Statistics of energy-averaged cross sections: "unknown unknowns" or neglected "unknown knowns"?

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  Brown & Kawano, EPJ — Web Conf 146, 12007 (2017)
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  Brody et al, Rev Mod Phys 53, 385 (1981)
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  Dietz et al, Phys Lett B 685, 263
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  Ericson et al, Phys Rev E 94, 042207 (2016)
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  Fröhner & Larson, Report No. NEA/WPEC-15

Theoretical estimate of cross section fluctuations

- Measure of importance of fluctuations:

$$R_{ab} = \frac{\sqrt{\mathrm{cov}(\sigma_{ab},\sigma_{ab})}}{\langle\sigma_{ab}\rangle} = \frac{\Delta(\sigma_{ab})}{\langle\sigma_{ab}\rangle}$$

where

$$\mathrm{cov}(\sigma_{ab},\sigma_{cd}) = \langle\sigma_{ab}\sigma_{cd}\rangle - \langle\sigma_{ab}\rangle\langle\sigma_{cd}\rangle$$

- Brown-Kawano result:

$$R_{ab}^2 = \frac{\pi\, d}{\Gamma_W}\frac{\mathcal{W}_{abab}}{\mathcal{W}_{ab}^2} - 1$$

Average resonance separation

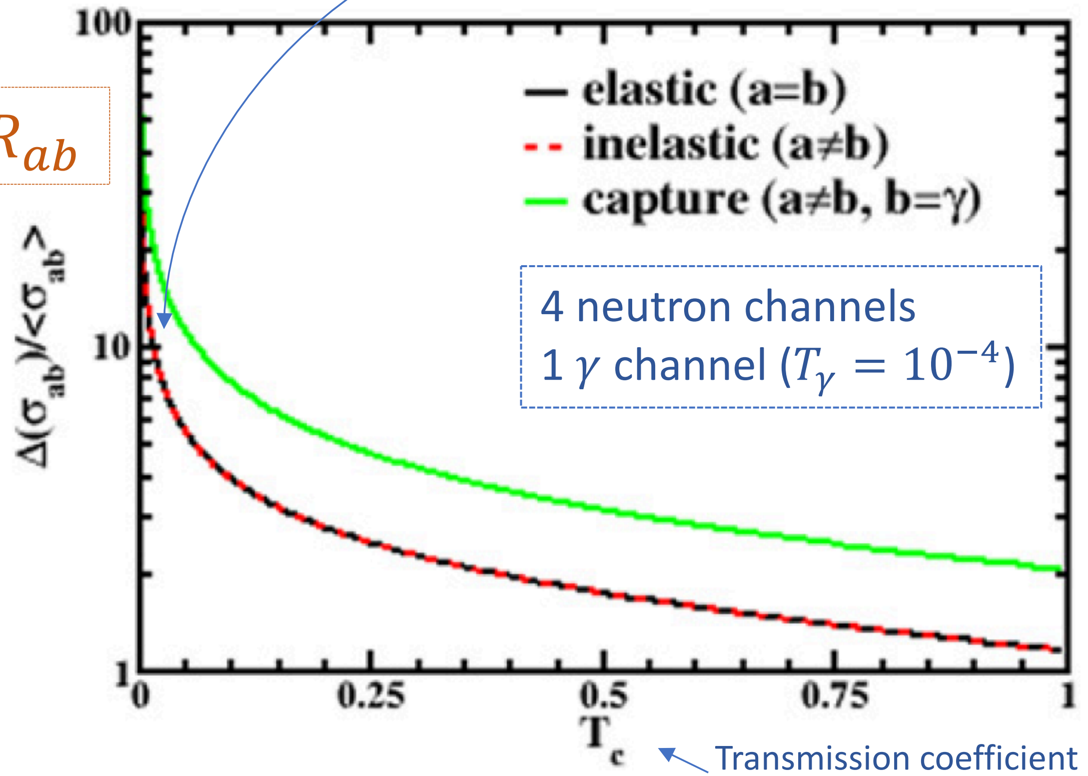
  - $\mathcal{W}_{ab}$: standard WFC
  - $\mathcal{W}_{abab}$: quartic generalization of WFC
  - Γ_W: Weisskopf correlation width

$$\Gamma_W = \frac{d}{2\pi}\sum_c T_c$$

Transmission coefficients

Resonance enhancement

R_{ab}



Transmission coefficient for each neutron channel

Fluctuations substantial!

Variance of energy-averaged cross section: an identity

- Model energy-averaged cross section as

$$\langle \sigma_{ab}(E) \rangle_\Delta = \frac{1}{\Delta} \int_{E-\frac{\Delta}{2}}^{E+\frac{\Delta}{2}} \sigma_{ab}(E')dE'$$

- Variance about theoretical (GOE) average $\bar{\sigma}_{ab}$:

Gaussian orthogonal ensemble of random Hamiltonian matrices

$$v_{ab}(\Delta) = \overline{(\langle \sigma_{ab}(E) \rangle_\Delta - \bar{\sigma}_{ab})^2} = \frac{2}{\Delta} \int_0^\Delta (\Delta - \varepsilon) C_{ab}(\varepsilon) d\varepsilon$$

where the auto-correlation function

$$C_{ab}(2\varepsilon) = \overline{\sigma_{ab}(E-\varepsilon)\sigma_{ab}(E+\varepsilon)} - (\bar{\sigma}_{ab})^2$$

What's known about autocorrelation functions? (Phys Lett B 685, 263)

- Numerical studies able to relate $C_{ab}(2\varepsilon)$ to $F_{ab}(2\varepsilon)$ $= \overline{(S_{ab}(E-\varepsilon-\delta_{ab})^2(S_{ab}^*(E+\varepsilon)-\delta_{ab})^2}$
  - Exact reduction possible of GOE average in F_{ab} to 3-dimensional integral (Phys Lett B 211, 379)

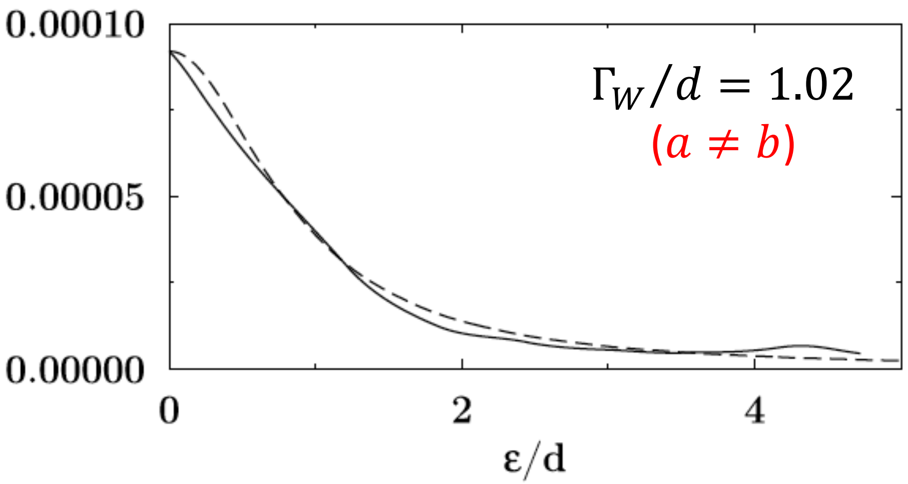
- Simple relations inferred – e.g., for $a \neq b$,

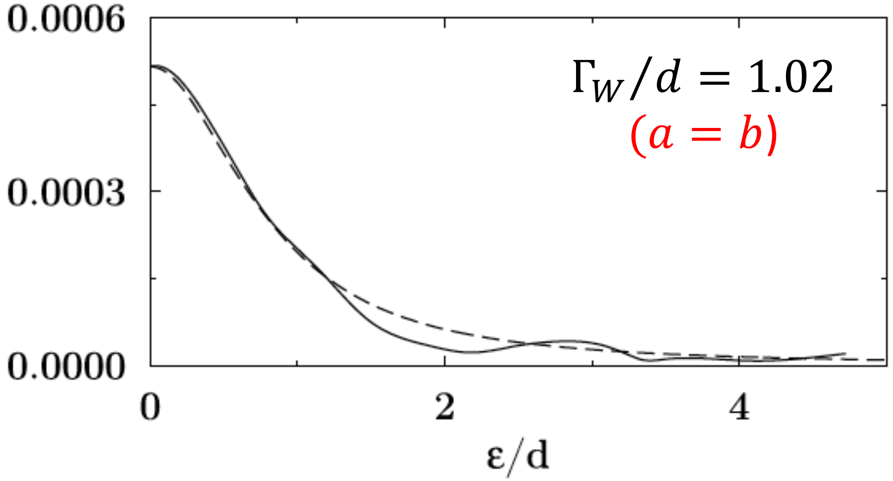
$$C_{ab}(\varepsilon) \approx \frac{R_{ab}^2}{R_{ab}^2+1}|F_{ab}(\varepsilon)| \qquad (\bigstar)$$

  - R_{ab} calculated with $F_{ab}(0)$ and $\bar{\sigma}_{ab}$

↑

Phys Rep 129, 367





Solid line: $C_{ab}(\varepsilon)$ [GOE-MC calc's]
Dashed line: rhs of (★) [analytical]
(32 equal T_c's)

$F_{ab}(\varepsilon) \quad (a \neq b)$

Similar to result for $\bar{\sigma}_{ab}$ in Phys Rep 129, 367

$$= \frac{1}{8}\int_0^\infty d\lambda_1 \int_0^\infty d\lambda_2 \int_0^1 d\lambda\, e^{-i\varphi(\lambda_1,\lambda_2,\lambda)}\, \mu(\lambda_1,\lambda_2,\lambda)\Pi(\lambda_1,\lambda_2,\lambda) f_a(\lambda_1,\lambda_2,\lambda) f_b(\lambda_1,\lambda_2,\lambda)$$

- $\mu(\lambda_1,\lambda_2,\lambda) = \frac{\lambda(1-\lambda)|\lambda_1-\lambda_2|}{(\lambda+\lambda_1)^2(\lambda+\lambda_2)^2\sqrt{\lambda_1(1+\lambda_1)\lambda_2(1+\lambda_2)}}$
- $\Pi(\lambda_1,\lambda_2,\lambda) = \prod_c \frac{1-T_c\lambda}{\sqrt{(1+T_c\lambda_1)(1+T_c\lambda_2)}}$
- $f_c(\lambda_1,\lambda_2,\lambda) = \frac{\lambda_1(1+\lambda_1)}{(1+T_c\lambda_1)^2} + \frac{\lambda_2(1+\lambda_2)}{(1+T_c\lambda_2)^2} + \frac{2\lambda(1-\lambda)}{(1-T_c\lambda)^2} + \frac{1}{2}(1-T_c)\left(\frac{\lambda_1}{(1+T_c\lambda_1)}+\frac{\lambda_2}{(1+T_c\lambda_2)}+\frac{2\lambda}{(1-T_c\lambda)}\right)^2$
- $\varphi(\lambda_1,\lambda_2,\lambda) = \pi\frac{\varepsilon}{d}(\lambda_1+\lambda_2+2\lambda)$

Not the most physically transparent result

(Useful comments on numerical evaluation in Phys Lett B 685, 263)

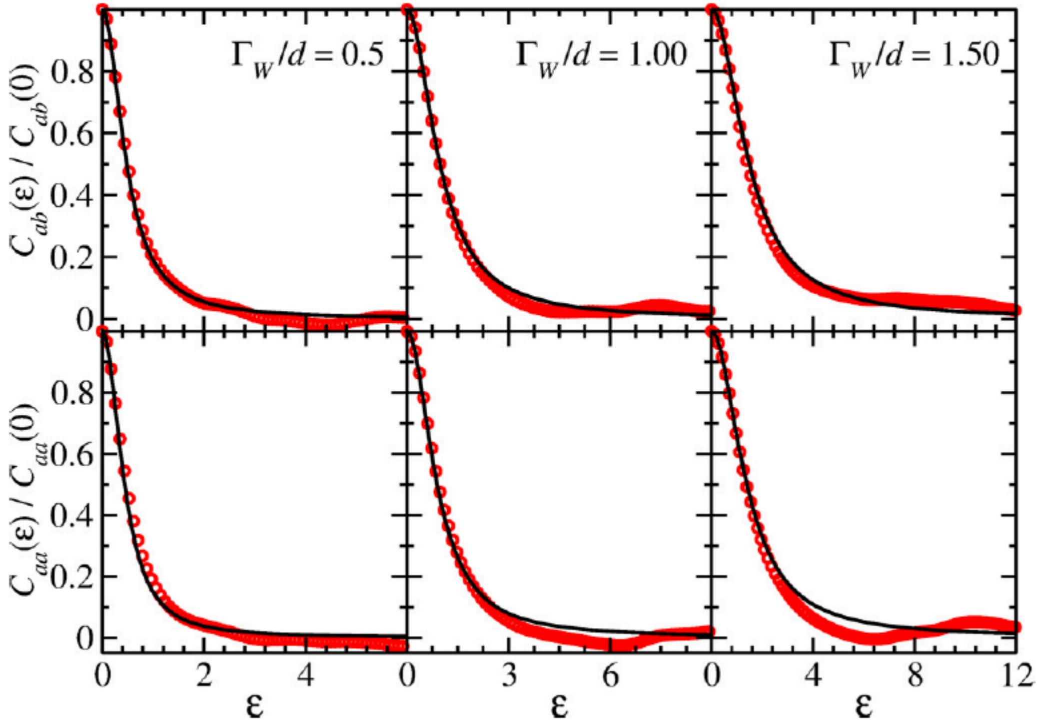
Alternative calculation of autocorrelation functions

Phys Rev E 94, 042207

Adopt statistical Breit-Wigner (SBW) model for S-matrix

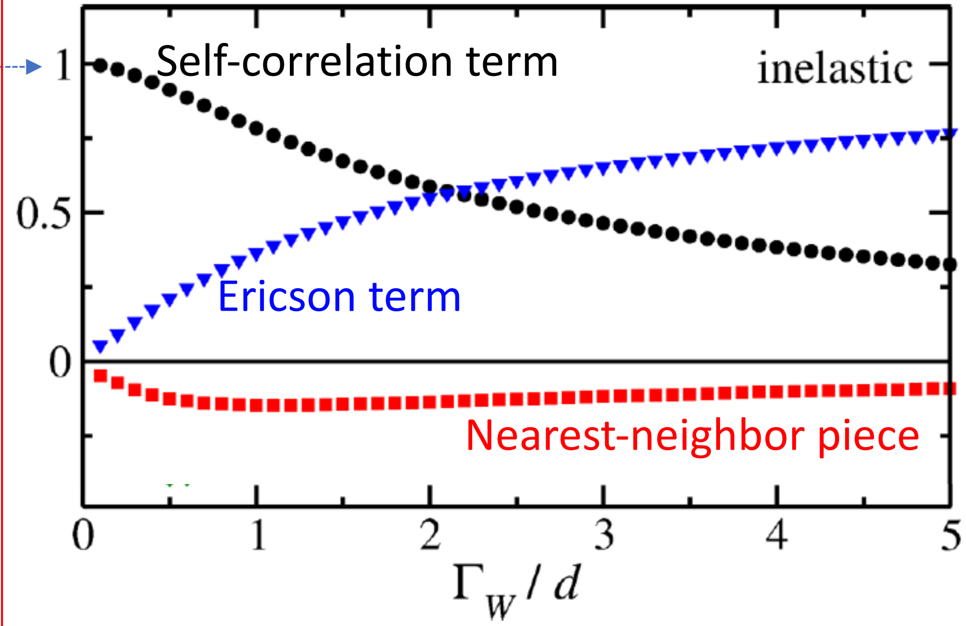
S-matrix = sum of Breit-Wigners with random parameters (distributed as in GOE)

Check of SBW



Red line: RMT-MC calc's
Black line: SBW model (52 equal T_c's)

Anatomy of $C_{ab}(\varepsilon)$



SBW → insight into $C_{ab}(\varepsilon)$

(Unity because scale choice)

A simple result for autocorrelation functions (lumping approximation)

Nucl Sci Eng 62, 756

$$\frac{C_{ab}(\varepsilon)}{(\bar{\sigma}_{ab})^2} = \left(\frac{d}{\pi\Gamma_W} + \frac{\Gamma_W}{\Gamma_W + d/\pi}\right)\frac{\Gamma_W^2}{\Gamma_W^2 + \varepsilon^2} - \frac{d}{\pi\Gamma_W}\left(\frac{\Gamma_W + d/\pi}{\Gamma_W} + \frac{\Gamma_W}{\Gamma_W + d/\pi}\right)\frac{\Gamma_W^2}{(\Gamma_W + d/\pi)^2 + \varepsilon^2} \quad (☆)$$

Resonance enhancement

Ericson term

Nearest-neighbor piece

Implication: ergodicity of σ_{ab} [$\because$ $C_{ab}(\varepsilon) \to 0$ as $\varepsilon \to \infty$]

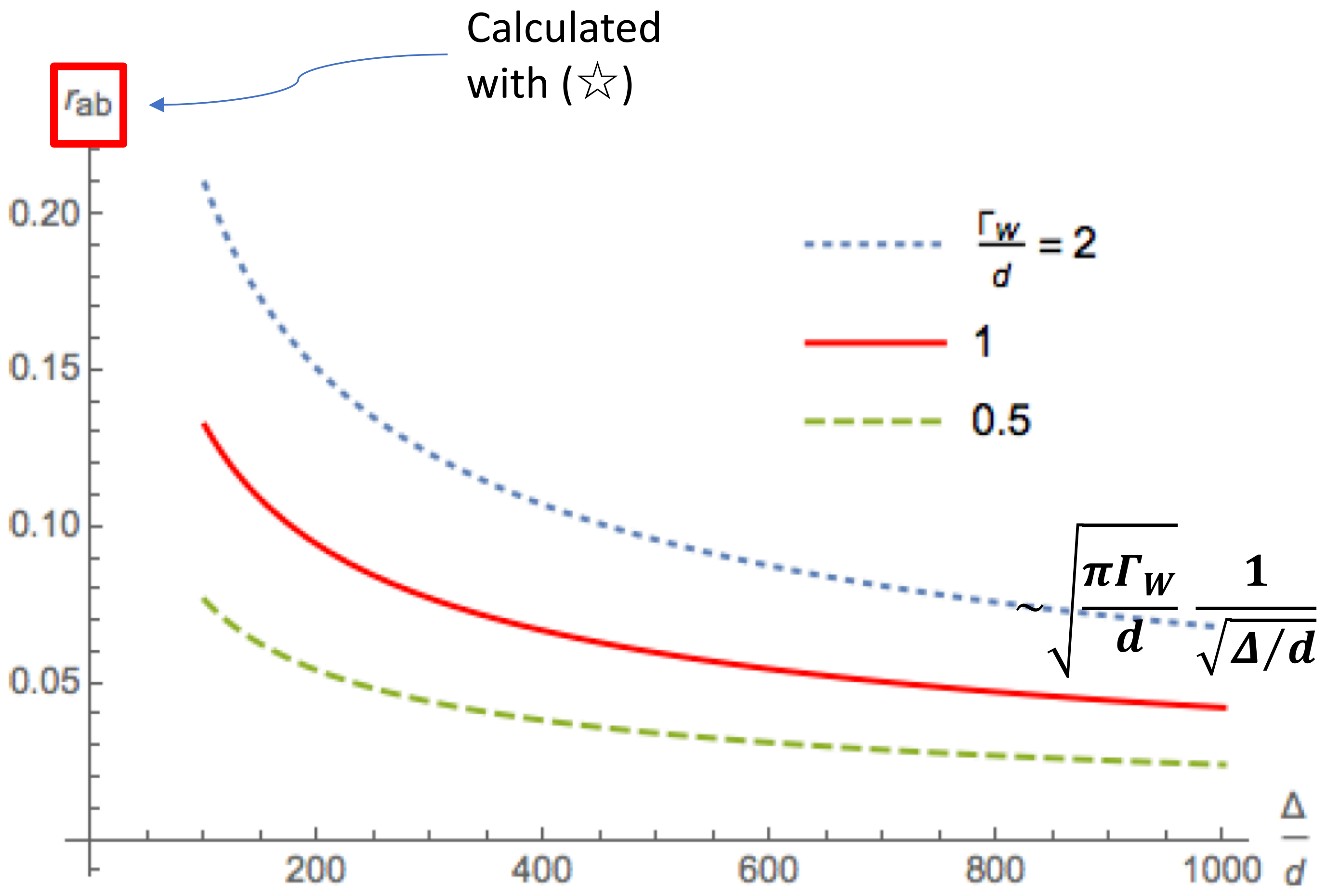
For large enough Δ, $\langle \sigma_{ab}(E) \rangle_\Delta = \bar{\sigma}_{ab}$

Behavior of $r_{ab} = \sqrt{v_{ab}(\Delta)}/\bar{\sigma}_{ab}$

Measure of deviation of $\langle\sigma_{ab}\rangle_\Delta$ from $\bar{\sigma}_{ab}$

To leading order in d/Δ,

$$r_{ab} = \frac{\Gamma_W}{\Gamma_W + d/\Gamma}\sqrt{\frac{\pi\Gamma_W}{\Delta}}$$



Deviations of energy-averaged cross section from theoretical average sizeable

(Convergence to ergodic limit slow)

An "unknown unknown"?

(or neglected "unknown known"?)

Closing thoughts on "unknown knowns"

- In unresolved resonance regime, unless averaging interval $\Delta > 10^4 \Gamma_W$, there is a sizeable probability ($\sim 30\%$) that *energy-averaged* cross section inferred from experiment and *theoretical ensemble* average should differ by $> 1\%$
- Distinction between ensemble and running averages impacts on uncertainties in the self-shielding correction factors used in the extraction of cross sections
  - Concern about MC estimates of self-shielding corrections is not new: in "[c]omparing calculation of measurement, we must keep in mind that the Monte Carlo distribution is an expectation value, i.e., an average over many sampled ladders, whereas the observed distribution comes from the one ladder realized in nature". (Fröhner & Larson, 1995)
  - Current view (EJP A 52, 170): "the uncertainty on [the self-shielding and multiple interaction] correction factor is $\leq 0.5\%$, as demonstrated in ref. [EJP A 50, 124]". This error estimate is based on the agreement of ratios of expectation values calculated with SESH and MCNP.

Thank you for your attention!