)$$

$$+ \sum_c \begin{cases} \gamma_{\lambda c}^2 S_{\lambda c} & \lambda = \mu \\ \gamma_{\lambda c}\gamma_{\mu c}\frac{S_{\lambda c}(E-E_\mu)-S_{\mu c}(E-E_\lambda)}{E_\lambda - E_\mu} & \lambda \neq \mu \end{cases},$$

where $S_{\lambda c} = S_c(E_\lambda)$.

- It is mathematically equivalent to the Lane-and-Thomas formalism.
- This is what is done by default in the AZURE2 code.

R-Matrix Boundary Conditions

The boundary conditions define the basis:

- $\rho \frac{u'}{u} |_{r=a} = B$ real, energy-independent $\rightarrow$ real E_λ, γ_λ
  Wigner, Lane, Thomas,… The basis vectors are orthogonal inside the channel radius.
- $\rho \frac{u'}{u} |_{r=a} = S(E) |_{r=a}$ real, energy-dependent $\rightarrow$ real E_λ, γ_λ
  Helps with interpretation of parameters, equivalent to above. The basis vectors are not orthogonal inside the channel radius.
- $\rho \frac{u'}{u} |_{r=a} = [S(E) + iP(E)]_{r=a}$ complex, energy-dependent $\rightarrow$ complex E_λ, γ_λ. Kapur and Peierls (1938), Siegert (1939): Gamow / Siegert states. Simple relationship to S matrix, but 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).

How Does One Define a Resonance?

- More specifically, how does one define a resonance energy, total width, and partial width?
- Is E_R where cross section peaks? Is Γ the FWHM of a cross section curve with a peak? Whatever I told you last week?
- There is no correct answer $\rightarrow$ be careful with values you take from the literature.
- All reasonable definitions converge to the same result, if the resonance is *narrow*.
- There is no ambiguity for the Asymptotic Normalization Constant (ANC).

A Convenient Definition

- In phenomenological R matrix, assuming $B_c = S_c(E_\lambda)$, it is convenient to define

$$E_\lambda = \text{resonance energy}$$
$$\Gamma_c = \frac{2\gamma_c^2 P_c}{1 + \sum_{c'} \gamma_{c'}^2 \left.\frac{dS_{c'}}{dE}\right|_{E_R}} \quad \text{partial width}$$
$$\Gamma = \sum_c \Gamma_c \quad \text{total width.}$$

  These result from making a one-level approximation and matching to the Breit-Wigner formula.

- For a resonance which is "not narrow," it may depend on the value of the channel radius.

- This is what is done in the AZURE2 code.

Poles of the Scattering Matrix

- An S-matrix pole at $\tilde{E} = E_R - i\Gamma/2$ defines a resonance energy and total width.
- The partial widths can be defined using the *residues* of these poles. They need not sum to the total width (but nearly do so for narrow resonances).
- Such a state decays exponentially in time:
  $|\Psi(t)|^2 \propto \exp(-\Gamma t/\hbar)$.
- This is commonly done in the field of particle physics. See G. F. Chew, *Resonances, Particles, and Poles from the Experimenter's Point of View*, 1966, https://escholarship.org/uc/item/445758sx.
- This definition is unambiguous. The only problem is that we do not perform experiments at complex energies…

Finding S-Matrix Poles from an R-Matrix

- Solve the non-linear eigenvalue problem $\boldsymbol{\mathcal{E}}(\tilde{E}_i)\boldsymbol{g}_i = \tilde{E}_i\boldsymbol{g}_i$, where
$$[\boldsymbol{\mathcal{E}}]_{\lambda\mu} = [\boldsymbol{A}^{-1}]_{\lambda\mu} + \tilde{E}\delta_{\lambda\mu}.$$
See G.M. Hale *et al.*, Phys. Rev. C **59**, 763 (1987).

- $\boldsymbol{\mathcal{E}}$ is complex, symmetric, and energy-dependent.

- Define $\tilde{\gamma}_{ic} \equiv \boldsymbol{g}_i^T\boldsymbol{\gamma}_c$. Then near the pole at $\tilde{E}_i$
$$S_{c'c} \approx 2i\frac{\rho_{c'}^{1/2}O_{c'}^{-1}\tilde{\gamma}_{ic'}\tilde{\gamma}_{ic}O_c^{-1}\rho_c^{1/2}}{(\tilde{E}_i - E)[\boldsymbol{g}^T\boldsymbol{g} + \sum_c \tilde{\gamma}_{ic}^2\frac{dL_c}{dE}(\tilde{E}_i)]},$$
where $O_c = \exp(-i\sigma_\ell + i\ell\pi/2)H_\ell^+$ and $L_c = \rho O_c'/O_c$.

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

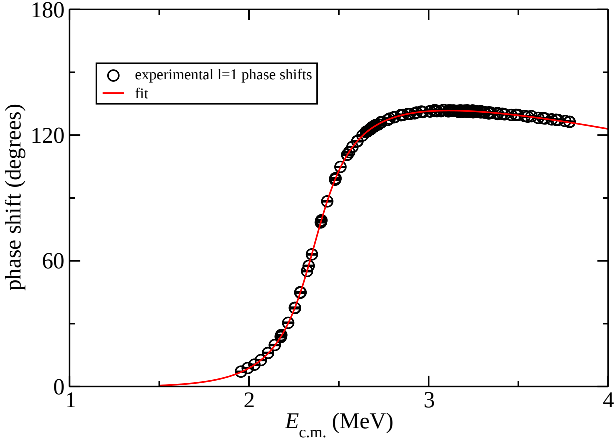
- Specifically, 170 $\ell = 1$ phase shift data points from P. Tishhauser *et al.*, Phys. Rev. C **79**, 055803 (2009).
- 3-level R-matrix fit: subthreshold resonance (-0.045 MeV), $\approx$ 2.4-MeV resonance, and a background pole.
- Only include $^{12}C + \alpha$ channel.
- Fix ANC of subthreshold 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:

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

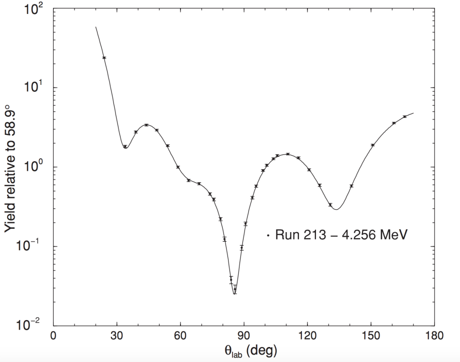
$$P_{\lambda c} = \mathrm{Im}[L_c(E_\lambda)]$$

- Extract S-matrix pole parameters.

Fit to Phase Shift Data

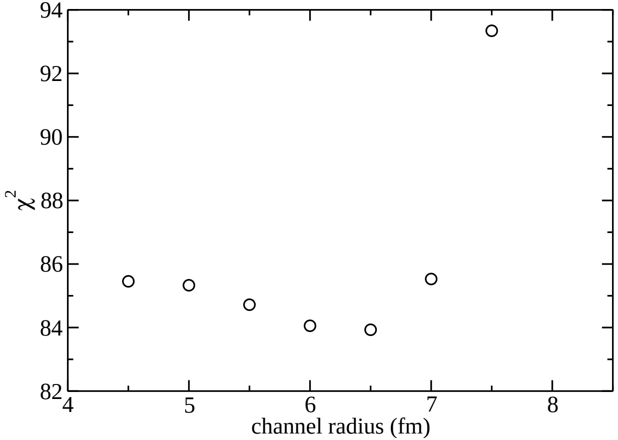


Fitting Cross Section Data is Better But...

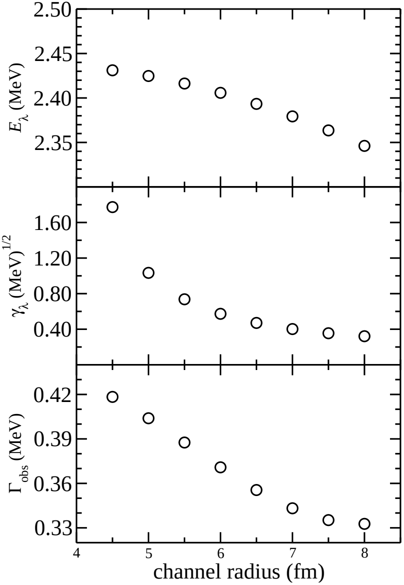


- Then you must model all partial waves.
- And average over energy of the measurement.
- This WAS done for the analysis in the deBoer *et al.* RMP article.

χ^2 Versus Channel Radius



Real Axis Parameters

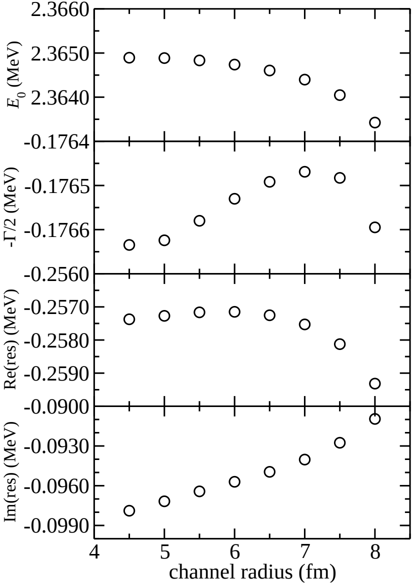


3.6% spread

138% spread

22.8% spread

S-Matrix Pole Parameters



0.051% spread

0.023% spread

0.75% spread

7.3% spread

To Conclude About S-Matrix Pole Parameters

- They provide results with minimal channel-radius sensitivity.
- However, the same is also true about the calculated S matrix, phase shifts, or cross section.
- There does not appear to be any practical way to use S-matrix pole parameters directly for fitting data.
- There is a good argument to be made that one should focus on observable quantities, such as cross sections, and not worry too much about how one defines the energy and width of a resonance.
- But it is human nature to try to reduce physics to just a small set of numbers…

Photon Channels

- Photon channels may also be described using R-matrix methods.

- Photon channels are labeled in a particular manner:
  - λ_f: the final state J^π, E_x,...
  - transition type: E for electric, M for magnetic
  - multipolarity: $L = 1, 2, 3\ldots$

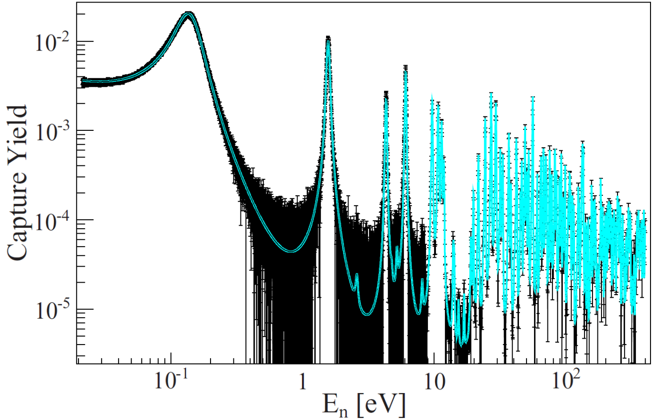
- The usual selection rules for electromagnetic transitions apply.

- The details of the implementation in R-matrix differ widely.

Heavy Nuclei

- For neutron capture on heavy nuclei, one is often presented with vary narrow resonances which are closely spaced.
- The photon channels may contribute significantly to the widths of levels $\rightarrow$ first-order perturbation theory is not applicable.
- The number final states may be very large, which requires some type of approximation. Most experiments do not resolve individual levels in the final state.
- Reich-Moore Approximation: C.W. Reich and M.S. Moore, Phys. Rev. **111**, 929 (1958).
- This is implemented in the code SAMMY.

Neutron Capture in Heavy Nuclei



^{176}Lu(n, γ) measured with the DANCE detector at the Los Alamos Neutron Science Center. The blue curve is a SAMMY fit. O. Roig *et al.*, Phys. Rev. **93**, 034602 (2016).

Light Nuclei

- The final states are almost always resolved.
- First-order perturbation theory is applicable (Γ_γ is small compared to other partial widths). In fact, this may be violated far below the Coulomb barrier, but then a single Breit-Wigner resonance is an excellent approximation.
- The matrix element calculated in perturbation theory may depend on the long-ranged parts of the wavefunctions. For electric (EL) transitions, one has $T \propto \langle \Psi_i | r_\alpha^L | \Psi_f \rangle$, at least for the large-radius contribution.
- Using R-matrix wavefunctions, the matrix element is naturally split into *internal* and *external* contributions.
- This was first introduced by R.G. Thomas in 1952 and then developed by many authors, culminating with F.C. Barker and T. Kajino, Aust. J. Phys. **44**, 369 (1991).

Barker-Kajino Formalism

- The internal part of the capture matrix element is described by a photon reduced width amplitude $\gamma_{\lambda p}$, which is just a matrix element of an electromagnetic operator between an R-matrix basis state and the final state.
- For EL transitions, the external contribution is calculated analytically, using Coulomb functions, an initial state constructed using the the R-matrix in nucleonic channels, and the Asymptotic Normalization Constant(s) for the final state.
- For many non-resonant reactions, particularly if they have low Q value, the external contribution dominates. This is the case for $^{3}\mathrm{He}(\alpha,\gamma)^{7}\mathrm{Be}$, $^{7}\mathrm{Be}(p,\gamma)^{8}\mathrm{B}$, and $^{16}\mathrm{O}(p,\gamma)^{17}\mathrm{F}$.
- In a phenomenological analysis, the $\gamma_{\lambda p}$ would simply be fit parameters.
- This is what is done in the AZURE2 code.

Thank you for your attention.