Multilevel Breit-Wigner (MLBW) elastic angular distributions

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a passion for discovery



Office of Science

Leakage from a critical assembly depends greatly on angular dists.

- A forward peaked distribution lets more particles escape from collision events on boundaries than an isotropic one
- Most evident in small critical systems

Shielding benchmark

ASPIS benchmark (iron)

Total Monte Carlo results obtained with the TRIPOLI code shows that **above 20 cm**, the flux attenuation is dominated by higher order polynomial coefficient uncertainties



What angular distributions are available in the resonance region?

| Format | Number occurrences | Number with angular distributions enabled |
|--------------------------|-----------------------|---|
| scattering radius only | 66 | 0 |
| SLBW | 8 | 0 |
| MLBW | 270 | 0 |
| Reich Moore (LRF=3) | 54 | 46 |
| R Matrix Limited (LRF=7) | 1 | 0 |
| URR only | 26 | 0 |



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| Reich Moore (LRF=; can we salvage these guys? | | | |
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MLBW Approximation to the R matrix

R matrix theory gets us the collision matrix (c=channel index)

$$U_{cc'} = e^{-i(\varphi_c + \varphi_{c'})} \left(\delta_{cc'} + i \sum_{\lambda,\mu} \Gamma_{\lambda c}^{1/2} A_{\lambda\mu} \Gamma_{\mu c'}^{1/2} \right)$$

in terms of the level matrix A:

$$(\mathbf{A}^{-1})_{\lambda\mu} = (E_{\lambda} - E)\delta_{\lambda\mu} - \sum_{c}\gamma_{\lambda c}L_{c}^{0}\gamma_{\mu c}$$

• Here, E_{λ} is the resonance energy, $\gamma_{\lambda c}$ is the reduced width and L^{0}_{c} is essentially the hard sphere shift and penetrability

MLBW Approximation to the R matrix

With just the scattering matrix, we can compute the total cross section

$$\sigma_c \equiv \sum_{c'} \sigma_{cc'} = 2\pi \lambda_c^2 (1 - \Re U_{cc})$$

and the cross section to channel c'

$$\sigma_{cc'} = \pi \lambda_c^2 g_c |\delta_{cc'} - U_{cc'}|^2$$



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MLBW Approximation to the R matrix

MLBW throws away off diagonal parts of the level matrix and renames things into the widths we are familiar with

$$(\mathbf{A}^{-1})_{\lambda\mu} = (E_{\lambda} - E - \sum_{c} L_{c}^{0} \gamma_{\mu c}^{2}) \delta_{\lambda\mu}$$
$$\equiv (E_{\lambda} + \Delta_{\lambda} - E - i\Gamma_{\lambda}/2) \delta_{\lambda\mu}$$

Result is that collision matrix no longer unitary; we can measure this with Frobenius norm:

$$||U||_{F} = \sqrt{\sum_{cc'} U_{cc'}^{*} U_{c'c}}$$

If U is unitary, $||U||_{F} = \sqrt{\dim(U)}$



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So MLBW is not unitary. Is this a problem?



ENDF's MLBW != R matrix MLBW

ENDF MLBW uses SLBW formulas for non-elastic cross sections

Bad

ENDF overrides use of potential scattering radius in phase-factor of scattering matrix

Meh

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ENDF's MLBW capture is clearly different



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This naturally impacts the total too



ENDF MLBW elastic is the same as the R matrix MLBW elastic



Blatt-Beidenharn shows us how to make angular distributions

According to Blatt-Biedenharn formalism, we only need a collision matrix in order to compute an angular distribution:

$$\frac{d\sigma_{\alpha,\alpha'}(E)}{d\Omega} = \frac{1}{k^2(2i+1)(2I+1)} \sum_{s,s'} \sum_{L=0}^{\infty} B_L(\alpha s, \alpha' s'; E) P_L(\mu)$$

where

$$B_{L}(\alpha s, \alpha' s'; E) = \frac{(-)^{s-s'}}{4} \sum_{c_{1}=\{\alpha \ell_{1}s_{1}J_{1}\}} \sum_{c'_{1}=\{\alpha' \ell'_{1}s'_{1}J'_{1}\}} \sum_{c_{2}=\{\alpha \ell_{2}s_{2}J_{2}\}} \sum_{c'_{2}=\{\alpha' \ell'_{2}s'_{2}J'_{2}\}} \bar{Z}(\ell_{1}J_{1}\ell_{2}J_{2}sL)\bar{Z}(\ell'_{1}J_{1}\ell'_{2}J_{2}s'L) \times \delta_{ss_{1}}\delta_{s's'_{1}}\delta_{J_{1}J'_{1}}\delta_{ss_{2}}\delta_{s's'_{2}}\delta_{J_{2}J'_{2}}(\delta_{c_{1}c'_{1}} - U_{c_{1}c'_{1}}(E))^{*}(\delta_{c_{2}c'_{2}} - U_{c_{2}c'_{2}}(E))$$



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$$U_{cc'} = e^{-i(\varphi_c + \varphi_{c'})} \left(\delta_{cc'} + \sum_{\lambda} \frac{i\Gamma_{\lambda c}^{1/2} \Gamma_{\lambda c'}^{1/2}}{E_{\lambda} + \Delta_{\lambda} - E - i\Gamma_{\lambda}/2} \right)$$

The MLBW formalism in ENDF is "broken", but it's elastic channel and the collision matrix are not

OK then, what does it look like?



The angular distribution directly from ENDF MLBW parameters



Try it on a more popular isotope: ⁹⁰Zr *distribution of level widths*



Try it on a more popular isotope: ⁹⁰Zr angular distribution



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Try it on a more popular isotope: ⁹⁰Zr *zoom in on angular distribution*



 $d\sigma_{el}/d\Omega = (4\pi)^{-1} \sum_{L} \sigma_{L} P_{L}(\mu)$

What next?

- Finish coding hooks in Fudge
- Get the distributions into an ENDF file (e.g. 90Zr)
- Compare to ^{nat}Zr µ
- Try it out in a benchmark

