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REPRESENTATION OF THE NEUTRON CROSS SECTIONS IN THE UNRESOLVED RESONANCE REGION*

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We discuss some limitations of the statistical approach to the representation of cross sections in the unresolved region and suggest that the actual Doppler-broadened cross sections should be used instead.

(Neutrons, cross sections, unresolved, resonances, reactors, ENDF/B)

Introduction

The low-energy neutron cross sections of the heavy elements can be described with resonance parameters. Those parameters may be obtained by analyzing the total and partial cross sections, although in many cases, and particularly for the fissile nuclei, the analysis does not yield unique values for the resonance parameters.

Above the resolved resonance region, there is an unresolved region where the cross sections show considerable structure but where the resonance parameters cannot be obtained because the resonances overlap. The widths of the levels broadened by the Doppler effect and the instrumental resolution are comparable to the level spacing.

It is important to represent the cross sections in the unresolved region as accurately as possible, because of the large contribution of this energy region to the Doppler coefficient of reactivity of fast reactors.

It has become the custom to describe the cross sections in the unresolved region by specifying average values and distribution functions of the resonance parameters. Resonance self-protection factors can then be computed by appropriate statistical techniques.

In this paper we review some of the limitations of this statistical approach. We then show that with present neutron cross section technology it is possible to perform measurements that have sufficient energy resolution to permit the direct calculation of the Doppler-broadened cross sections needed for reactor calculations. This direct use of the actual cross sections would avoid some of the problems associated with the statistical approach, and hence it should be preferred.

The Statistical Approach and Its Limitations

The statistical treatment of the unresolved region has been described by Greebler and Hutchins,[1] Brissenden and Durston,[2] Dyos,[3] Levitt,[4] and others.[5] It is based on the statistical theory of nuclear reactions.[6] The cross sections are specified by the average values and distribution functions of the resonance parameters; the required statistical properties of the cross sections can then be obtained numerically, by the generation of ladders of pseudo resonances, and in some cases analytically.[7]

The development of this statistical approach was initiated at a time when very few good-resolution measurements above a few keV were available, and before intermediate structure in heavy nuclei had been observed.

Kelber and Kier,[8] and Dyos and Stevens[9] have investigated the statistical uncertainty inherent in the statistical approach: even if the average resonance parameters and the distribution functions could be known exactly, the computed reactor parameters would have a statistical uncertainty, since they are functions of a finite sample of resonances which may have properties differing from those of the average resonances. For example, Dyos and Stevens have shown that when the partial infinitely dilute resonance integral of ^{238}U between 4 and 5 keV is computed by the statistical approach, the probable statistical error is about 10%. Kelber and Kier have shown that the probable error in the statistical computation of the fissile component of the Doppler coefficient of reactivity is almost as large as the magnitude of this component!

In addition to this error inherent in the statistical approach, there are large uncertainties in the values of the average resonance parameters and some questions about the validity of the model from which the distribution functions of the resonance parameters are derived.

The average values of the resonance parameters in the unresolved region must be obtained by extrapolating values obtained in the resolved region and by analyzing the average cross sections and the fluctuations of the cross sections around their average values. However, the values of the resonance parameters in the resolved region often have very large uncertainties, particularly for the fissile isotopes where the multi-level analysis is not unique[10] and where a large percentage of the levels are missed.[11] Furthermore, for the fissile isotopes, only s-wave parameters may be obtained; even for the fertile isotopes some p-wave parameters (such as the radiation widths) cannot be determined reliably; hence the extrapolation of the resolved resonance parameters to higher energies and angular momenta must heavily rely on theoretical models.

The analysis of the average cross sections[12] and of the fluctuations[13] yields relations between the average resonance parameters, but these relations are usually not sufficient to determine uniquely all the average parameters.

In recent years intermediate structure has been observed in a number of heavy nuclei cross sections particularly important for reactor calculations,[14-17] such as the fission and capture cross sections of ^{235}U, ^{238}U, ^{239}Pu, and ^{240}Pu. This intermediate structure may be caused by doorway states in the entrance (neutron) channel[18] or by the coupling of the levels of the first and second wells of the fission potential barrier.[19]

The intermediate structure complicates considerably the statistical representation of the cross sections: First, the distribution laws of the resonance parameters are based on the statistical model of nuclear reactions which is inconsistent with intermediate structure, particularly where the strength function varies rapidly with energy. Second, the fluctuations of the cross sections are caused partly by changes in the average value of the resonance parameters, due to the doorway states, and partly by the fluctuations of the individual parameters around their average values. In general, there is no way to separate clearly these two causes of fluctuations.

A number of improvements in the statistical representation of cross sections have been suggested: "forced sampling" may be used in the construction of ladders to ensure that the pseudoresonances reproduce low resolution experimental data.[2,3] This technique is limited to the construction of ladders and is not very practical when the fluctuations in the cross sections exceed the expected value, because they are due to intermediate structure.

In the ENDF/B-IV description of some cross sections, the "average" resonance parameters are made to vary rapidly with energy: The ^{235}U average parameters are redefined at five energies between 82 and 100 eV, hence "average parameters" apply only to about six levels! Such an approach must make an arbitrary division between fluctuations in the average parameters due to intermediate structure and fluctuations of the parameters around their average values. There is no guarantee that such a representation will yield the correct probability distribution of the cross sections, and hence the correct self-shielding factors.

An additional important objection to the statistical representation of cross sections is that this treatment is based on the assumption that the actual value of the cross section at a given energy is unimportant, the only relevant quantity being the probability distribution of the cross section. This assumption does not seem reasonable. Figure 1 shows the total cross section of iron,[20] and Fig. 2 shows two measurements of the capture cross section of ^{238}U;[21] in the core of a fast reactor which contains much iron, the neutron flux will "peak" at the position of the minimum in the iron cross section near 24 keV. It seems relevant to ask whether the iron cross section minimum "lines up" with a maximum or a minimum of the ^{238}U capture cross section. Clearly, the ENDF/B-IV statistical representation of the ^{238}U cross sections shown in Fig. 2 cannot provide an answer to such a question.

We have reviewed a few of the problems associated with the statistical approach to the unresolved region. We will now show how the results of measurements could be used directly (that is, without going through the step of generating statistical resonance parameters) to obtain those cross sections needed for reaction calculations.

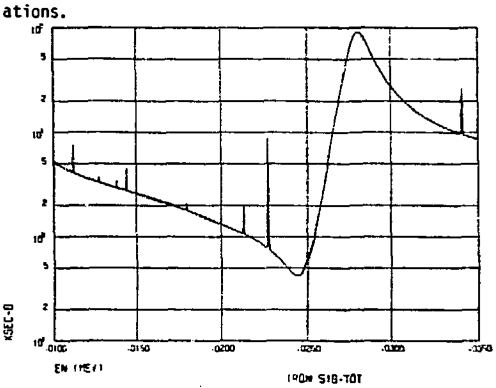

FIG. 1. Iron total cross section (10-35 keV).

Doppler Broadening and Resolution Broadening

Harris[22] and Fröhner[23] have given elegant proofs of the fact that if a Doppler broadened cross section is known for a temperature, T_1, the Doppler broadened cross section for any higher temperature, T_2, can be obtained by an appropriate convolution. If the broadening kernel is approximated by a Gaussian, the relation follows from a well-known property of the convolution of two Gaussians, and can be expressed as:

$$\sigma_\Delta(E,T_2) = \frac{E^{-1/2}}{\pi^{1/2}\Delta}\int E'^{1/2}\ \sigma_\Delta(E',T_1)e^{-[(E-E')/\Delta]^2}dE' \quad (1)$$

and

$$\Delta^2 = \frac{4k(T_2 - T_1)}{A}E \quad , \quad T_2 > T_1 \quad , \quad (2)$$

where we use common notation.

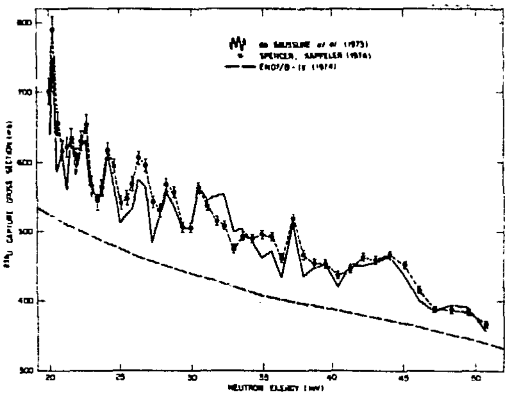

FIG. 2. ^{238}U capture cross section (20-50 keV).

Fröhner also noted that often the resolution broadening may be approximated by a Gaussian convolution of 1/e - width, W. In this case Eq. (1) still holds with:

$$\Delta^2 = \frac{4k(T_2-T_1)}{A}E - W^2 \quad , \quad T_2 > T_1\left(1 + \frac{AW^2}{4kT_1E}\right) \quad . \quad (3)$$

In fact as long as $AW^2 \le 4kT_1E$ the effect of the resolution broadening can be "unfolded" with fair accuracy, as we will show later.

For most time-of-flight measurements W is given by:[24]

$$W^2 = \frac{2}{3}\left[\left(\frac{\ell}{L}\right)^2 E^2 + \left(\frac{\tau}{\mu L}\right)^2 E^3\right] \quad , \quad (4).$$

where L is the length of the flight path, ℓ is the length uncertainty due to the thicknesses of the detector and of the neutron source, τ is the time uncertainty resulting from the finite duration of the source pulse and the resolution of the detector, and μ = 72.3 μs/m at 1 eV is the neutron flight time at the reference energy. If the source neutrons are slowed down by an hydrogeneous moderator, the moderation process introduces a broadening equivalent to that of a length uncertainty of approximately 2.4 cm.[25]

Figure 3 shows the room temperature Doppler width, Δ, for a typical heavy element (A = 240), as well as the resolution width, W, for three different instrumental conditions. The upper curves were computed for ℓ = 2.4 cm, τ = 5 nsec, and flight path L or 40 and 160 m respectively. The lowest curve is also for a 160 m flight path, for ℓ = 1.0 cm (no moderator) and τ = 5 nsec.

We see from Fig. 3 that in the energy region which contributes most to the Doppler effect, i.e., below 50 keV, the resolution width at a flight path of 160 m can be made smaller or comparable to the Doppler width at

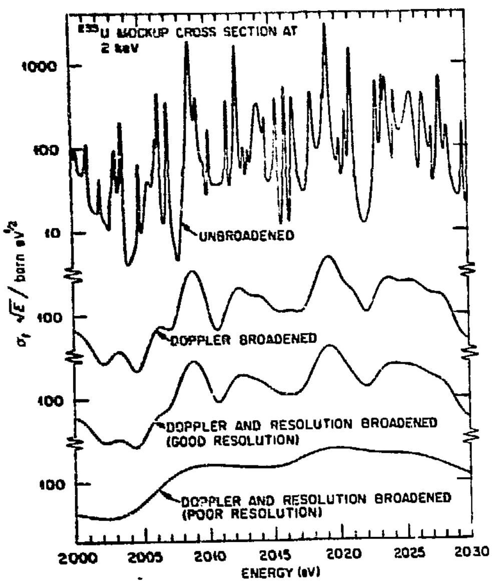

FIG. 4. ^{235}U mockup cross section at 2 keV.

300°K, although above 25 keV this requires measurements without moderator.

The direct use of cross sections measured with good resolution to compute Doppler-broadened cross sections for reactor calculations is illustrated in Figs. 4 and 5. The upper curve in Fig. 4 represents a mock-up of the fission cross section of ^{235}U between 2000 and 2030 eV. The resonance parameters at 2 keV are not known and the mock-up was obtained by selecting the same sequence of spacings and reduced widths that is found between 0 and 30 eV. This is reasonable since at 2 keV the cross section is still dominated by the s-wave contribution and since the s-wave average parameters would not be expected to change much over the small change in excitation energy. The second curve of Fig. 4 was obtained by Doppler broadening the upper curve to a temperature of 300°K; this is the cross section that might be required in a reactor calculation. The third curve of Fig. 4 shows the cross section as it would be obtained with the good resolution obtainable on an 80 m flight path at ORELA. The lowest curve shows the cross section as it would be obtained with the poorer resolution corresponding to a 20 m flight path at ORELA.

It is apparent from Fig. 4 that if only the "poor resolution measurement," shown in the lowest curve, is available, the Doppler broadened cross section cannot be reliably obtained by unfolding the resolution broadening; in this case the most reasonable approach is probably to generate ladders of pseudoresonances (such as that shown in the upper curve of Fig. 4) and Doppler broadening the ladders to obtain the probability distribution of the Doppler broadened cross section. On the other hand, if the "good resolution measurement" shown in the third curve of Fig. 4 is available, then an accurate estimate of the actual Doppler-broadened cross section may be obtained by unfolding the broadening due to the instrumental resolution. The resolution width, W, of the "good resolution measurement" of Fig. 4 is approximately equal to the Doppler width, Δ. In Fig. 5 we illustrate a possible technique to remove the effect of the resolution broadening.

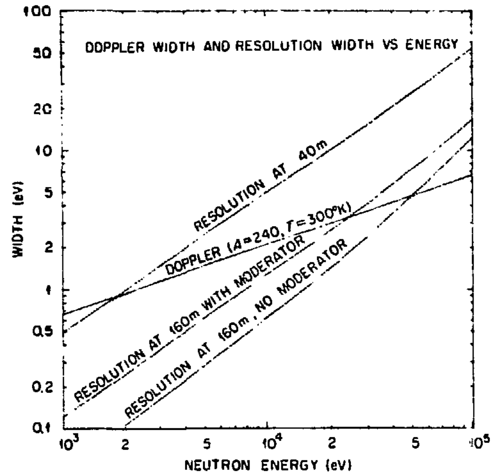

FIG. 3. Doppler width and resolution width vs energy.

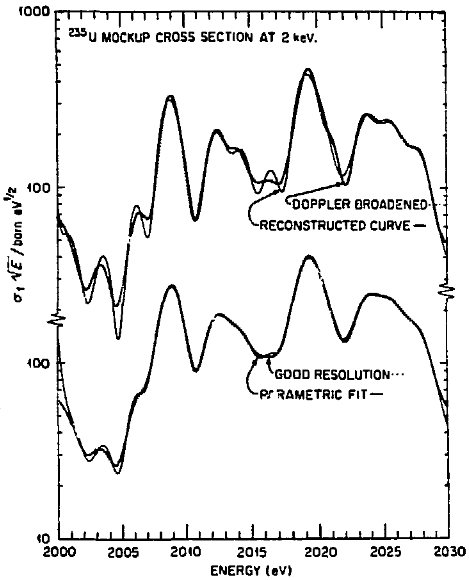

FIG. 5. ^{235}U mockup cross section at 2 keV.

In the lower part of Fig. 5 we show the "good resolution measurement" (third curve of Fig. 4) fitted by a linear combination of the form:

$$\sigma E^{1/2} = \sum_k \frac{1}{\nu_k} [G_k \psi(x_k, \beta_k^*) + H_k \phi(x_k, \beta_k^*)] \qquad (5)$$

and

$$x_k = \frac{E-\mu_k}{\nu_k} \qquad \beta_k^* = \frac{(\Delta^2 + W^2)^{1/2}}{\nu_k} \quad , \qquad (6)$$

where the ψ and ϕ are the usual Voigt profiles.[26] The values of μ_k, ν_k, G_k and H_k were obtained by a least squares fit. In the upper part of Fig. 5 we compare the "unbroadened" cross section, obtained in setting $W = 0$ in Eqs. (5) and (6) to the "actual" Doppler broadened cross section (the second curve of Fig. 4).

The resolution unfolding illustrated in Fig. 5 is not exact but, with the limitation that $W \lesssim \Delta$, it provides a fairly accurate description of the actual Doppler-broadened cross section. Other, perhaps more powerful, methods exist to unfold resolution,[27] but the technique used here is convenient and also provides a parametric description of the Doppler broadened cross section.

Discussion and Conclusions

Until recently partial cross section measurements could be done only with the moderate resolution corresponding to flight paths of 20 to 50 m, because of the limited intensity of pulsed neutron sources. However, in recent years powerful neutron time-of-flight facilities have been developed which allow a great improvement in instrumental resolution.[28] For instance, the cross sections most important for the calculation of the Doppler coefficient of reactivity in fast reactors could be measured at ORELA with the resolution corresponding to the lowest curve in Fig. 3. Yet very few high resolution measurements have been reported, and none, to our knowledge, are used directly in reactor calculations.[29] The high resolution measurements are difficult and time consuming, and hence may not be performed unless requested by reactor designers.

The storage requirements for evaluated data consisting of actual Doppler broadened cross sections would be appreciable; if on the average n points per Doppler width are required to represent the Doppler broadened cross section, then the total number of points required to represent a cross section in the unresolved range is:

$$N = n\int_{E_1}^{E_2} \frac{dE}{\Delta(E)} = n\sqrt{\frac{A}{kT}}\;\left(E_2^{1/2} - E_1^{1/2}\right) \quad , \qquad (7)$$

where E_1 and E_2 are the limit of the unresolved range. The Doppler broadened curve shown on Fig. 4 covers a range of 33 Doppler widths and can be represented to 3% accuracy by a linear interpolation with 35 points, indicating that for this type of cross section $n \approx 1$ or 2. For $n = 1$, Eq. (7) shows that approximately 2300 points would be required to represent a Doppler-broadened cross section up to 50 keV. This is a fairly large number of points, but the processing of a cross section represented by data points should be faster than the processing of average resonance parameters.

It appears to us that the expected increase in precision, particularly in the calculation of the Doppler coefficient of reactivity, makes it desirable to abandon the statistical approach to the unresolved region for the most important nuclides and to replace it as soon as possible by the use of the actual Doppler broadened cross sections obtained directly from high resolution measurements.

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1. P. Greebler and B. A. Hutchins, Proc. Seminar on Physics of Fast and Intermediate Reactors 3, 121, IAEA, Vienna (1962).

2. R. J. Brissenden and C. Durston, The Calculation of Neutron Spectra in the Doppler Region, Proc. Conf. Application of Computing Methods to Reactor Problems, p. 51, ANL-7050, Argonne National Lab. (1965).

3. M. W. Dyos, Nucl. Sci. and Eng. 34, 181 (1965).

4. L. B. Levitt, Nucl. Sci. and Eng. 49, 450 (1972).

5. Much of the early work on the subject is discussed in the six papers of the Proc. Invited Session on Resonance Cross Sections in the Unresolved Resonance Region, Meeting of ANS and CNA, CONF-680601, ANS-RPD-1, 1968.

6. "Statistical Theory of Spectra Fluctuation," Ed. C. E. Porter, Academic Press, New York, 1965. See also, C. E. Porter and R. G. Thomas, Phys. Rev. 104, 483 (1956).

7. R. N. Hwang, Nucl. Sci. and Eng. 36, 67 and 82 (1969).

8. C. N. Kelber and P. H. Kier, Nucl. Sci. and Eng. 24, 383 (1966) and 26, 67 (1966).

9. M. W. Dyos and C. A. Stevens, Nucl. Sci. and Eng. 25, 294 (1966).

10. M. S. Moore and C. W. Reich, Phys. Rev. 118, 718 (1960), D. W. Bergen and M. G. Silbert, Phys. Rev. 166, 1178 (1968), and G. de Saussure, R. B. Perez, and W. Kolar, Phys. Rev. C7, 2018 (1973).

11. D. R. Koenig and A. Michaudon, J. Nucl. Energy 25, 273 (1971), J. D. Garrison, Phys. Rev. Lett. 29, 1185 (1972), and E. Melkonian, J. P. Felvinci, and W. W. Havens, submitted to Phys. Rev. Lett. (1975).

12. A. M. Lane and J. E. Lynn, Proc. Phys. Soc. (London) A70, 557 (1957).

13. P. A. Egelstaff, J. Nucl. Energy 7, 35 (1958) and Proc Phys. Soc. (London) 71, 910 (1958).

14. B. H. Patrick, M. G. Sowerby, and M. G. Schomberg, J. Nucl. Energy 24, 269 (1970).

15. R. B. Perez and G. de Saussure, "Intermediate Structure in the ^{238}U Neutron Capture Cross Section," this conference (BAPS II, 20, 161, 1975).

16. J. Blons, H. Derrien, and A. Michaudon, Proc. Second Intern. Conf. Nucl. Data for Reactors I, 513, IAEA Vienna (1970).

17. E. Migneco and J. P. Theobald, Nucl. Phys. A112, 603 (1968).

18. H. Feshbach and A. K. Kerman, Comments on Nuclear Particle Physics II, 4, 125 (1968).

19. H. Weigmann, Zeitschrift für Physik 214, 7 (1968).

20. Courtesy of F. G. Perey, 1975.

21. R. R. Spencer and F. Käppeler, Proc. Specialist Meeting on Resonance Parameters of Fertile Nuclei and ^{239}Pu, Saclay, May 20-22, 1974.

22. D. R. Harris, "Bettis Technical Review," WAPD-BT-30 41 (1964).

23. F. H. Fröhner, Nucl. Instr. and Methods 49, 89 (1967).

24. F. H. Fröhner and E. Haddad, Nucl. Phys. 71, 129 (1965).

25. J. Rainwater et al., Rev. Sci. Instr. 31, 481 (1960); A. Michaudon, Reactor Sci. and Tech. 17, 168 (1963).

26. W. Voigt, S. B. Bayer Akad Wiss, p. 603 (1912); A. W. Solbrig, Am. J. Phys. 29, 257 (1961).

27. For instance, J. W. Cooley, "Applications of the Fast Fourier Transform Method," Proc. IBM Scientific Computing Symp., Yorktown Heights, N. Y. (1966).

28. E. Rae, in Experimental Neutron Resonance Spectroscopy, Ed. J. A. Harvey, Academic Press, New York (1970) p. 66.

29. S. C. Cohen, p. 247 in ANL-7320 (1966).