Recent Advances in R-matrix Data Analysis

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1 R-matrix Theory

R-matrix theory is designed to describe individual resonances in two-body scattering even when overlapping, and the non-resonant background between them. It describes all the asymptotic properties of the relative wave function outside some fixed radius a in terms of pole energies e_p and reduced width amplitudes $\gamma_{p\alpha}$ for each partial-wave channel α and pole p. The $\gamma_{p\alpha}$ can be calculated from some structure theory, or fitted to data.

R-matrix theory is the starting point for compound-nucleus models. It is the basis for making statistical approximations, such as the Reich–Moore approximation, and Hauser-Feshbach models. It can be used to check the accuracy of those approximate models, as well as models for the width-fluctuation corrections.

The foundation of R-matrix theory is summarized in the landmark paper of Lane and Thomas [1]. In that paper is the foundational "R-matrix Theorem": For Hermitian $H = T + V + \hat{B}$ with Bloch operator $\hat{B} = \delta(r-a)(\frac{d}{dr} - \frac{B}{r})$, with $V \neq 0$ only for $r \in [0, a]$ and E-independent, then the exact scattering solution $H\psi = E\psi$ can be represented by a R-matrix at $r = a$ with a set of pole energies e_p and reduced width amplitudes $\gamma_{p\alpha}$ as

$$R_{\alpha\alpha'}(E) = \sum_{p=1}^{\infty} \frac{\gamma_{p\alpha}\gamma_{p\alpha'}}{e_p - E}. \tag{1}$$

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2 Phenomenological R-matrix

The "phenomenological R-matrix method" that is followed in the remainder of this paper does not start from a Hamiltonian and does not have an infinite series of poles. Rather it uses a finite number P of R-matrix pole energies e_p, with reduced width amplitudes $\gamma_{p\alpha}$ as parameters in the familiar *finite* sum

$$R_{\alpha\alpha'}(E) = \sum_{p=1}^{P} \frac{\gamma_{p\alpha}\gamma_{p\alpha'}}{e_p - E}, \tag{2}$$

to be adjusted to fit experimental scattering data. Positive-energy poles are again aligned with scattering resonances. Other poles are "background poles" at higher positive energies to attempt to represent the effects of all the remaining terms missing in comparison with expression (1).

Both the exact and phenomenological R-matrix expressions yield (a) unitary S-matrix at each energy, and (b) orthogonal scattering wave functions at different energies. When we come to the approximations often used in R-matrix theory, they should only be accepted if at least they still yield those features. Both conditions derive from having a Hermitian and energy-independent Hamiltonian.

The Reich–Moore approximation [2], by contrast, has imaginary damping widths for missing channels, so condition (a) is not satisfied. It is perhaps satisfactory if a specific meaning is given to the missing flux, e.g., capture or fusion.

Another convenient approximation changes the boundary conditions in the Bloch operator, so B is not constant but is set equal to the shift function at each energy: $B = S(E)$. But now condition (b) is not satisfied since $H = T + V + \hat{B}$ is energy-dependent.

The "alternative parametrization" of Brune [3] is much better than using $B = S(E)$ for making R-matrix pole energies close the energies of cross-section peaks and resonances, since the Brune basis is transformable to and from the Lane and Thomas formalism.

3 Verification of R-matrix Codes

An inter-comparison of the capabilities of the R-matrix codes AMUR [4], AZURE2 [5], EDA (LANL), FRESCOX [6], GECCCOS (TU Vienna), SAMMY [7], and CONRAD [8] was performed [9] following a series of IAEA consultants meetings since 2015 [10–13]. As the codes were developed initially for the solution of different problems, each one has its particular features, strengths, and weaknesses, an inter-comparison is particularly valuable.

I have written a python program FERDINAND.PY, to translate between most of the input and output formats of these codes, using GNDS [14] as the intermediate structure. It is also able to make ENDF output sections in the MT= 151 format for evaluations. This kind of interchangeability makes it much easier to track down discrepant details, and to verify and build on each other's work.

4 Example in A = 7 Scattering

As an example of R-matrix fits, Fig. 1 shows the FRESCOX results for ^{4}He+^{3}He elastic scattering, with the p+^{6}Li channel also included. A code-to-code comparison for this data "based on fixed R-matrix parameters" is shown by ratios in Fig. 2. Agreement is almost all better than 0.5%, the level of accuracy needed for R-matrix standard cross-sections. The original fit was done with $B = -L$ boundary conditions, but we can easily and reversibly transform to the Brune basis.

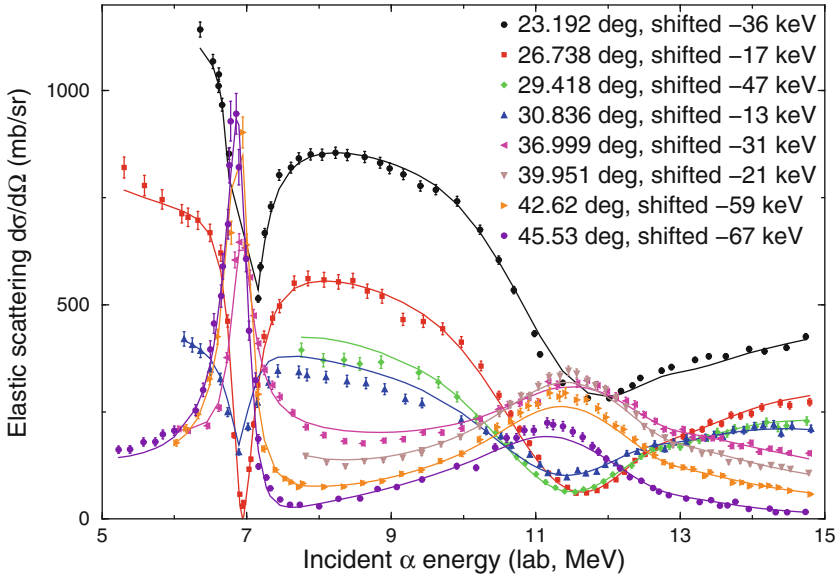

Fig. 1 Fitted cross-sections ^{3}He$(\alpha,\alpha)^3$He reaction to the data of [15]. The separate curves are for each scattering laboratory angle, with preferred data shifts shown by the listed keV values. Tombrello quoted a systematic uncertainty of 5%. Taking this as a 1σ value, the overall fit preferred a systematic increase of the data by 8%

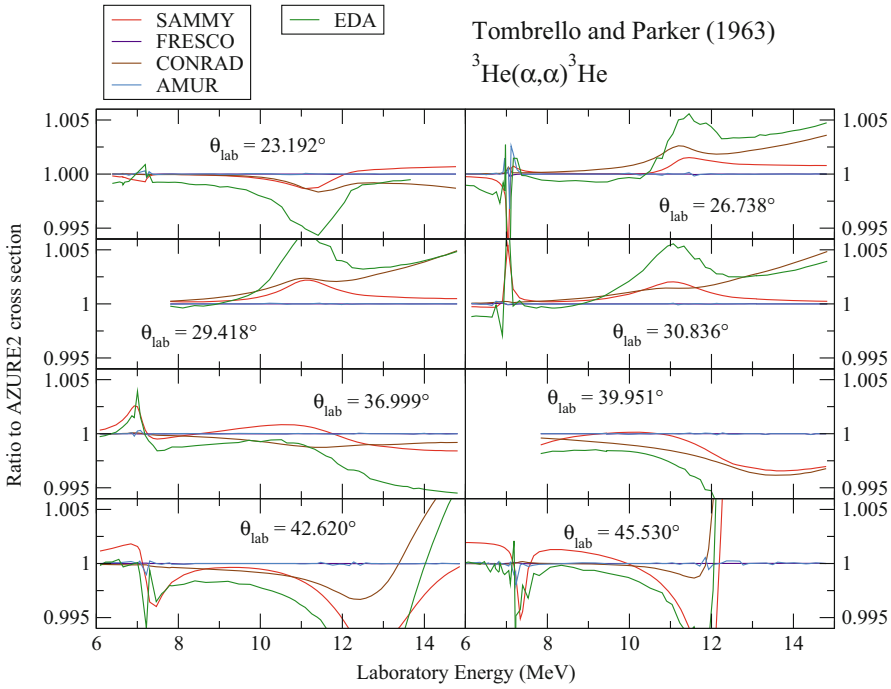

Fig. 2 Comparison of calculations to AZURE2 results for the ^{3}He$(\alpha, \alpha)^3$He reaction using the energies and angles of the [15] data

5 An "Optical" R-matrix Model

At higher incident energies, there are more and more inelastic or transfer two-body channels. Numbers of partial waves increase, but this is still manageable using standard R-matrix theory. But when breakup channels begin to open, these are more difficult to model as they need three-body dynamics. Sometimes these can be well approximated by cascaded two-body channels [16], or by using hyper-spherical harmonics to model the three-body kinematics in full detail. In the meantime, we could perhaps settle for using damping widths Γ_α to describe loss of flux to outside the two-body model space in generalization of the Reich–Moore approximation.

Such damping widths Γ_α describe loss of flux to outside the model space like an optical model, generalizing Reich–Moore for missing particle channels, as in

$$R_{\alpha\alpha'}(E) = \sum_{p=1}^{P} \frac{\gamma_{p\alpha}\gamma_{p\alpha'}}{e_p - E + i\Gamma_\alpha/2}. \tag{3}$$

This could be allowed, as mentioned earlier, if there are specific physical channels missing from the model (never for bound states). Then the missing flux (from the

unitarity defect) could (for example) be fed into a Hauser-Feshbach decay model built only on the missing physics channels.

But if the total width of a damped resonance is large, then the flux will be missing at lower energies, even below the known threshold for the excluded channels! In that case, absorption would still be present below the threshold of the missing channels, and that would be unphysical.

I therefore consider energy-dependent damping widths, which allows me to describe the energy dependence of flux going to an excluded channel with known threshold E_0. This makes the damping width energy-dependent, $\Gamma_\alpha(E)$. Ideally, we would like the energy dependence to mimic a set of missing level widths, each behaving as the formal R-matrix widths $\Gamma = 2\gamma^2 P_L(E-E_0)$. So I used, for each R-matrix level p above threshold, a formula which cuts off the width below threshold:

$$\Gamma_\alpha(E) = \tilde{\Gamma}_\alpha \frac{P_L(E - E_0)}{P_L(e_p - E_0)}, \tag{4}$$

for penetrability functions $P_L(E - E_0)$. This cuts off the damping for $E < E_0$, and gives $\Gamma_\alpha(e_p) = \tilde{\Gamma}_\alpha$ as a parameter to be fitted. Making this work depends on having good experimental data for angular distributions above the E_0 threshold. We may also need to choose the e_p energy in the Brune basis in order to keep it at the right energy above the threshold.

If we know the physics of missing channels we can estimate L and Coulomb barriers in the penetrability functions. This would even allow many-body exit channels, in particular three-body ($M = 3$) channels such as (p, pn). If these are described by hyper-spherical harmonics, then there is a new quantum number $K \geq 0$ that describes the ratios of the new three-body coordinates for given moment of inertia ρ. For each value of K there is a centrifugal barrier $L(L + 1)/\rho^2$ where $L = K + (3M - 6)/2$. For 3-body breakup channels this gives $L = K + 3/2$. If a particular K dominates in an exit channel, then the corresponding L-value should be used in Eq. (4).

As an example fit with energy-dependent damping, I refitted ^{4}He+^{3}He data from Tombrello [15] with only the elastic channel, and no explicit p+^{6}Li channel which should open above 10 MeV. The effect of the missing channel is to be represented by the new fitted damping parameters. I fitted the e_p energy in the Brune basis, keeping $L = 0$. The result is shown in Fig. 3, with a fit quality of χ^2/df= 4.25 compared with 2.63 in the full R-matrix fit.

This first attempt at least gives (blue line on the right) transfer cross-sections that are close to the average of the more complete model (black line). It has no absorption below 10 MeV, unlike what we would get from fixed damping widths (red line).

This kind of treatment is reminiscent of optical models for elastic scattering, where energy-dependent imaginary terms are added even though the total Hamiltonian is no longer Hermitian or even energy-dependent. It is available as a resort above the energy range of a strict Lane and Thomas model, by generalizing the Reich–Moore approximation to particle channels.

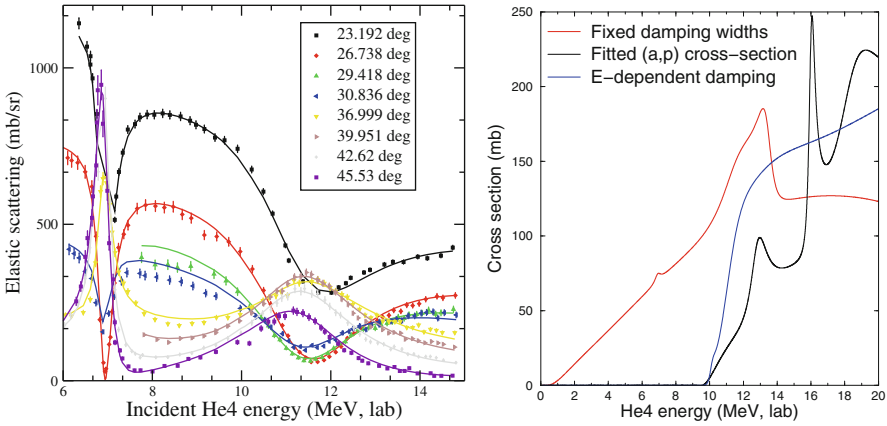

Fig. 3 (Left) Fitted cross-sections $^{3}\mathrm{He}(\alpha,\alpha)^{3}\mathrm{He}$ reaction to the data [15], without an explicit p+^{6}Li channel, but with energy-dependent damping. (Right) Absorption cross-sections from the elastic channel, with red, black, and blue lines from Eqs. (3), (2), and (4), respectively

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