Phenomenological *R*-Matrix
Introduction

Carl R. Brune

Ohio University

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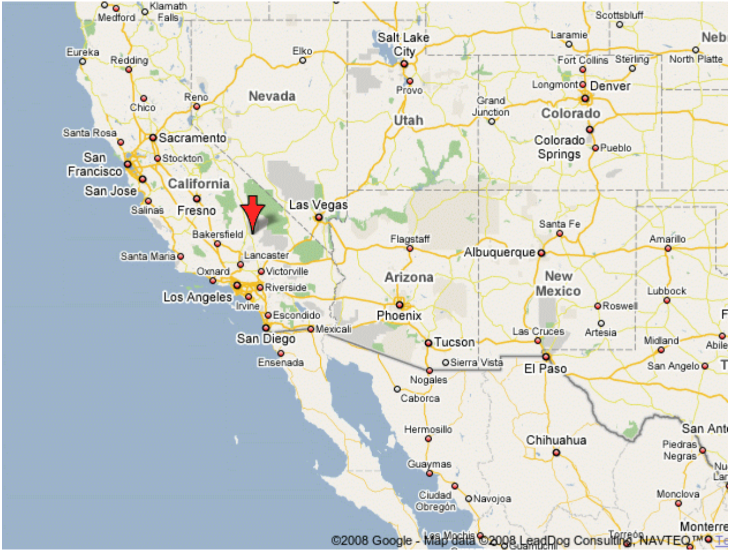
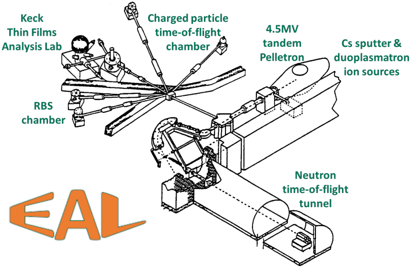
Where do I come from?



I was born and raised in Ridgecrest, CA – in the Mojave Desert!

Where am I now?

Google Maps

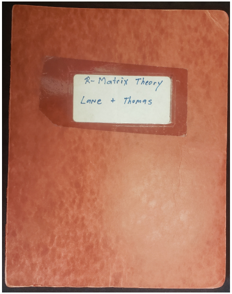


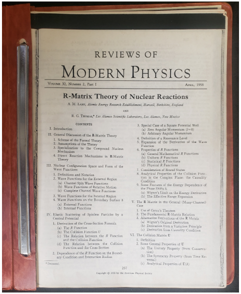
Ohio University in Athens, Ohio

Edwards Accelerator Laboratory (4.5 MV tandem accelerator)
Research focus: Nuclear Astrophysics, Reactions, Structure, and Applications
Faculty: CRB, Steve Grimes, Tom Massey, Cody Parker, Andrea Richard, and Alexander Voinov

How did I get here?

Lecturing on R-matrix methods in Edinburgh…





Xerox copy of key RMP article made when I was a grad student, circa 1992.

Plus knowledgeable people answered my questions!
Thanks: Dick Azuma, Fred Barker, Gerry Hale, and Jean Humblet.

Broad Outline for Lectures

- Introduction
- Coulomb Functions
- Photon channels (capture reactions)
- Thresholds, Scattering Lengths, ...
- Isospin and Mirror Symmetry
- Relating Transfer Reactions to R matrix
- Open Questions
- ... (time permitting)

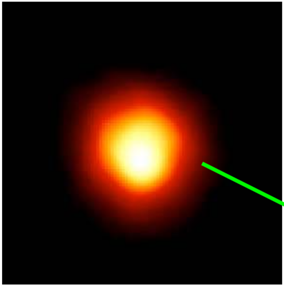
What is the Phenomenological R-matrix ?

- A way to describe two-body nuclear reactions using adjustable parameters of nuclear energy levels.

- As much quantum mechanics as possible is put in:.
  - Angular momentum and parity conservation.
  - Long-range Coulomb interaction.
  - Probability conservation (unitarity).
  - Time-reversal invariance.

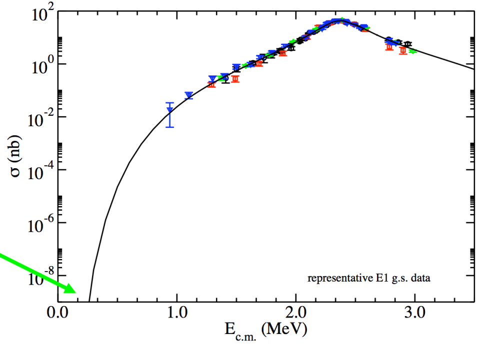
The Challenge

Red Giant



T=(1-3)x10^8 K

The Lab



- Extrapolation to low energies is required. More challenging than the typical data evaluation problem.

Some Important Literature for Nuclear Reaction Phenomenology with R-Matrix

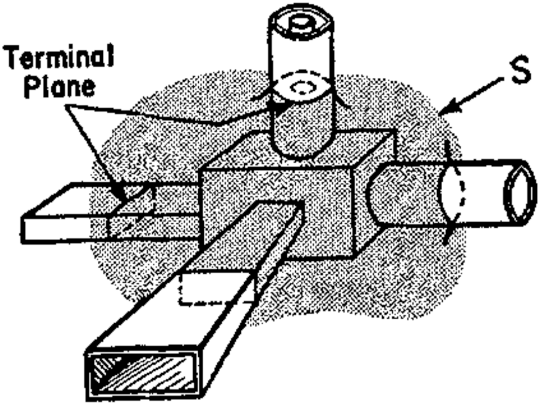
Original Literature

- G. Breit and E. Wigner, *Capture of Slow Neutrons*, Phys. Rev. **49**, 519-531 (1936).
- P.L. Kapur and R. Peierls, *The dispersion formula for nuclear reactions*, Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences, **166**, Issue 925, pp. 277-295, (1938).
- A.J.F. Siegert, *On the Derivation of the Dispersion Formula for Nuclear Reactions*, Phys. Rev. **56**, 750-752 (1939).
- E.P. Wigner and L. Eisenbud, *Higher Angular Momenta and Long Range Interaction in Resonance Reactions*, Phys. Rev. **72**, 29-41 (1947).
- C. Bloch, *Une formulation unifiée de la théorie des réactions nucléaires*, Nucl. Phys. **4**, 503-528 (1957).
- A.M. Lane and D. Robson, *Comprehensive Formalism for Nuclear Reaction Problems. I. Derivation of Existing Reaction Theories*, Phys. Rev. **151**, 774-787 (1966).
- F.C. Barker, *The boundary condition parameter in R-matrix theory*, Australian Journal of Physics **25**, 341-348 (1972).
- G.M. Hale, R.E. Brown, and N. Jarmie, *Pole structure of the $J^\pi = 3/2^+$ resonance in ^{5}He*, Phys. Rev. Lett. **59**, 763-766 (1987).
- C.R. Brune, *Alternative parametrization of R-matrix theory*, Phys. Rev. C **66**, 044611 (2002).

Review Articles

- A.M. Lane and R.G. Thomas, *R-Matrix Theory of Nuclear Reactions*, Reviews of Modern Physics **30**, 257-353 (1958).
- P. Descouvemont and D. Baye, *The R-matrix theory*, Reports on Progress in Physics **73**, 036301 (2010).
- R.J. deBoer, CRB *et al.*, The $^{12}C(\alpha,\gamma)^{16}O$ reaction and its implications for stellar helium burning, Reviews of Modern Physics, **89**, 035007 (2017).

An Intuitive Picture for Nuclear Reactions



"A transmission line (waveguide) junction"
E.P. Wigner, *Nuclear Reactions and Level Widths*,
American Journal of Physics **17**, 99-109 (1949).

Scattering Matrix

- If there is incoming flux in channel c, then the wavefunction Ψ_c is given asymptotically by

$$\Psi_c \propto I_c - \sum_{c'} S_{c'c} O_c,$$

  where I_c and O_c are incoming and outgoing waves, respectively.
- And $S_{c'c}$ is the *Scattering Matrix*. The notation $U_{c'c}$ is often used in the R-matrix literature.
- $S_{c'c}$ is *unitary*, $\rightarrow \boldsymbol{S^\dagger S = 1}$, provided the underlying Hamiltonian is Hermitian. This ensures conservation of probability.
- $S_{c'c}$ is symmetric in c and c' if time-reversal invariance holds.
- $S_{c'c}$ is block diagonal with respect to the total angular momentum J and parity π, assuming these quantities are conserved.
- **We assume all of the above.**
- If $S_{c'c}$ is diagonal, we have $S_{c'c} = \delta_{c'c} \exp(2i\delta_c)$,
  with real phase shifts δ_c (δ_c includes the Coulomb phase shift here).
- It is sometimes useful to think about these channels labeled by "c" abstractly, like on the previous slide, but what are they, really?

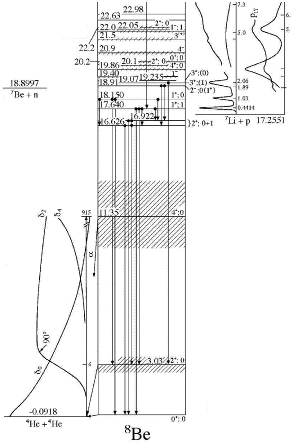
Definition of Channels

- We assume there are only two bodies asymptotically, and label the *particle pair* with α.
- We then perform an angular momentum decomposition. The intrinsic spins of the particle pair are coupled to form the *channel spin* s.
- The orbital angular momentum ℓ of the particle pair are then coupled to form the *total angular momentum* J. This step also defines the *parity* of the channel, since this parity will be $(-1)^\ell$ times the intrinsic parity of each member of the particle pair.
- Normally, we will assume $c \equiv \alpha s \ell$, with the J^π value also implicit.
- For photon channels, we replace sl with multipolarity: $(E/M)L$. Photons are special, and we will talk about them more later.

Truncating the Number of Channels

- In principle, there are a very large number of possible particle pairs, and $0 \leq \ell < \infty$. In order to keep this tractable, we must truncate.
- (1) Limit consideration only to those particle pairs which are energetically "open" in the energy range of interest.
- (2) Limit ℓ to the lowest few values, keeping in mind the angular momentum barrier.
- These assumptions may be tested to some extent by relaxing them.
- In phenomenological R-matrix, these decisions are partially driven by quantity and quality of data available to constrain the calculation.

Example of Channels: ^{8}Be



http://www.tunl.duke.edu/nucldata/

spins and parities:

"particle"	J	π
p	1/2	+
^{4}He	0	+
^{7}Li	3/2	-
^{7}Li*(0.48)	1/2	-

channels

α	s	ℓ	J	π
^{4}He + ^{4}He	0	0	0	+
^{4}He + ^{4}He	0	2	2	+
$p + {}^{7}$Li	1	0	1	-
$p + {}^{7}$Li	2	0	2	-
$p + {}^{7}$Li	1	1	0,1,2	+
$p + {}^{7}$Li	2	1	1,2,3	+
$p + {}^{7}$Li*(0.48)	0	0	0	-
$p + {}^{7}$Li*(0.48)	1	0	1	-
$p + {}^{7}$Li*(0.48)	0	1	1	+
$p + {}^{7}$Li*(0.48)	1	1	0,1,2	+

Let's practice with channels a little bit

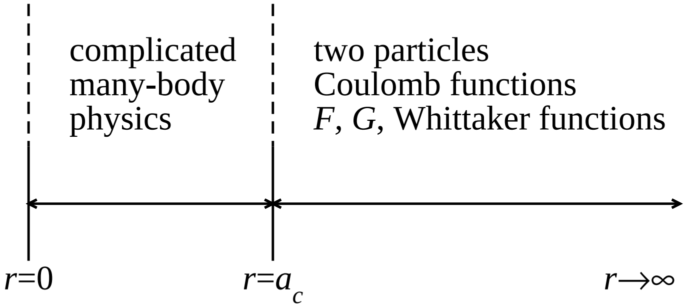
Consider the nuclear reaction $^{3}\mathrm{H}(d,n)^{4}\mathrm{He}$. Answer the following:

- After $^{3}\mathrm{H} + d$ and $n + {}^{4}\mathrm{He}$, should any other particle pairs should be considered?
- Enumerate all of the possible two-particle channels with $\ell \leq 2$, in terms of α, s, ℓ, J, and π.
- Which channels would you expect to be the most important for the $^{3}\mathrm{H}(d,n)^{4}\mathrm{He}$?

When and Why to use Phenomenological R-matrix

- Ab initio or other theoretical approaches may
  - lack the desired precision
  - not be possible
- Parametrization of data for astrophysics, etc...
- Extrapolation / interpolation of data into regions without data
- When dealing with resonances
  - particularly when dealing with more than one
  - particularly when resolved with widths are non-negligible
    - $\rightarrow A < 25$
    - $\rightarrow$ neutron-induced reactions at low energies
- Low energies (few channels)
- When incorporating information from multiple sources:
  - cross section data
  - spectroscopic information (excitation energy, spin,...)
  - transfer reactions (ANCs, spectroscopic factors)
  - theoretical calculations

Basic Idea of the R-Matrix Approach



- Inside the channel radii, a basis of states $|\lambda JM\rangle$ is used.
- The basis is orthogonal and normalized *inside* the channel radii:

$$\langle \lambda' J' M' | \lambda JM \rangle = \delta_{\lambda'\lambda}\delta_{J'J}\delta_{M'M}$$

- The basis is assumed to be complete (but this cannot be exactly true if the number of basis states is finite).
- Bound and scattering states enter on the same footing.

More on the R-Matrix Basis

- Define a channel surface operator:

$$|\mathcal{S}cJM\rangle = \left(\frac{\hbar^2}{2\mu_\alpha a_c}\right)^{1/2} \frac{\delta(r_\alpha - a_c)}{a_c} \times \left[|\psi\rangle_{\alpha s\nu} \otimes i^l Y_{\ell m}(\hat{r}_\alpha)\right]_{JM},$$

  where $\psi\rangle_{\alpha s\nu}$ are channel-spin wavefunctions.
- Then the basis states are defined by requiring that they satisfy

$$\langle \mathcal{S}cJM|\frac{\partial}{\partial r_\alpha} r_\alpha|\lambda JM\rangle = B_c\langle \mathcal{S}cJM|\lambda JM\rangle,$$

  and the Schrödginer equation. The B_c are real energy-independent boundary condition constants.
- We also have

$$B_c = \frac{a_c}{u_{\lambda c}} \frac{du_{\lambda c}}{dr_\alpha}\bigg|_{r_\alpha = a_c},$$

  where $\frac{1}{r}u_{\lambda c}(r_\alpha)$ is the radial part of the projection of $|\lambda JM\rangle$ onto the two-body channel c.
- We thus say that eigenfunctions satisfy a boundary condition on the logarithmic derivative of the radial wavefunction.

Even More on the R-Matrix Basis

- The real energy-independent B_c make this like a Sturm-Liouville eigenvalue problem (precisely so for a single-channel problem with a local central potential).
- Finite volume inside the channel radii
  $\rightarrow$ discrete real eigenvalues $\rightarrow E_\lambda$.
- We define the *reduced width amplitudes*

$$\begin{aligned}\gamma_{\lambda c} &= \langle \mathcal{S} c J M | \lambda J M \rangle \\ &= \left(\frac{\hbar^2}{2\mu_\alpha a_c} \right)^{1/2} u_{\lambda c}(a_c)\end{aligned}$$

- Time-reversal invariance $\rightarrow \gamma_{\lambda c}$ can be defined to be real.
- The J dependence of E_λ and $\gamma_{\lambda c}$ is understood, and is usually not written explicitly.
- This choice of basis is not the only one that can be made:
  - the basis functions do not need to solve the Hamiltonian (calculable R matrix)
  - other boundary conditions

Coulomb Functions

- The Scattering Matrix is determined by the $r \to \infty$ wavefunction.
- Our basis describes the wavefunction at the channel radii.
- $\to$ we need Coulomb functions at $r_\alpha = a_c$.
- We define, using $\rho_\alpha \equiv k_\alpha r_\alpha$, $\rho_c \equiv k_\alpha a_c$ and $' \equiv d/d\rho_\alpha$:

$$\begin{aligned} H_\ell^+(\rho_\alpha) &= G_\ell(\rho_\alpha) + iF_\ell(\rho_\alpha) \\ L_c &= \rho_\alpha \frac{H_\ell^{+\prime}}{H_\ell^+}\bigg|_{\rho_\alpha=\rho_c} = S_c + iP_c \\ \phi_c &= \tan^{-1} F_\ell(\rho_c)/G_\ell(\rho_c), \end{aligned}$$

  where P_c, S_c, and ϕ_c are known as the *penetration*, *shift*, and *phase* factors, respectively. The quantity $-\phi_c$ is sometimes called the hard-sphere phase shift.
- We also need the relative Coulomb phase shift, $\omega_{\alpha\ell} \equiv \sigma_{\alpha\ell} - \sigma_{\alpha 0}$.
- The channel-space matrices $\boldsymbol{B}$, $\boldsymbol{L}$, $\boldsymbol{P}$, and $\boldsymbol{\Omega}$ are defined to be diagonal, with elements B_c, L_c, P_c, and $\exp[i(\omega_{\alpha\ell} - \phi_c)]$, respectively.

The R and S Matrices

- The R-matrix is defined to be

$$R_{c'c} = \sum_{\lambda} \frac{\gamma_{\lambda c'}\gamma_{\lambda c}}{E_\lambda - E}.$$

- Note that $\boldsymbol{R}$ depends on E.
- The most elegant derivation of the S matrix from the R matrix utilizes the Bloch operator; see for examples Eqs. (52)-(66) of Lane and Robson, Phys. Rev. **151**, 774 (1966). https://doi.org/10.1103/PhysRev.151.774
- The result in terms of channel-space matrices is

$$\boldsymbol{S} = \boldsymbol{\Omega}\left[\mathbf{1} + 2i\boldsymbol{P}^{1/2}[\mathbf{1} - \boldsymbol{R}(\boldsymbol{L} - \boldsymbol{B})]^{-1}\boldsymbol{R}\boldsymbol{P}^{1/2}\right]\boldsymbol{\Omega}.$$

- This form for $\boldsymbol{S}$ is automatically unitary and symmetric.
- In practice, $\boldsymbol{R}$ and $\boldsymbol{S}$ are calculated separately for each J^π (block diagonality).

Phenomenological R Matrix

- Adjust E_λ and $\gamma_{\lambda c}$ to describe data!
- These parameters are (mostly) related to to the level energies partial widths of those levels.
- Interestingly, observable quantities, i.e., the S matrix, only depend upon a few properties of discrete eigenfunctions: the energy eigenvalues and the amplitudes at the channel radii.
- The number of levels must be severely truncated.
- Fortunately, the truncations in levels and channels do no destroy the unitarity and time-reversal invariance properties of the S matrix. This is a key reason why the phenomenological R-matrix approach is so useful.

Choosing the Channel Radius

- Formally, the channel radii should be chosen large enough so that nuclear interactions have become negligible.
- However, in a phenomenological analysis, using channel radii which are "too large" cause problems: the states corresponding to a particle in spherical box start coming into play.
- In practice, one typically wants to use a radius just a little bit larger than the "surface" of the nucleus.
- $a_c = 1.4(A_1^{1/3} + A_2^{1/3})$ fm is a reasonable starting point.
- The sensitivity of any conclusions to the adopted radii should be investigated. A large sensitivity indicates that the number of levels has been overly truncated and that an additional (background) level should be included.
- Because there may be some nuclear interactions beyond the radii used in practice, the $\gamma_{\lambda c}$ should be considered to be renormalized quantities, that do not necessarily correspond exactly to the true wavefunction at the channel radii.

Choosing the Boundary Condition Constants

- All choices of the B_c lead to formally equivalent physics: F.C. Barker, Australian Journal of Physics **25**, 341-348 (1972).
- It is not obvious that this is true – that's why it took nearly 30 years after the invention of R-matrix theory for it to be realized.
- There is still confusion about this point, because it is not in Lane and Thomas.
- The choice $B_c = S_c(E_\lambda)$ for a particular level is a useful choice. It provides for a simple interpretation of the parameters associated with that level.
- The alternative basis, to be discussed later, removes the boundary condition choice.

The Single Channel Case

- Now, the R and S matrices are just numbers:

$$\begin{aligned} R &= \sum_\lambda \frac{\gamma_\lambda^2}{E_\lambda - E} \\ S &= \exp[2i(\omega_\ell + \delta)] = \exp[2i(\omega_\ell - \phi_\ell)] \left[1 + \frac{2iP_\ell R}{1 - R(S_\ell + iP_\ell - B)}\right]. \end{aligned}$$

- A little algebra yields

$$\delta = \tan^{-1} \frac{P_\ell R}{1 - R(S_\ell - B)} - \phi_\ell.$$

S-wave Neutrons

- For no Coulomb interaction, we have

$$\begin{aligned} F_\ell(0,\rho) &= \rho\, j_\ell(\rho) \\ G_\ell(0,\rho) &= -\rho\, n_\ell(\rho). \end{aligned}$$

- For $\ell = 0$, this becomes

$$\begin{aligned} F_0(0,\rho) &= \sin(\rho) \\ G_0(0,\rho) &= \cos(\rho) \end{aligned}$$

- and $P_0 = \rho$, $S_0 = 0$, $\phi_0 = \rho$.

- The single-channel case is now very simple (assuming $B = 0$):

$$\delta = \tan^{-1}(\rho R) - \rho.$$

S-wave Neutrons, No Interaction

- This is easily solved analytically:

$$
\begin{aligned}
\delta &= 0 = \tan^{-1}(\rho R) - \rho \quad , \text{ or} \\
R &= \frac{\tan\rho}{\rho} = \sum_{\lambda=1}^{\infty} \frac{\gamma_\lambda^2}{E_\lambda - E} \quad , \\
E_\lambda &= \frac{\pi^2 \hbar^2 (\lambda - 1/2)^2}{2\mu a^2} = \frac{(\hbar k_\lambda)^2}{2\mu} \quad , \quad \lambda = 1, 2, 3, \ldots , \\
\gamma_\lambda &= (-1)^{\lambda+1} \left(\frac{\hbar^2}{\mu a^2} \right)^{1/2} , \quad \text{and} \\
u_\lambda(r) &= \frac{\sin(k_\lambda r)}{\left[\int_0^a \sin^2(k_\lambda r)\, dr \right]^{1/2}} = \sqrt{\frac{2}{a}} \sin(k_\lambda r) \quad .
\end{aligned}
$$

- The R matrix in non-zero, even if there are no interactions! This is related to the problem that arises when the channel radius is too large: the R matrix must compensate for the large hard-sphere phase shift.

The Single Channel Case: Single Level

- Assume we are near the level energy $\rightarrow R = \frac{\gamma^2}{E_R - E}$.
- Adopt $B = S_\ell(E_R)$ and define $\delta = \delta_R - \phi_\ell$.
- Approximate $S_\ell - B \approx \left.\frac{dS_\ell}{dE}\right|_{E_R}(E - E_R)$.
- Then

$$\delta_R = \tan^{-1}\frac{\Gamma/2}{E_R - E}$$

and

$$\Gamma = \frac{2\gamma^2 P_\ell}{1 + \gamma^2 \left.\frac{dS_\ell}{dE}\right|_{E_R}}.$$

- This is how R-matrix parameters may be interpreted as resonance parameters.

What About Bound a Bound State?

- For bound channels, we have $P_c = 0$ and

$$S_c = \frac{r_\alpha}{W_\ell} \left. \frac{dW_\ell}{dr_\alpha} \right|_{r_\alpha = a_c},$$

  where W_ℓ is the exponentially-decaying Whittaker function.
- Adopting $B_c = S_c(E_R)$ is now just the usual bound-state condition.
- The radial part of the projection of the asymptotic wavefunction of a bound state onto the channel c is $\frac{C_c}{r} W_\ell(r_\alpha)$, where C_c is the Asymptotic Normalization Constant (ANC).
- Specifically, $N^{1/2} u_c(a_c) = C_c W_\ell(a_c)$, where $N^{1/2}$ changes the normalization from inside the channel radii to all space.
- One can show that $N^{-1} = 1 + \sum_c \gamma_c^2 \left. \frac{dS_c}{dE} \right|_{E_R}$, and thus

$$C_c = \frac{(2\mu_\alpha a_c)^{1/2}}{\hbar W_\ell(a_c)} N^{1/2} \gamma_c$$

- Note the analogy: C_c^2(bound state) $\longleftrightarrow$ Γ_c(unbound state).

Calculation of Observables

- Once the scattering matrix is known, any observable (e.g., differential cross section) can be calculated.

- One may think about this as

  R Matrix $\to$ S Matrix $\to$ Scattering Amplitudes $\to$ Observables

- Being able to to fit or predict as many experimental observables as possible can be important. Differential cross section and polarization data are particularly useful for untangling various J^{π} contributions (partial wave analysis).

- As an example of what can be done, James deBoer and I have worked out how to calculate the angular distribution of secondary γ rays from reactions.

Calculation of Observables, continued

- Observables generally involve bi-linear products of S-matrix elements, and possibly Coulomb amplitudes.
- Note that levels with the same J^π will interfere as a function of *energy*, while levels of differing J^π will interfere as a function of *angle*, but not energy.
- The cross section for $\alpha \to \alpha'$, when $\alpha \neq \alpha'$, is given by

$$\sigma_{\alpha\alpha'} = \frac{\pi}{k_\alpha^2} \sum_{J, c \ni \alpha, c' \ni \alpha'} \frac{2J+1}{(2J_{\alpha 1}+1)(2J_{\alpha 2}+1)} |S^J_{c'c}|^2.$$

The General Single-Level Case

- The S matrix is given by

$$S_{c'c} = \Omega_{c'}\Omega_c \left[\delta_{c'c} + 2i(P_{c'}P_c)^{1/2} \frac{\gamma_{c'}\gamma_c}{E_R - E - \sum_{c''}\gamma_{c''}^2(S_{c''} + iP_{c''} - B_{c''})}\right]$$

- Adopt $B_c = S_c(E_R)$, $S_c - B_c \approx \frac{dS_c}{dE}\big|_{E_R}(E - E_R)$, and ignore $\Omega_{c'}\Omega_c\delta_{c'c}$.
- Then we have (assuming $\alpha \neq \alpha'$)

$$\sigma_{\alpha\alpha'} = \frac{\pi}{k_\alpha^2} \sum_{c\ni\alpha, c'\ni\alpha'} \frac{2J+1}{(2J_{\alpha 1}+1)(2J_{\alpha 2}+1)} \frac{\Gamma_c\Gamma_{c'}}{(E-E_R)^2 + (\Gamma/2)^2},$$

where

$$\Gamma_c = \frac{2\gamma_c^2 P_c}{1 + \sum_{c'}\gamma_{c'}^2 \left.\frac{dS_{c'}}{dE}\right|_{E_R}} \quad \text{and} \quad \Gamma = \sum_c \Gamma_c.$$

- The famous Breit-Wigner formula with partial and total widths!

The $\boldsymbol{S}$ 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.

$\boldsymbol{R}$ matrix versus $\boldsymbol{A}$ matrix

- Is better to use the $\boldsymbol{R}$ matrix or the $\boldsymbol{A}$ matrix to calculate $\boldsymbol{S}$?
- If the the number of channels is $\gg$ than the numbers of levels for a given J^π, then it will be more efficient to use the $\boldsymbol{A}$ matrix. Note that the computation effort required to invert a matrix typically increases as the cube of the number of rows (or columns).
- Likewise, if the number of levels is $\gg$ than the number of channelse, then the $\boldsymbol{R}$ matrix will be more efficient.

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 $^{12}C(\alpha, \gamma)^{16}O$, 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) https://doi.org/10.1103/PhysRevC.66.044611 .
- 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 $S_{\lambda c} = S_c(E_\lambda)$.
- This approach is known as the alternative or Brune basis.
- This is what is done by default in the AZURE2 code.

Features of the alternative basis

- It is mathematically equivalent to the Lane-and-Thomas formalism.
- Level shifts are eliminated, so that exact excitation energies can be easily implemented.
- Interpretation of fit parameters in terms of excitation energies, partial widths, and/or ANCs is straightforward.
- Parameter correlations are reduced. This feature is important for fitting and/or random-walk parameter searching.
- One normally only considers using the $\boldsymbol{A}$ matrix in this formalism. There are cases where it could be more efficient to convert the parameters to the Wigner-Lane-Thomas formalism and then to use the $\boldsymbol{R}$ matrix.

Thank you for your attention.