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Statistical Estimates of Thermal Neutron Capture Cross Sections

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Abstract —*Fluctuations of neutron resonance parameters result in the observed distribution of the thermal neutron capture cross sections. The statistical approach allowing for quantitative estimates of unknown thermal cross sections is presented. The calculated distribution of the cross sections is compared with recent data.*

Estimations statistiques de sections efficaces de capture de neutrons thermiques

Résumé —*Les fluctuations de paramètres de resonance neutronique résultent dans la distribution observée des sections efficaces de capture des neutrons thermiques. Une methode statistique est présentée ici permettant d'estimer quantitativement des sections efficaces thermiques inconnues. La distribution calculée des sections efficaces est comparee aux données acquises récemment.*

Statistische Schatzungen der Einfangquerschnitte thermischer Neutronen

Zusammenfassung —*Schwankungen der Neutronenresonanzparameter fiihren zu der beobachteten Verteilung der Einfangquerschnitte thermischer Neutronen. Hier wird ein statistischer Ansatz fur quantitative Schätzungen unbekannter thermischer Querschnitte aufgezeigt. Die berechnete Querschnittsverteilung wird mit neue Daten verglichen.*

At thermal energies neutron cross sections can differ by several orders of magnitude even for neighboring nuclei, and their exact values are unpredictable. This results from (a) variations of the strength functions from one nuclide to another, and (b) random fluctuations of the positions and widths of the low-lying resonances that dominate the thermal cross section.

In Ref. 1, the statistical approach to the thermal cross-section estimates was developed following the idea suggested by Gurevich,[2] and later independently by Cook and Wall.[3]

In this Note, we demonstrate that thermal neutron cross sections obey some universal distribution in the same way as the reduced neutron widths follow the well-known Porter-Thomas law. The main points of the statistical approach are discussed with respect to its application for practical estimates. We find the calculated distribution of thermal capture cross sections to be in good agreement with recent data[4-6] (see Fig. 1).

The main idea of the statistical approach is to account for the random fluctuations of resonance parameters by introducing the universal probabiliry distribution $P_r(z)$. Here, the quantity $z \equiv \sigma_r/\sigma_r^*$ is the ratio of the actual cross section of the reaction r to its "expected" value σ_r^*, the latter being calculated for each nuclide individually through its own average parameters. In particular, the expected value of the thermal

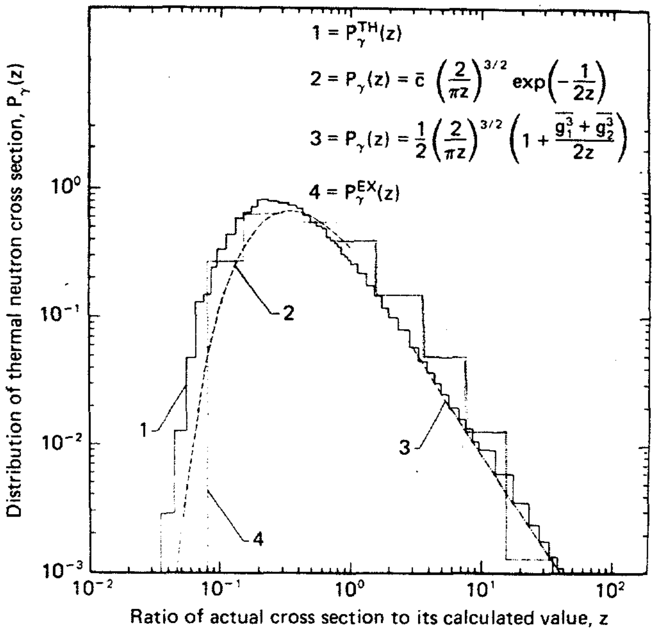

Fig. 1. The calculated distribution of the thermal neutron cross sections $P_\gamma^{TH}(z)$ compared to data $P_\gamma^{EX}(z)$. The dashed lines show the asymptotic estimates neglecting the fluctuations of the spacings. Data include 180 nuclides,“‘ 94 having zero spin I. The average values of I-dependent coefficients are $\overline{g_1^3} + \overline{g_2^3} = 0.67$ and $\bar{c} = 1.13$.

capture cross section is expressed through the strength functions of s resonances — S_0 for neutrons and $S_{\gamma 0}$ for photons:

$$\sigma_\gamma^* = \pi_3\left(\frac{A+1}{A}\right)^2 ƛ_T^2 \cdot (E_T/E_0)^{1/2} S_0 \cdot S_{\gamma 0}$$
$$= 0.40 \times 10^8 \left(\frac{A+1}{A}\right)^2 \cdot S_0 \cdot S_{\gamma 0} \qquad (1)$$

Here, A is the atomic weight of the target nucleus, $E_T = 0.0253$ eV is the thermal energy, and $E_0 = 1$ eV. In Eq. (1) we assume the following:

1. All reaction widths are equal to the corresponding mean values.
2. The energy spacings between the resonances of the same spin are constant.
3. The resonances are located symmetrically with respect to the zero neutron energy point.

Equation (1) can also be derived from Eq. (5) of Ref. 3 in the limiting case of narrow resonances ($S_\gamma \ll 1$), which is a rather good approximation at thermal energies.

If the resonance parameters were not fluctuating at all, the distribution of thermal cross sections could be described by the delta function $P_\gamma(z) = \delta(z-1)$, so that the thermal capture cross section would be exactly calculable with Eq. (1). This is not the case, however, because the fluctuations transform the delta function into a broad distribution $P_\gamma(z)$.

An exact analytical expression for $P_\gamma(z)$ can be obtained in the equidistant resonance model that takes into account the Porter-Thomas distribution for the reduced neutron widths and the random position of the thermal energy point between the resonances.' At large z, $P_\gamma(z)$ is[a]

$$P_\gamma(z) \approx \frac{1}{\pi z}\left(\frac{2}{\pi z}\right)^{1/2}\left(1 + \frac{g_1^3 + g_2^3}{2z} + \ldots\right) ,$$

$$g_1 = \frac{I+1}{2I+1} , \quad g_2 = \frac{I}{2I+1} , \tag{2}$$

where I is the spin of the target.

At small z up to $z = 1$, one can use the following approximation:

$$P_\gamma(z) \approx c(2/\pi z)^{3/2} \exp(-1/2z) , \quad c = \begin{cases} 1 , & I = 0 \\ 4/\pi , & I \neq 0 \end{cases} . \tag{3}$$

Now let us make some historical notes. The first term in the asymptotic Eq. *(2)* was obtained long ago by Gurevich[2] [without the factor $(2/\pi)^{1/2} = 0.8$ rising due to the fluctuations in the reduced neutron widths unknown at that time]. Later, Musgrove[7] derived the analytic expressions for the thermal cross-section moments. For the realistic values of S_γ ($S_\gamma \ll 1$), the extremely large variances made "useful predictions of the absorption probability for thermal neutrons impossible."' (Note that in our model the variance of thermal cross sections is infinite, but this does not prevent quantitative predictions of the probability to find the unknown thermal cross section within the given range.) Cook and Wall[3] used the Monte Carlo simulation of the thermal capture cross sections to obtain $P_\gamma(z)$. They did not take into account, however, the random position of the first resonance and the fluctuations of spacings between the adjacent resonances. Analytic expression for $P_\gamma(z)$ (neglecting the fluctuations of resonance spacings) was first derived in Ref. 1.

The Wigner distribution of resonance spacings was taken into account by the Monte Carlo simulation of the cross sections. In Fig. 1, the calculated distribution is given, which accounts for 400 resonances. Estimates, based on asymptotic formulas *(2)* and **(3)**, which neglect the fluctuations of spacings, are presented for comparison. It can be seen from the figure that these simple formulas are sufficiently accurate. Thus, we recommend using Eqs. *(2)* and *(3)* for the approximate estimates of the probability of the possible deviations of the actual cross sections σ_γ from their expected values σ_γ^*.

In Ref. 1, the calculated distribution $P_\gamma(z)$ was compared with data[4,5] for 105 nuclei for which both the thermal neutron capture cross sections and average parameters are known. Because of an insufficient number of such nuclides, we were forced to compare not the probabilities $P_\gamma(z)$ but rather the cumulative distribution functions

$$S_\gamma(z) = \int_0^z P_\gamma(y)\, dy .$$

A compilation[6] containing far more complete and reliable data became available recently, so we can extend our statistics to 180 nuclides ($A \geq 40$) and obtain the probability distribution $P_\gamma(z)$ itself.

We conclude that the agreement of the calculated thermal cross-section distribution $P_\gamma^{TH}(z)$ with experiment is rather satisfactory (Fig. 1), although splitting of data into z intervals still remains too coarse for detailed comparison.

[a]In Eq. (2), the erroneous coefficients of Eq. **(22)** of Ref. 1 were corrected. Besides, the term $1/(8\bar{\bar{Z}}^2)$ must be replaced by $5/(8\bar{\bar{Z}}^2)$.

Fluctuations of neutron resonance parameters following from the statistical model[8] are responsible for the broad distribution of the thermal capture cross sections. This distribution is observed experimentally. Hence, the statistical approach can be applied to the excited states located near the neutron binding energy for all medium and heavy nuclei. The probability distribution $P_\gamma(z)$, together with **Eq.** (1), can be used for the quantitative estimates of the probability to find the unknown thermal cross section within the given limits.

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An Efficient Algorithm for Nodal-Transport Solutions in Multidimensional Geometry

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Abstract —*An algorithm is derived for implementing nodal-transport methods in multidimensional geometries more efficiently than with current algorithms. The cellwise storage and computational penalties of the nodal methods are reduced significantly. Central processing unit time is reduced two to four times over the direct nodal algorithm with a constant surface-flux approximation, and the number of coefficients required is reduced twofold. The corresponding reductions are even greater when the new algorithm is utilized in the linear surface flux nodal method. Results of testing in two- and three-dimensional rectangular geometry are presented.*