SAMMY Workshop Part 4.1b

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Part 4.1b, Approximations to R-Matrix

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Common Approximations to the Scattering Matrix

- **Reich-Moore Formalism (RM)**
- **Multilevel Breit-Wigner (MLBW)**
- **Single-level Breit-Wigner (SLBW)**
- **Adler-Adler Formalism (AA)**

- **Alternative Formulation – Multipole (MP)**
  - **Not an approximation, just a different view**

Reich Moore

- **The method of choice for most evaluations**
- **Derived from the A-Matrix by assuming no off-diagonal terms for gamma channels**

$$A^{-1}_{\mu\lambda} \approx \left(E_\lambda - E - i\overline{\Gamma}_{\lambda\gamma}/2\right)\delta_{\mu\lambda} - \sum_{\substack{c = \\ \text{particle} \\ \text{channels}}} \gamma_{\mu c} L_c \gamma_{\lambda c}$$

Reich Moore, cont.

- **R-Matrix is**

$$R_{cc'} = \left[\sum_{\lambda} \frac{\gamma_{\lambda c}\, \gamma_{\lambda c'}}{E_{\lambda} - E - i\bar{\Gamma}_{\lambda\gamma} / 2} \right] \delta_{JJ'}$$

- **X is given in terms of R as**

$$X = P^{1/2} L^{-1} \left(L^{-1} - R \right)^{-1} R\, P^{1/2}$$

- **Cross sections are written in terms of X**

Using X is not "standard operating procedure" or standard notation, but it is a reliable method for calculating cross sections. The more common method (using $W = 1 + 2iX$) has problems with numerical stability.

Reich Moore, cont.

- **Total cross section is**

$$\sigma_{total}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \left[\frac{1}{2} \sin^2 \varphi_c + X_{cc}^i \cos(2\varphi_c) - X_{cc}^r \sin(2\varphi_c) \right]$$

where summation over c includes only the appropriate (incident) channels

Reich Moore, cont.

- **Elastic cross section is**

$$\sigma_{elastic}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \Big[\sin^2 \varphi_c \left(1 - 2X_{cc}^i\right) - X_{cc}^r \sin\left(2\varphi_c\right) + \sum_{c'} \left\{ X_{cc'}^{i\,2} + X_{cc'}^{r\,2} \right\} \Big]$$

where again sum over c includes only incident channels

Reich Moore, cont.

- **Reaction cross section is**

$$\sigma_{reaction}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_c \sum_{c'} \left[X_{cc'}^{i\,2} + X_{cc'}^{r\,2} \right]$$

where sum over c includes incident channels, sum over c' includes reaction channels

- **Capture cross section is**

$$\sigma_{capture}(E) = \frac{4\pi}{k_\alpha^2} \sum_J g_{J\alpha} \sum_{inc\,c} \left[X_{cc}^{i} - \sum_{all\,c'} \{ X_{cc'}^{i\,2} + X_{cc'}^{r\,2} \} \right]$$

Reich Moore, cont.

- **Can we write cross sections directly in terms of the resonance parameters?**
- **For example: one-level two-channel case…**

$$\sigma_{elastic}(E) = \frac{2\pi}{k_\alpha^2}\sum_J g_{J\alpha}\sum_c\left[1-\cos 2\varphi_c\left(1-\frac{\Gamma\Gamma_1}{2d}\right)\right.$$
$$\left.-\sin 2\varphi_c\frac{(E-E_\lambda)\Gamma_1}{d}-\frac{\Gamma_1(\Gamma_\gamma+\Gamma_2)}{2d}\right]$$

For more of this example, see the SAMMY manual.

Multilevel Breit Wigner

- **The method of choice 30 or 50 years ago**
- **Derived from the A-Matrix by assuming no off-diagonal terms for *any* channels**

$$A^{-1}_{\mu\lambda} \approx \left(E_\lambda - E - \sum_{all\ c} L_c \gamma^2_{\lambda c} \right) \delta_{\mu\lambda}$$

$$= \left(\left(E_\lambda - \sum_{all\ c} \left(S_c - B_c \right) \gamma^2_{\lambda c} \right) - E - i \sum_{all\ c} P_c \gamma^2_{\lambda c} \right) \delta_{\mu\lambda}$$

$$= \left(E^{BW}_\lambda - E - i\Gamma_\lambda / 2 \right) \delta_{\mu\lambda}$$

Multilevel Breit Wigner, cont.

- **Reaction cross section is**

$$\sigma_{cc'}^{MLBW} = \frac{4\pi g_J}{k^2} \sum_{\lambda} \frac{\Gamma_{\lambda c}\Gamma_{\lambda c'}}{\Gamma_{\lambda}^2} \left(\mathrm{Re}\, M_{\lambda}^{cc'} \psi_{\lambda} + \mathrm{Im}\, M_{\lambda}^{cc'} \chi_{\lambda} \right)$$

where psi & chi functions are given by

$$\psi_{\lambda} = \frac{\Gamma_{\lambda}^2 / 4}{\left(E_{\lambda}^{BW} - E \right)^2 + \Gamma_{\lambda}^2 / 4} \qquad \chi_{\lambda} = \frac{\left(E_{\lambda}^{BW} - E \right) / 4}{\left(E_{\lambda}^{BW} - E \right)^2 + \Gamma_{\lambda}^2 / 4}$$

with

$$M_{\lambda}^{cc'} = 1 + \sum_{\lambda' \neq \lambda} \frac{\gamma_{\lambda' c}}{\gamma_{\lambda c}} \frac{i\Gamma_{\lambda}}{E_{\lambda'}^{BW} - E_{\lambda}^{BW} + i\left(\Gamma_{\lambda'} + \Gamma_{\lambda} \right) / 2} \frac{\gamma_{\lambda' c'}}{\gamma_{\lambda c'}}$$

Multilevel Breit Wigner, cont.

- **Elastic cross section is**

$$\sigma_{cc}^{MLBW} = \frac{4\pi g_J}{k^2}\left\{\left(1-\cos\left(2\varphi_c\right)\right)\left(\frac{1}{2}-\sum_{\lambda}\left[\frac{\Gamma_{\lambda c}}{\Gamma_{\lambda}}\psi_{\lambda}\right]\right)\right.$$

$$+\sin\left(2\varphi_c\right)\sum_{\lambda}\left[\frac{\Gamma_{\lambda c}}{\Gamma_{\lambda}}\chi_{\lambda}\right]$$

$$\left.+\left(\sum_{\lambda}\left[\frac{\Gamma_{\lambda c}}{\Gamma_{\lambda}}\chi_{\lambda}\right]\right)^2+\left(\sum_{\lambda}\left[\frac{\Gamma_{\lambda c}}{\Gamma_{\lambda}}\psi_{\lambda}\right]\right)^2\right\}$$

Single Level Breit Wigner

- **Drop all level-level interference ➔ $M \approx 1$**

- **Reaction cross section becomes**

$$\sigma_{cc'}^{SLBW} = \frac{4\pi g_J}{k^2} \sum_{\lambda} \frac{\Gamma_{\lambda c}\Gamma_{\lambda c'}}{\left(E_{\lambda}^{BW} - E\right)^2 + \Gamma_{\lambda}^2 / 4}$$

Single Level Breit Wigner, cont.

- **Drop all level-level interference ➔ Elastic cross section is**

$$\sigma_{cc}^{SLBW} = \frac{4\pi g_J}{k^2}\left\{\left(1-\cos\left(2\varphi_c\right)\right)\left(\frac{1}{2}-\sum_{\lambda}\left[\frac{\Gamma_{\lambda c}}{\Gamma_{\lambda}}\psi_{\lambda}\right]\right)\right.$$

$$+\sin\left(2\varphi_c\right)\sum_{\lambda}\left[\frac{\Gamma_{\lambda c}}{\Gamma_{\lambda}}\chi_{\lambda}\right]$$

$$\left.+\sum_{\lambda}\left[\frac{\Gamma_{\lambda c}}{\Gamma_{\lambda}}\chi_{\lambda}\right]^2+\sum_{\lambda}\left[\frac{\Gamma_{\lambda c}}{\Gamma_{\lambda}}\psi_{\lambda}\right]^2\right\}$$

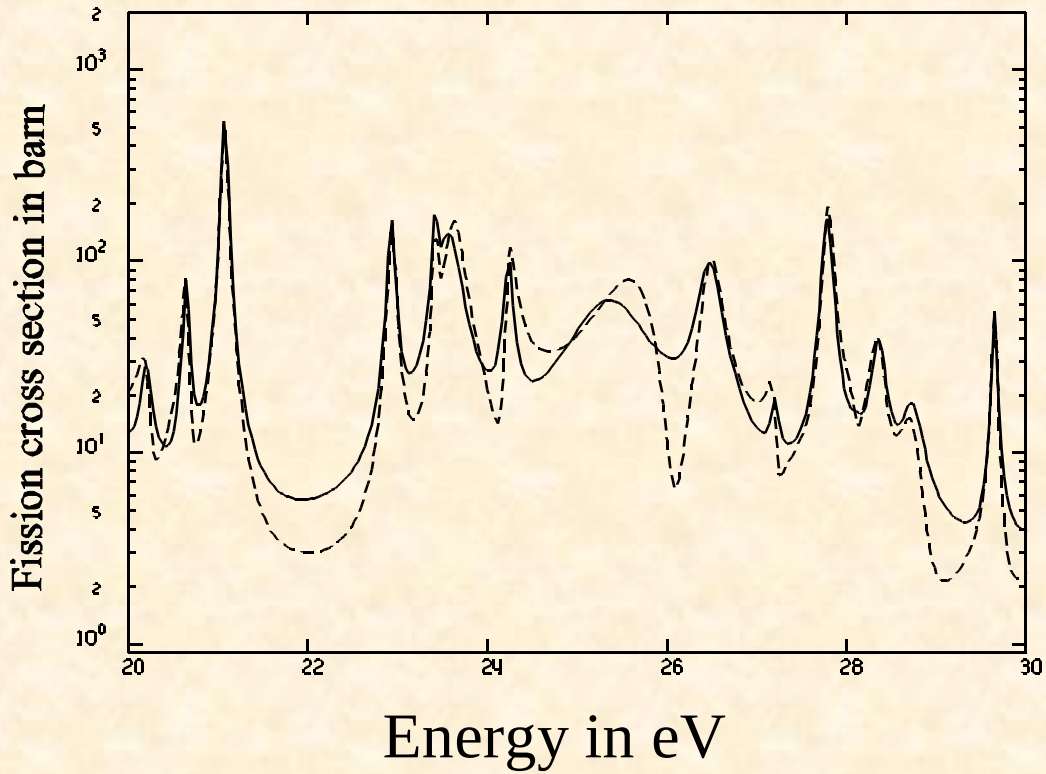
Square is inside the summation

Breit Wigner vs. Reich Moore

- **MLBW is more restrictive than Reich-Moore**
- **MLBW does not give interference for fission**

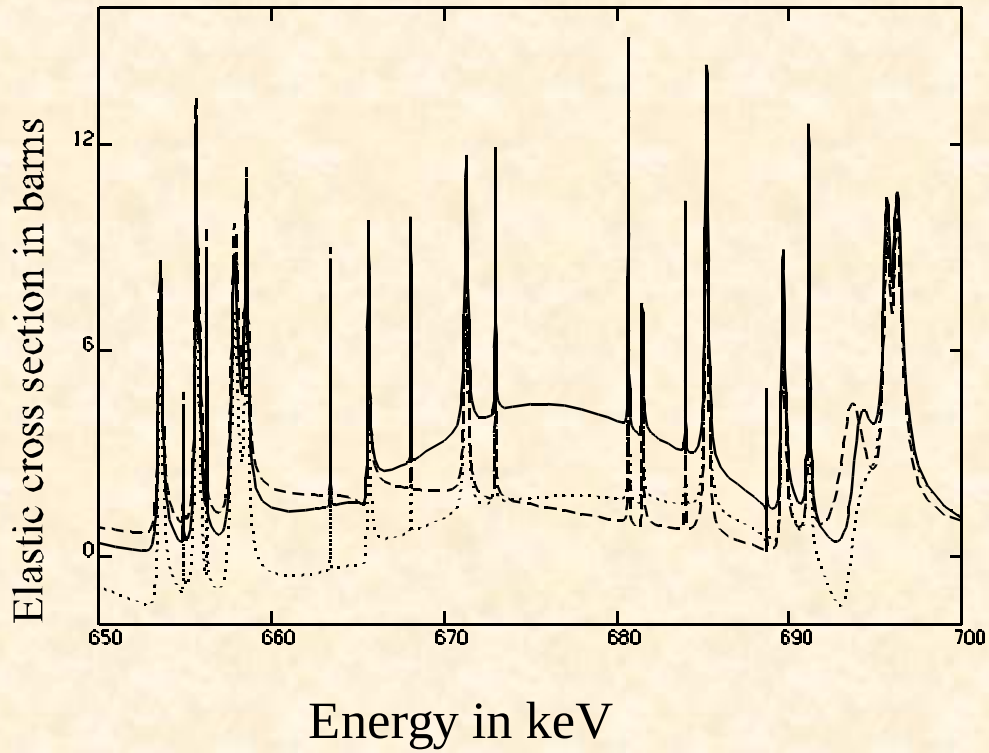
- **SLBW is more restrictive than MLBW**
- **SLBW can give non-physical cross sections (negative values)**

^{235}U fission: RM vs. BW



Fission cross section for ^{235}U from 20 to 30 eV. Dotted curve is calculated with Reich-Moore formalism; solid curve is calculated from the Breit Wigner formalism using the same resonance parameters.

^{56}Fe elastic: RM vs MLBW vs SLBW



Elastic cross section for ^{56}Fe, as calculated from the same resonance parameters using three different approximations to the R-matrix. The solid curve is Reich-Moore, the dashed is multilevel Breit Wigner, and the dotted is single-level Breit Wigner.

ENDF's "MLBW"

- **Caution: ENDF's "MLBW" is only partly "multi"**
  - **Elastic = MLBW**
  - **Reaction = SLBW**

- **SAMMY's "MLBW" is ENDF's**
  - **(was created to be used with ENDF files)**

Adler-Adler

- **Energy-dependence of *S* and *P* is neglected**
- **Involves complex eigenvalues**

- **Not used in SAMMY**

Alternative formulation: Multipole (MP)

- **NOT an approximation**
- **Valid for any angular momentum *l***
  - **(s-, p-, d-waves, etc)**
- **MP parameters are obtained by transformation from energy-space to momentum-space**
- **Developed by Richard Hwang at Argonne ('90s)**
- **Not used in SAMMY but used in AMPX at ORNL**
  - **(AMPX = processor code like NJOY developed by Maurice Greene, Mike Dunn, Dorothea Wiarda)**

SAMMY options for calculating σ

- **Reich Moore approximation to R-Matrix**
  - **Contribution from external levels calculated via**
    - **Dummy resonances**
    - **Logarithmic parameterization of R-function**
  - **Can be "tricked" into behaving like full R-matrix**
- **Breit Wigner approximation**
  - **Multilevel or single level for elastic**
  - **Single level for everything else**

RECOMMENDATION: Use Reich Moore

Or something better

- **Multilevel Breit Wigner is often wrong. Single-level Breit Wigner is usually wrong.**
- **When it's right, MLBW gives identical results to Reich Moore !!**
- **"Ease of Programming" is no longer a good excuse for using MLBW.**
  - **Neither is a slow computer.**
  - **Neither is the need to Doppler-broaden.**

ENDF FORMATS

Caveat: ENDF nomenclature can be misleading!

- ENDF's MLBW is not quite MLBW to the rest of the world –
  - Only elastic cross section is truly MLBW
  - Other partial cross sections are SLBW

- ENDF's "Reich Moore Format" (LRF=3) is a highly restricted version of Reich Moore –
  - at most four channels (gamma, n, two fission)
  - channel radius is identical for all particle channels
  - no angular-momentum admixture
  - no channel-spin admixture
  - no Coulomb penetrabilities & shift factors

ENDF FORMATS, cont.

Caveat: ENDF nomenclature can be misleading!

- ENDF's new "R-Matrix Limited" format (LRF=7)
  - can be use for full R-Matrix or Reich Moore
  - can be used for all SAMMY evaluations

- NOTE:
  - SAMMY's MLBW is actually ENDF's MLBW, except that more channels are permitted
  - SAMMY's RM is far more general than ENDF's so-called Reich-Moore format