Interchange, Extension and Validation of R-matrix fits for gamma production

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Abstract. The R-matrix method of Lane and Thomas is the standard procedure for modeling resonances at low energies, to determine widths and angular distributions needed for nuclear evaluations. Many different codes have been written with different input and output file formats, so a new code FERDINAND is available to interchange parameters. The standard procedure requires fixed boundary condition constants, so the ansatz of allowing energy-dependence for such ‘constants’ should be deprecated. The future need for larger R-matrix fits with more target excited states, to enable better prediction of gamma-rays from the decays of those states, will almost certainly be facilitated by the GPU parallel methods that are now appearing.

1 R-matrix methods

The R-matrix method of Lane and Thomas [1] is the standard procedure for modeling resolvable resonances at low energies, at least for two-body channels. The methods can be used to solve quantum problems defined by a Hamiltonian confined within a specific R-matrix radius. It provides a discrete basis for the interior wave functions that easily enables exterior scattering wave functions to be found by means of R-matrix pole energies and reduced width amplitudes at each pole for all the coupled partial wave channels. It can describe both resonant and non-resonant behaviors.

R-matrix phenomenology fits resonances and data between resonances not from a Hamiltonian, but by directly adjusting the pole energies and reduced widths to fit known data of cross sections and angular distributions. This is extensively used for low-energy ranges of resolved neutron resonances on many targets to give the continuous cross sections and angular distributions in our nuclear data libraries. The ‘limited R-matrix’ format in the ENDF6 [2] data specification is in fact not limited, since it is quite sufficient to store all R-matrix parameters, including for charged-particle reactions.

2 Codes for fitting and translating

Many different codes have been written to fit R-matrix parameters to experimental data, but they have different input and output file formats. To ensure that results can be communicated and replicated, I make available a python code FERDINAND[3] using FUDGE [4] to read and write ENDF6, GNDS [5] standard formats, to read AMUR, AZURE [6], EDA, FRESCOX [7, 8] and RAC formats, and to write AZURE, EDA, FRESCOX, HYRMA and latex formats. This code greatly facilitated the recently-published code comparison of Thompson et al [9]. It functions by translating all the input formats to and from the new GNDS format as an intermediate. At the GNDS stage, we can convert to and from the Brune basis [10], and hence also change the boundary condition constants $B_\alpha$ in each partial wave channel $\alpha$. It can convert between reduced width amplitudes and reduced widths, add or remove Reich-Moore channels, and also reconstruct point-wise distributions for cross-sections and/or angular distributions from the R-matrix parameters.

3 Non-standard boundary conditions

Many historical neutron evaluations have been fitted using the $B = S(E)$ ansatz where the boundary-condition constant $B$ has been non-physically replaced by the shift function $S(E)$, which is in fact a function of energy $E$. The advantages of this are that arithmetic is simplified for point-wise reconstructions, and that $s$-wave resonance peaks are very close to the R-matrix pole energies which makes it easy to construct a non-uniform energy grid with more densely-placed points in the peak regions.

However this $B = S(E)$ ansatz is not within the Lane and Thomas framework. It is non-physical because it leads to scattering wave functions which are no longer orthogonal to each other at different energies. It also means that we can no longer inter-convert such R-matrix parameter sets to other options such as $B = \text{constant}$, $B = -L$, or the Brune basis.

For these reasons the use of this ansatz should be deprecated and ultimately removed. Some codes already have alternative options in place (AZURE, FRESCOX, and EDA). Other codes such as SAMMY [11] are currently being adapted to use and fit physical boundary condition configurations.
4 Comparison of R-matrix codes

The comparison of R-matrix codes consists first of verifying that they use the same Coulomb wave functions to calculate shift functions, penetrabilities and hard-sphere phase shifts. Secondly we verify the physical constants and masses. Are the masses for nuclei, or do they include the electrons as atomic masses? Are the $Q$-values consistent relativistically with the given masses? Thirdly we compare the coupling orders, whether the codes use $LS$ or $SL$ for example? Do they include (somewhere) the $^2$Hub phases [12]? If the codes use different conventions for these phases, then correction factors can be easily included in the FERDINAND translation code. The FRES-COX code, for instance, does not build the Huby phases into the definition of the nuclear states, but includes them as a factor of the channel couplings. They thus have to be coded in the FERDINAND translations.

Lastly the comparison consists of verifying that the codes give the same cross sections for the same input R-matrix parameters. The publication Thompson et al. [9] shows the agreements between some existing codes. Fig 1 shows, for example, the ratios of the code’s outputs to the AZURE2 predictions. The ratios are slightly further from unity around the resonance at 7 MeV where the cross sections vary more rapidly with energy.

![Figure 1](https://example.com/figure1.png)

**Figure 1.** Comparison of calculations to AZURE2 results for the $^3$He$(\alpha,\alpha)^3$He reaction using the energies and angles of the [13] data. Here the vertical axis is scaled to a uniform 1%.

5 Gamma production

Because of the increasing need for gamma production information, R-matrix codes are being extended to include primary and secondary gammas and predict the angular distributions for both of kinds. Lighter nuclei tend to produce larger-energy gamma rays because of lower typical level densities, and such gammas are easier to detect experimentally. The R-matrix method is useful when low level densities mean that individual resonances can be distinguished by energy, spin and parity: this is the ‘resolved resonances region’ (RRR). To predict secondary gamma-ray intensities, however, more excited states of residual nuclei need to be included in the fits, since these are the levels (e.g. the excited states shown in Fig. 2 for $n+^{14}$N), that decay to produce many of the observed secondary gamma decays.

![Figure 2](https://example.com/figure2.png)

**Figure 2.** Hauser-Feshbach predictions (averaged over resonances) for inelastic n,n' exit energy distributions at 14 MeV incident neutron energy, for the first 9 excited states in $^{14}$N.

Many historical R-matrix fits stop at an upper energy which does not give too many open channels, but for gamma-ray production it is precisely these additional channels from excited-state production that do need to be included. This places additional computational demands on the codes. The use of GPUs should enable faster calculations, especially if the computational method is organized to calculate all scattering energies in parallel – as is possible on such devices. I find that using the Tensorflow framework [14] enables the development of efficient GPU codes. The LLNL code RFLOW [15] will soon be available for fitting excitation functions and angular distributions.

6 Connecting R-matrix with statistical models at higher neutron energies

The level densities increase at higher excitation energies, where individual resonances can no longer be resolved in experiments. There are two possible methods here. We can extrapolate spin-dependent level densities from lower to higher energies following the same statistical trends. This gives an ‘unresolved resonance region’ (URR) where resonances now have to be probabilistically produced to give a probability distribution for each of the needed channel cross sections. The other method is to move to the Hauser-Feshbach (HF) statistical approximation [16], which tries to calculate just the average cross sections. This HF approximation can be derived from the R-matrix method by neglecting all the resonance interference terms, and by using optical potentials to give physical values of the ratios of average level widths to average level spacings. The HF method also replaces an average of width ratios by a ratio of average widths, but often include a ‘width fluctuation correction’ to compensate for the error caused by this change of averaging.
In most nuclear evaluations there is a need to include higher-energy resonances in the compound nucleus, above the RRR. This will require theory consistency checks to ensure smooth transitions from unresolved and/or overlapping resonances in an R-matrix code to Hauser-Feshbach predictions that are based on transmission coefficients derived from optical potentials. A good connection between these two methods should be possible because the Hauser-Feshbach method may be derived as an approximation to R-matrix resonance descriptions.

7 Conclusions

New tools are available for the interchange of R-matrix fits between the multiple international codes. My utility FERDINAND [3] allows such fits to be easily verified between codes, and thus to be validated by the same standard methods to compare evaluated cross sections with experimental data such as from EXFOR.

I argue that R-matrix codes should use boundary condition constants that are indeed constant, and not made to track any non-constant shift functions $S(E)$. Constant boundary conditions enable parameter sets to be translated to other $B$ values, and also converted to the Brune basis [10], since they follow then the Lane and Thomas standard.

Finally, I observe that the needs to predict secondary gamma-ray production from the decays of target excited states modeled by R-matrix fits will require the inclusion of many more excited states in these fits than have been common up to now. I suggest that search procedures using GPUs to solve all scattering energies in parallel will prove to be very useful.

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References

[16] W. Hauser, H. Feshbach, Phys. Rev. 87, 366 (1952)