II.B.2. Simulation of Full R-Matrix

While SAMMY does not yet have the ability to calculate the full (unapproximated) R-matrix of Lane and Thomas [AL58], it is possible to use the Reich-Moore approximation in such a way that it mimics the full R-matrix with a high degree of accuracy. This is necessary, for example, in cases where there are interference effects between the (incident) neutron channel and a gamma channel – that is, for some low-mass nuclides.

The Reich-Moore approximation involves an aggregate treatment ("eliminated channels") for the gamma widths (capture widths). Therefore, to approximate the full R-matrix, one sets the Reich-Moore gamma width to a very small number and uses an exit channel to define the actual gamma channel:

1. Set the SAMMY gamma-channel widths to a very small number, perhaps 0.001.

2. Define an exit channel to be the actual capture channel and assign appropriate values for the widths. Quantum numbers for this channel will be the same as those for fission channels (in particular, set LPENT = 0).

3. When calculating capture cross sections, set the IFEXCL flag to 1 for all other (non-gamma) exit channels. (See Section II.B.1.c and card set 10.1 or 10.2 of Table VIA.1 for details.) When calculating other reaction cross sections, set the IFEXCL flag to 0 for the reaction channels of interest, to1 for the capture channels, and to 1 for any other reaction channels to be excluded.

When utilizing this option, SAMMY users should take care that results are not unduly influenced by the approximation in step 1 above. To test this, make radical changes in the value used for the gamma widths (e.g., set the value to 100.0 or 10^{-6}) and recalculate the cross section. Note that it is not possible to set these values to zero; doing so results in numerical overflow problems (because computers do not know how to calculate zero divided by zero).

Comparisons between cross sections calculated by SAMMY and those generated by the R-matrix code EDA [GH75] using the same R-matrix parameters have shown agreement to ~5 significant digits [INDC03]. Some of the runs for those comparisons are now assembled into SAMMY test case tr125.

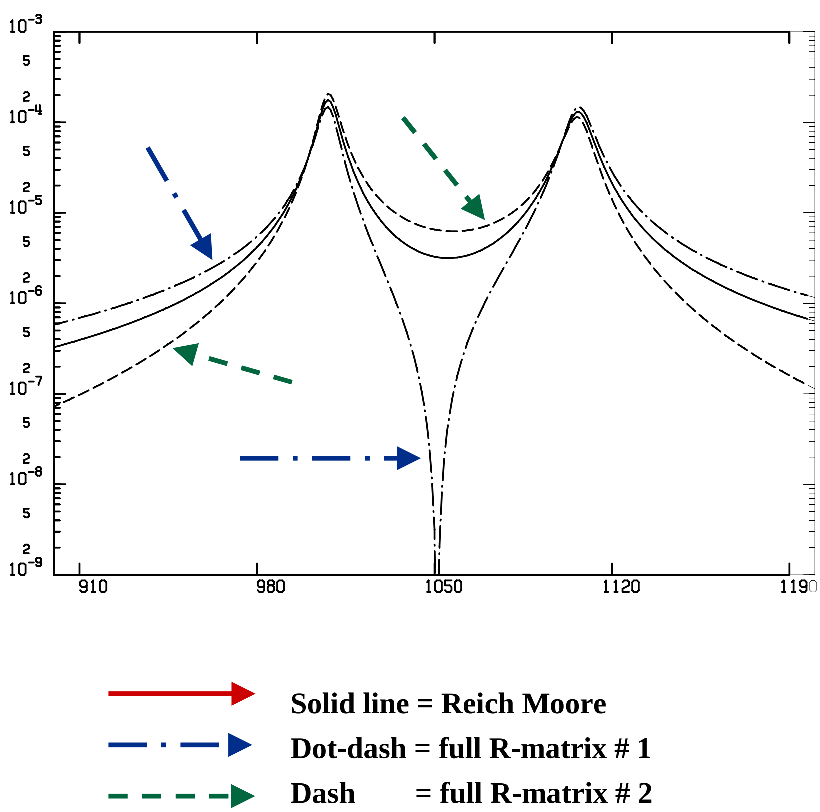
Test case tr110 shows an artificial but extreme example of a situation in which use of the Reich-Moore approximation gives very different results from those obtained via the full R-matrix. For this example, there are two resonances with parameter values as shown in Table II B2.1; plots of the curves calculated with those parameters are shown in Figure II B2.1. As evident from the figure, the Reich-Moore curve lies between the two extreme R-matrix curves which show constructive (dashed curve) and destructive (dot-dash curve) interference.

Table II B2.1. Parameter values used to illustrate Reich-Moore vs. full R-matrix calculations

	λ	Energy (MeV)	$\overline{\Gamma}_{\lambda\gamma}$ (eV)	$\Gamma_{\lambda n}$ (eV)	Sign $\times\, \Gamma_{\lambda\gamma}$ (eV)[a]
Reich Moore	1	1.0	1.0	10000.	
	2	1.1	1.1	11000.	
Pseudo-full R-matrix # 1	1	1.0	10^{-8}	10000.	1.0
	2	1.1	10^{-8}	11000.	1.1
Pseudo-full R-matrix # 2	1	1.0	10^{-8}	10000.	1.0
	2	1.1	10^{-8}	11000.	−1.1

[a] Remember that the value given in the SAMMY PARameter file is not the partial width Γ (which is always a positive number); rather, it is the sign of the reduced-width amplitude γ multiplied by the partial width Γ. Hence, the negative sign in the final entry of this table is actually associated with the reduced-width amplitude for the capture channel. See Section II.B.1 for further discussion.

Figure II B2.1. Reich-Moore approximation vs. full R-matrix for artificial example of test case tr110.



Different treatments for different capture channels

Occasionally it may be convenient to treat certain gamma widths individually while treating most gamma widths in aggregate fashion. This can be accomplished by defining "particle" channels for the individual widths (as described above), and using the Reich-Moore capture channel (eliminated width) for the aggregate width.

To calculate the capture cross section in this situation, it is not sufficient to specify the data type as "CAPTURE", because that would give only the contribution from the aggregate width. To obtain the contribution from the individual widths, specify the data type as "REACTION" or (preferably) as "FINAL state pairs =" followed by the exact names specified for the gamma-channel particle-pairs. (See card sets 4 and 8 of Table VI A.1 and Section II.B.1.c for details.)

To calculate the complete capture cross section, use "FINAL state pairs =" for the data type, and add the command line

```
ADD ELIMINATED CAPTUre channel to final state
```

This will cause SAMMY to add the contributions from the individual capture channels plus the contribution from the aggregate channels.

The formula used to calculate the capture cross section is similar to Eq. (II B1 a.6), with only the non-capture exit channels included in the summation over c',

$$\sigma_{capture}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[X_{cc}^i - \sum_{\substack{c' = \text{non-capture} \\ \text{exit channels}}} \left\{ X_{cc'}^{i\;2} + X_{cc'}^{r\;2} \right\} \right] \quad . \qquad \text{(II B2.1)}$$