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Can cross sections be accurately known a priori?

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Distinct maxima and minima in the neutron total cross section uncertainties were observed in our large scale covariance calculations using a spherical optical potential. In this contribution we investigate the physical origin of this oscillating structure. Specifically, we analyze the case of neutron reactions on ^{56}Fe, for which total cross section uncertainties are characterized by the presence of five distinct minima at 0.1, 1.1, 5, 25, and 70 MeV. To investigate their origin, we calculated total cross sections by perturbing the real volume depth V_v by its expected uncertainty $\pm\Delta V_v$. Inspecting the effect of this perturbation on the partial wave cross sections we found that the first minimum (at 0.1 MeV) is exclusively due to the contribution of the s-wave. On the other hand, the same analysis at 1.1 MeV showed that the minimum is the result of the interplay between s-, p-, and d-waves; namely the change in the s-wave happens to be counterbalanced by changes in the p- and d-waves. Similar considerations can be extended for the third minimum, although it can be also explained in terms of the Ramsauer effect as well as the other ones (at 25 and 70 MeV). We discuss the potential importance of these minima for practical applications as well as the implications of this work for the uncertainties in total and absorption cross sections.

I. INTRODUCTION

Excitation curves of neutron total cross sections often show broad and well-defined maxima and minima in the energy region above 0.1 MeV. This effect is experimentally observed up to 100 MeV and has been explained theoretically by various optical-model calculations with varying degrees of success. This nuclear phenomenon is seen as the result of the interference between the part of the neutron wave which has traversed the nucleus with the part which has gone around. The positions of the broad maxima depend on the size of nucleus and their shifting is related to the parameters of the real potential well rather than to the depth of the imaginary potential well.

In our large scale covariance calculations [1, 2] neutron total cross section uncertainties were derived from the perturbation of optical model parameters using a spherical potential. The most striking features found in the relative uncertainties of the total cross section were the presence of distinct minima related to the oscillations in the cross sections. The presence of these minima at certain energies reflects our perfect knowledge of the cross sections calculated with a specific nuclear model. Therefore, experimental data can be used to estimate the nuclear model uncertainty via the relation

$$(\delta\sigma_{\rm mod})^2 = [\sigma_{\rm mod}(\hat{E}) - \sigma_{\rm exp}(\hat{E})]^2 \,, \qquad (1)$$

where $\sigma_{\rm mod}(\hat{E})$ and $\sigma_{\rm exp}(\hat{E})$ are respectively the model and the experimental cross sections calculated at the energies $\hat{E}$ where the minima occur.

The purpose of this paper is to investigate the physical basis of the oscillating structure in the total cross section uncertainties. We start the analysis in the framework of a global spherical optical potential. Some general properties of the potential are shown by perturbing the real volume depth V_v and the nuclear radius r_v. We then inspect the effect of this perturbation on the partial wave cross sections.

The paper is organized as follows. In Section II, we describe the methodology used to calculate the cross section uncertainties, while Sections III and IV discuss, respectively, the sensitivity analysis and the results. Our findings are summarized in Section V.

II. METHODOLOGY

Our calculations are based on the coupled-channels code ECIS95 [3], using bash scripts written to extract efficiently the calculated cross sections and the related S-matrix elements. For this work, we used optical-model calculations based on the recent global potential of Koning and Delaroche [4], which was based on an extensive set of experimental data for spherical nuclei (or nearly spherical ones). The energy as well as other dependences, such as a mass-dependence, of potential parameters that were employed by those authors are more flexible than those used in previous similar analyzes. This feature engenders a reasonable description of total and elastic cross sections, as well as elastic angular distributions for spherical nuclei across the periodic table. The energy range extends well above non-relativistic energies and we adopt 200 MeV as the upper energy since this is the limit of Koning-Delaroche optical potential.

To better describe the two basic model parameters the real volume depth, V_v, and the nuclear radius, r_v, considered in our calculations and the sensitivity analysis on the scattering matrix, we briefly outline the nuclear optical potential, the S-matrix formalism, and the definition of cross section uncertainties.

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A. Spherical optical potential

The optical model for nucleon-nucleus interaction is the starting ingredient in calculating cross sections. This model allows us to determine neutron elastic scattering as well as absorption cross sections. The spherical optical model potential is usually defined as

$$\mathcal{U}(r,E) = -\mathcal{V}_v(r,E) \; - \; i\mathcal{W}_v(r,E) - i\mathcal{W}_s(r,E) + \mathcal{V}_{so}(r,E)\ell\cdot s + i\mathcal{W}_{so}(r,E)\ell\cdot s\,. \tag{2}$$

Here, all components are separated into energy-dependent well depths and energy-independent radial parts according to

$$\begin{aligned}
\mathcal{V}_v &= V_v(E) f(r,R_v,a_v)\,,\\
\mathcal{W}_v &= W_v(E) f(r,R_v,a_v)\,,\\
\mathcal{W}_s &= -4a_s W_s(E)\frac{\mathrm{d}}{\mathrm{d}r} f(r,R_s,a_s)\,,\\
\mathcal{V}_{so} &= V_{so}(E)\left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r} f(r,R_{so},a_{so})\,,\\
\mathcal{W}_{so} &= W_{so}(E)\left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r} f(r,R_{so},a_{so})\,,
\end{aligned} \tag{3}$$

where the indices v, s, and so refer, respectively, to volume-central, surface-central, and spin-orbit potential. The form-factor is given by the frequently used Woods-Saxon shape

$$f(r,R_i,a_i) = \{1+\exp[(r-R_i)/a_i]\}^{-1}, \tag{4}$$

where the geometric parameters are the radius $R_i = r_i A^{1/3}$ and the diffuseness, a_i, with A being the atomic mass number.

B. S-matrix formalism

The optical potential allows us to compute the energy-averaged S-matrix, or equivalently the complex phase shifts $\eta_\ell^\pm$. These are related by

$$S_\ell^\pm(E) = e^{2i\eta_\ell^\pm(E)} = \alpha_\ell^\pm(E)\, e^{i\beta_\ell^\pm(E)}\,, \tag{5}$$

where $\alpha_\ell^\pm, \beta_\ell^\pm$ are real. The superscript $\pm$ refers to those elements where the possible values of ℓ for a given j are $j\pm 1/2$. In term of these and with $E \propto 1/\lambda\!\!\!^{-2}$, the total and absorption cross sections are given by

$$\begin{aligned}
\sigma_{\text{tot}}(E) &= 2\pi\lambda\!\!\!^{-2}\sum_{\ell=0}^{+\infty}(\ell+1)(1-\mathrm{Re}[S_\ell^+]) + \ell(1-\mathrm{Re}[S_\ell^-])\,,\\
\sigma_{\text{abs}}(E) &= \pi\lambda\!\!\!^{-2}\sum_{\ell=0}^{+\infty}(\ell+1)(1-|S_\ell^+|^2) + \ell(1-|S_\ell^-|^2)\,,
\end{aligned}$$

respectively. The elastic cross section can be obtained by subtracting σ_{abs} from the total cross section.

C. Cross section uncertainties

The uncertainty of any cross section σ due to uncertainties in a set of parameters, $\mathbf{p} = \{p_1,\ldots,p_\mu,\ldots,p_\nu,\ldots\}$, is given in linear approximation by the square root of

$$\langle(\delta\sigma)^2\rangle = \sum_\mu\sum_\nu \frac{\partial\sigma}{\partial p_\mu}\langle\delta p_\mu\,\delta p_\nu\rangle\frac{\partial\sigma}{\partial p_\nu}\,, \tag{6}$$

where $\langle\delta p_\mu\,\delta p_\nu\rangle$ is an element of the covariance matrix of the parameters, and where the sensitivity coefficients, $\partial\sigma/\partial p_\mu$, are to be calculated with the best estimates of p_μ. In our work the sensitivity coefficients were numerically computed as first-order partial derivatives assuming a linear dependence of the parameters on the cross sections for small perturbations $\pm\Delta p_\mu$.

III. CROSS SECTION SENSITIVITY

We carried out sensitivity calculations by varying several of the optical model parameters. In this paper, we concentrate on the results obtained for the uncertainties in the depth and radius of the real volume potential. Both V_v and r_v contribute significantly to the results for total and absorption (or absorption) cross sections, and we will show their correlation, which is significant.

We quantify the effect of the perturbation of the model parameter p on the cross section via the dimensionless ratio

$$\mathcal{S}(E,p) = \frac{\sigma(E,p^+)-\sigma(E,p^-)}{\sigma(E,p)}\,, \tag{7}$$

where $\sigma(E,p)$ is the cross section calculated for the central value of p, while

$$\sigma(E,p^\pm) = \sigma(E;p\pm\Delta p) \tag{8}$$

are the cross sections calculated with the value of the parameter p perturbed by the quantity $\pm\Delta p$. A very similar analysis for dimensionless sensitivity parameters was recently carried out by Fessler *et al.* [5].

As an example, in Fig. 1, we discuss neutron reactions on ^{56}Fe and the response of the (n,tot) and (n,abs) cross sections to the variation of the volume nuclear radius (r_v) and the real volume depth (V_v) of the Koning-Delaroche optical potential [4]. There are remarkably different levels of sensitivity between two reactions, and strong energy dependences. All sensitivities change sign several times between 1 keV and 200 MeV. The immediate consequence of this behavior is that at these zero-crossing points the parameter uncertainties (even if arbitrarily large) will not contribute to uncertainty in the cross section.

The sensitivities plotted in Fig. 1 for (n,tot) depict the strong correlation between r_v and V_v (continuous black and red lines) as well as the principal dependence of the structure of the total cross sections, i.e., $V_v r_v^2$ above $\sim$ 10 MeV. Fig. 1 also shows the cross section sensitivities of (n,abs). We note that the parameter correlation is still seen although it is limited

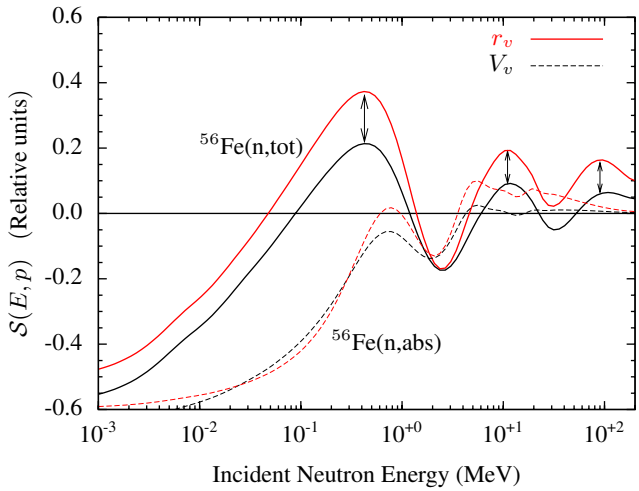

FIG. 1: Relative sensitivity of the ^{56}Fe+n total (continuous lines) and absorption (dashed lines) cross section to $\pm 5\%$ perturbation of volume nuclear radius, r_v, and the real volume depth, V_v.

to a few energy intervals. Finally, as shown in Fig. 2, it appears clear that the zero-crossing points in (n,tot) and (n,abs) are uncoupled.

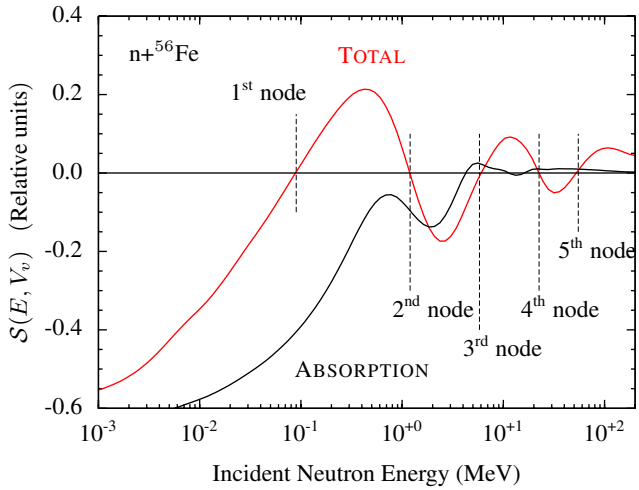

FIG. 2: Relative sensitive of the ^{56}Fe+n total and absorption cross section to $\pm 5\%$ perturbation of the real volume depth, V_v. It is also shown that zero-crossing points (or nodes) in (n,tot) and (n,abs) are clearly uncoupled.

IV. CALCULATIONS AND RESULTS

A. Nuclei from ^{27}Al to ^{210}Bi

We calculated the neutron total and absorption cross section uncertainties for 648 isotopes, defined by the list of the European Activation Files (EAF), at 54 incident energies between 1 keV and 200 MeV, by perturbing the real volume depth, V_v. In the calculations we used the Koning-Delaroche global optical potential and we confirm our previous results [1, 2] about the oscillating structure of the cross section uncertainties.

To present the overall picture of our results, we plotted contours in a single figure of the full set of nuclei over the entire range of incident energies studied. These plots show relative cross section uncertainties represented by different colors, from 0% shown in black to 100% shown in yellow. Using these plots, we depict in Figs. 3-4 the relative cross section uncertainties for the considered reaction types. The horizontal axis refers to the mass numbers of the complete list of materials, while the vertical axis to all incident neutron energies.

For both total and absorption cross sections, exceptionally high uncertainties are found at incident energies below 100 keV for nuclei between Cs and Sm and for materials in the region of Tantalum. This effect was recently observed in our large scale covariance calculations [1, 2] and might be traced to the structure observed in the s- and/or d-wave neutron strength functions. We note that we have used the spherical optical potential model for all nuclei considered, including the deformed ones. For the two reaction channels, we also note very similar patterns characterized by regions where the uncertainties are particularly small. This effect triggered our analysis and it will be discussed in detail for ^{56}Fe in the next subsection.

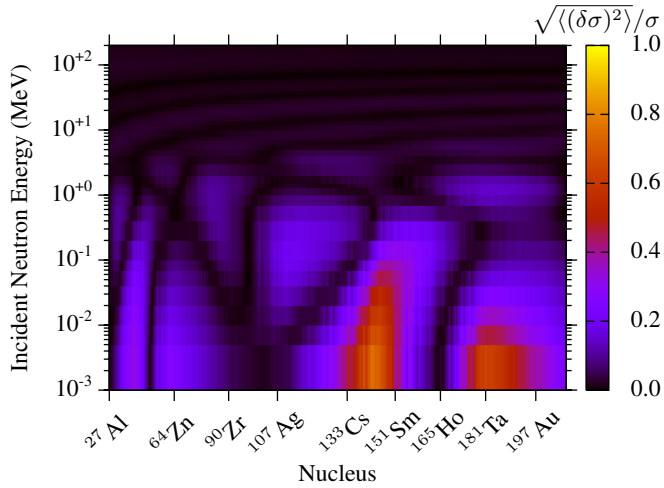

FIG. 3: Relative uncertainties for neutron total cross sections on 648 materials obtained with the Koning-Delaroche spherical optical potential.

B. Analysis of ^{56}Fe+n

We focus on ^{56}Fe+n where the relative cross section uncertainties are obtained by perturbing the real volume depth of the Koning-Delaroche global optical potential. We start our discussion by showing the effect of this perturbation on the cross

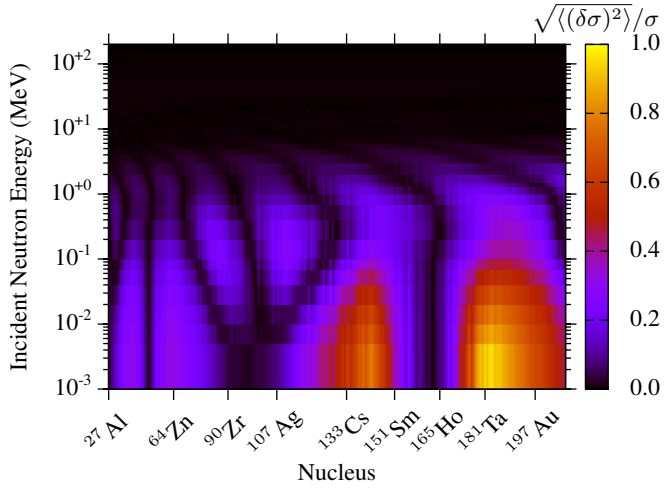

FIG. 4: Relative uncertainties for neutron absorption cross sections on 648 materials obtained with the Koning-Delaroche spherical optical potential.

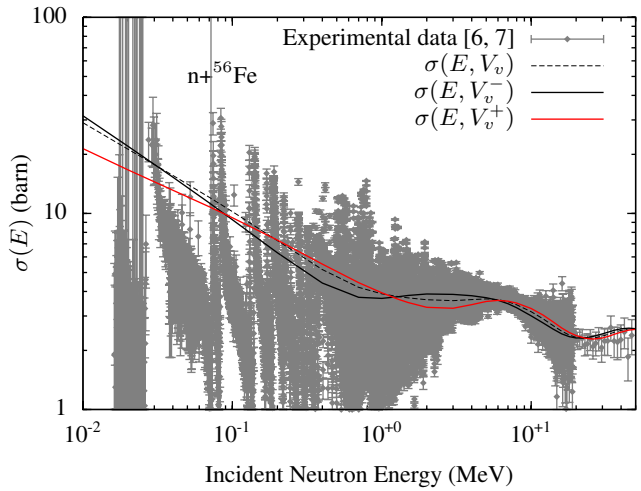

FIG. 5: Cross sections of ^{56}Fe+n obtained by perturbing the real volume depth, V_v, by $\pm 5\%$ (continuous red and black lines, respectively). Also show are cross sections calculated for the best estimate of V_v (dashed black line) compared with selected experimental data [6, 7].

sections, then we investigate the origin of the zero-crossing points in the relative cross section uncertainties.

Fig. 5 shows the response of the total cross sections for ^{56}Fe to the variation of the optical parameter V_v by the quantity $\Delta V_v = \pm 5\%$. In particular, we point to the presence of distinct crossing points at about 0.1, 1.1, 5, and 25 MeV. Fig. 5 also displays the total cross sections calculated with the central value of V_v (dashed line) along with selected experimental data [6, 7]. The oscillating structure in $\sigma(E, V_v)$ as well as in $\sigma(E, V_v^{\pm})$ results from the interference of the incident neutron wave traversing the nucleus with the wave which was scattered. This quantum-mechanical feature is naturally incorporated in the optical model. The widths and the positions of the cross section humps are directly related to the volume depth of the real potential well, V_v, and the nuclear radius, r_v.

The relative sensitivity defined by Eq. (7) can be written in terms of the partial wave sensitivities,

$$\mathcal{S}(E, V_v) = \frac{1}{\sigma} \sum_{\ell=0}^{+\infty} \tilde{\mathcal{S}}_\ell(E, V_v)\,, \tag{9}$$

where, for total cross section,

$$\begin{aligned} \tilde{\mathcal{S}}_\ell \propto (\ell+1)\ \ &\{\mathrm{Re}[S_\ell^+(V_v^-) - S_\ell^+(V_v^+)]\}\ + \\ \ell\ \ &\{\mathrm{Re}[S_\ell^-(V_v^-) - S_\ell^-(V_v^+)]\} \end{aligned} \tag{10}$$

is related to S-matrix elements via the Eqs. (5-6). Fig. 6 exhibits the effect of $\mathcal{S}_\ell$ on ^{56}Fe(n,tot) for different partial waves. As expected, in the low-energy range where we found the first minimum (at 0.1 MeV), the relative sensitivity results exclusively from the contribution of the s-wave. Differently, at intermediate energies above 1 MeV, other contributions are observed. Fig. 6 shows that the minimum at 1.1 MeV is the result of the interplay among s-, p-, and d-waves. Namely, the change in the s-wave happens to be counterbalanced by changes in the p- and d-waves. Similar considerations can be extended to the third minimum at 5 MeV where the d-wave is replaced by the f-wave (positive) contribution. This minimum can be also interpreted by another effect. In fact, at this and higher energies the presence of the minima can be explained in terms of the single-phase model, or nuclear Ramsauer effect [8–10]. The nuclear Ramsauer model is a semi-classical model where all partial waves are assumed to have the same phase shifts. This phase shift corresponds to an average of the actual phase shifts from $\ell = 0$ to the maximum given by the kinematics. The model yields an effective S-matrix,

$$S_{\mathrm{eff}}(E) = e^{2i\eta(E)} = \alpha(E)\, e^{i\beta(E)}\,, \tag{11}$$

where $0 < \alpha < 1$ generally reflects both the absorption and the averaging of various phase shifts, and β represents the relative phase between the wave that passes through the nucleus and the waves that go around. Therefore, the total cross section is given by,

$$\sigma_{\mathrm{tot}} = 2\pi(R + \lambda\!\!\!^{-})^2(1 - \mathrm{Re}[S_{\mathrm{eff}}])\,, \tag{12}$$

where R is the nuclear radius and $\lambda\!\!\!^{-}$ is the reduced wavelength of the neutron.

V. DISCUSSION AND CONCLUSIONS

We produced a very comprehensive set of neutron cross section uncertainties for total and absorption on 648 materials from ^{27}Al to ^{210}Bi in the energy range between 1 keV and 200 MeV using the Koning-Delaroche global spherical optical potential. These results confirm, in a broader view,

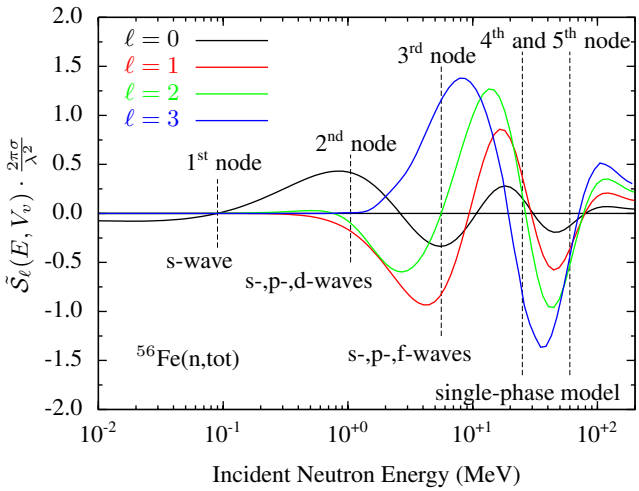

FIG. 6: Relative sensitivity of the ^{56}Fe+n total cross section to $\pm 5\%$ perturbation of the real volume depth, V_v. Also shown is the effect of this perturbation on the partial wave sensitivities.

previous notions about the structure of the uncertainties plotted as a function of the incident energy and mass number. In particular, we note patterns very similar to those observed in our recent model-based covariance calculations. The uncertainties were derived perturbing the real volume depth and the analysis of partial wave cross sections has been carried out in detail for ^{56}Fe. In this example, the presence of minima showing up in the total cross sections uncertainties at energies below a few MeV arises from different reasons. Except for the minimum at 0.1 MeV, which is exclusively due to the contribution of the s-wave, the minima up to 5 MeV appear to be the result of the interplay between different partial waves. At higher energies up to 70 MeV, the presence of two remaining minima can be explained in terms of the single-phase model (Ramsauer effect).

The calculated uncertainty minima, if confirmed, would have impact on the theoretical and experimental nuclear physics and could, in principle, influence precision of the nuclear data affecting nuclear applications. One should be able to identify narrow energy regions in which total and absorption cross sections can be predicted with particularly high precision and reliability. Such regions would be perfect for defining standards and for calibrating experimental setups or normalizing relative measurements. Precise experiments carried out in the minima could be used to investigate intrinsic model deficiencies since effect of the uncertainties on the model parameters would be largely suppressed. On the other hand, the experimentalist should avoid these energy ranges when deriving parameters of the optical potential.

Thus, can cross sections be accurately known a priori? Taking into account the quantum-mechanical origin of the discussed structure and well proven applicability of the optical model, we expect that the uncertainty minima are a natural consequence of quantum-mechanical scattering and that there are regions in which cross sections can be known precisely, even if respective measurements are not available. More studies are needed, however, to affirm such conclusion. First of all, one has to demonstrate that the observed structure is universal, i.e., it shows up with any optical potential. If this is the case, how stable are the positions of the minima? Finally, will the same arguments hold for deformed nuclei realistically treated with the coupled-channel approach rather than with the spherical optical model? We are carrying out a more extended studies in order to address these questions.

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