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On the Methodology to Calculate the Covariance of Estimated Resonance Parameters

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Principles to determine resonance parameters and their covariance from experimental data are discussed. Different methods to propagate the covariance of experimental parameters are compared. A full Bayesian statistical analysis reveals that the level to which the initial uncertainty of the experimental parameters propagates, strongly depends on the experimental conditions. For high precision data the initial uncertainties of experimental parameters, like a normalization factor, has almost no impact on the covariance of the parameters in case of thick sample measurements and conventional uncertainty propagation or full Bayesian analysis. The covariances derived from a full Bayesian analysis and least-squares fit are derived under the condition that the model describing the experimental observables is perfect. When the quality of the model can not be verified a more conservative method based on a renormalization of the covariance matrix is recommended to propagate fully the uncertainty of experimental systematic effects. Finally, neutron resonance transmission analysis is proposed as an accurate method to validate evaluated data libraries in the resolved resonance region.

I. INTRODUCTION

Evaluated cross section data together with full uncertainty information are of primary importance for the performance and safety assesment of nuclear energy systems. Despite the increasing request from users and the ongoing effort to improve evaluated data libraries, the number of cross section data with covariance information for neutron induced reactions in the resonance region are rather scarce. In addition, when covariance data are present in the resonance region, they mostly result in rather low uncertainties. For example, the capture cross sections of ^{37}Cl, ^{235}U, ^{238}U and ^{239}Pu are recommended in the ENDF/B-VII.1 library with uncertainties of 1% and lower [1, 2]. Such uncertainty levels are below the accuracy that can be reached with the most up to date capture cross section measurement methods that are presently available [3]. In this contribution the origin of these low uncertainties is investigated.

II. PARAMETERIZATION OF CROSS SECTIONS IN THE RESONANCE REGION

Cross sections in evaluated data libraries are parameterized in terms of nuclear reaction theory. In the resonance region the R-matrix formalism is applied [4–6]. In the resolved resonance region (RRR) cross sections are parameterised by parameters of individual resonances. Each resonance is characterized by the resonance energy E_R, the total width Γ, the partial reaction widths (e.g. the neutron width Γ_n, the capture width Γ_γ, the fission width Γ_f, ...), the total angular momentum J, the orbital angular momentum of the original neutron-nuclear system ℓ and the channel spin s. For a complete description of the cross sections scattering radii R_ℓ are also required.

In the unresolved resonance region (URR) cross sections are mostly described by the Hauser-Feshbach formalism including a width fluctuation correction [7, 8] or more rigorously by solving the triple integral over the Gaussian Orthogonal Ensemble (GOE) of resonances. Independent of the method that is used, they all rely on average parameters such as scattering radii, neutron strength functions S_ℓ or capture transmission coefficients T_γ. The parameters can be derived from a statistical analysis of parameters of resolved resonances [6]. Some of them, such as the neutron strength functions, can even be obtained from optical model calculations [9]. However, to arrive at a reasonable accuracy level, in particular for the capture channel, an adjustment of the parameters by fitting to experimental data is required [9–11].

III. ANALYSIS OF EXPERIMENTAL DATA

Accurate resonance parameters, in particular those required for the parameterization of cross sections in the RRR, can only be derived from experimental data. Var-

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ious methods, i.e. least-squares fitting, full Bayesian statistical analysis, and Monte Carlo sampling, can be applied. All these methods involve the calculation of the χ^2, which is defined by

$$\chi^2(\vec{\theta}) = \left(\vec{Z}_{\rm exp} - \vec{Z}_m(\vec{\theta})\right)^T \mathbf{V}_{\vec{Z}}^{-1} \left(\vec{Z}_{\rm exp} - \vec{Z}_m(\vec{\theta})\right), \quad (1)$$

where $\vec{Z}_m(\vec{\theta})$ is a model describing the experimental data $\vec{Z}_{\rm exp}$, with covariance matrix $\mathbf{V}_{\vec{Z}}$, and $\vec{\theta}$ a set of model parameters, with $\vec{\theta} = (\vec{\eta},\vec{\kappa})$. In the RRR a model $\vec{Z}_m(\vec{\theta})$ is required that includes the R-matrix theory and a model to account for experimental effects. Consequently, the model depends on the resonance parameters $\vec{\eta}$ and a set of experimental parameters $\vec{\kappa}$ [3]. The experimental parameters $\vec{\kappa}$ include e.g. details about the sample, detector and the time-of-flight (TOF)-spectrometer. Therefore, the covariance of the resonance parameters is influenced by both the covariance of the experimental data $\mathbf{V}_{\vec{Z}}$ and the covariance of the experimental parameters $\mathbf{V}_{\vec{\kappa}}$. The dependence on $\mathbf{V}_{\vec{\kappa}}$ complicates the procedure compared to e.g. the fast region, where model cross sections are directly compared with experimental cross sections and only $\mathbf{V}_{\vec{Z}}$ is involved.

The methodologies to determine the experimental observables together with their full covariance information ($\vec{Z}_{\rm exp}$, $\mathbf{V}_{\vec{Z}}$) are well established [3]. To process the data and produce their full covariance information, the AGS (Analysis of Geel Spectra) concept has been developed at the EC-JRC-IRMM. The use of this concept, which is described in detail in Ref. [12], has been recommended in a consultants' meeting organized by the IAEA [13] to report TOF cross section data in the EXFOR library [14]. However, the propagation of the experimental covariance $\mathbf{V}_{\vec{\kappa}}$ is not evident. A comparison of results obtained with different methods in Ref. [3] reveals that the final covariance of the resonance parameters strongly depends on the experimental conditions, the resonance structure and the method that is used to propagate $\mathbf{V}_{\vec{Z}}$ and $\mathbf{V}_{\vec{\kappa}}$.

A. Least-squares Fit

Resonance parameters are mostly obtained from a least-squares fit to experimental data, that is by minimizing the χ^2 (Eq. (1)). For a linear model the minimum is found for

$$\vec{\theta} = \left(\mathbf{G}_{\vec{\theta}}^T \mathbf{V}_{\vec{Z}}^{-1} \mathbf{G}_{\vec{\theta}}\right)^{-1} \left(\mathbf{G}_{\vec{\theta}}^T \mathbf{V}_{\vec{Z}}^{-1} \vec{Z}_{\rm exp}\right). \quad (2)$$

The sensitivity matrix $\mathbf{G}_{\vec{\theta}}$ has as elements the partial derivatives of $\vec{Z}_{\rm exp}$ with respect to $\vec{\theta}$. The covariance of the estimated parameters based on conventional uncertainty propagation (CUP) is given by

$$\mathbf{V}_{\vec{\theta}} = \left(\mathbf{G}_{\vec{\theta}}^T \mathbf{V}_{\vec{Z}}^{-1} \mathbf{G}_{\vec{\theta}}\right)^{-1}. \quad (3)$$

For non-linear models Eq. (2) and Eq. (3) can be solved by iteration. As noticed in Ref. [6, 15], the solutions of Eq. (2) and Eq. (3) are the result of a Bayesian inference or generalized least-squares (GLSQ) when the prior ($\vec{\theta}_0, \mathbf{V}_{\vec{\theta}}$) is considered as a part of the experimental data. This also removes any restriction on the correlation between the prior and the experimental data.

When experimental covariances are propagated a distinction has to be made between experimental effects resulting from the data reduction, i.e. included in $\mathbf{V}_{\vec{Z}}$, and those that can only be included in the model or $\mathbf{V}_{\vec{\kappa}}$. At present the models in the resonance region are not yet at a level that pure counting spectra can be reproduced such that all systematic experimental effects can be included in the parameters $\vec{\kappa}$, such that $\mathbf{V}_{\vec{Z}}$ only contains uncorrelated uncertainties due to counting statistics. When a parameter that would introduce a correlated uncertainty in $\mathbf{V}_{\vec{Z}}$ can be considered as a model parameter, its uncertainty as experimental parameters $\mathbf{V}_{\vec{\kappa}}$ can be propagated in exactly the same way as if it was included in the correlated part of $\mathbf{V}_{\vec{Z}}$. This offers the advantage that [3]:

- Peelle's Pertinent Puzzle is avoided;
- the impact of its initial uncertainty on the reaction model parameters can be verified; and
- all correlations between experimental data and priors can be taken into account.

The possibility to account for all possible correlations between priors and additional experimental data avoids that unrealistic low uncertainties are produced when a sequential Bayesian evaluation is applied incorrectly on a set of correlated data. This can not be done with the Bayesian updating procedures implemented in e.g. SAMMY [2, 16] and KALMAN [17, 18].

In Ref. [3] it has been demonstrated that applying CUP based on Eq. (3), the covariance $\mathbf{V}_{\vec{\kappa}}$ (e.g. in case of a normalization factor) does not always fully propagate to $\mathbf{V}_{\vec{\eta}}$ and consequently to the covariance of the model cross section. Also the Propagated Uncertainty Parameter (PUP) method applied in SAMMY [16], which is fully based on CUP, will not always fully propagate the uncertainty of the systematic effects to the covariance of the resonance parameters.

A full impact on $\mathbf{V}_{\vec{\eta}}$ of an uncertainty component that creates a correlated component in $\mathbf{V}_{\vec{Z}}$ can be realized by the marginalization procedure of Habert *et al.* [19]. However, this procedure is very limited. It can only be applied to account for uncertainties on parameters involved in the data reduction process (e.g. normalization and background) and can not propagate uncertainties on most of the other experimental effects included in $\mathbf{V}_{\vec{\kappa}}$. In addition, as shown in Ref. [3], results obtained with this procedure are not fully understood and a further investigation is required before it can be implemented.

An alternative is a coupling of Monte Carlo sampling with GLSQ and CUP, as proposed by De Saint Jean *et al.* [20]. This procedure, which will be referred to as