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Inherent Limitations and Current Status of the Unresolved Resonance Treatment*

by

R. N. Hwang

Applied Physics Division
Argonne National Laboratory
9700 S. Cass Avenue
Argonne, IL 60439

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The treatment of the resonance self-shielding effect in the unresolved energy region is essentially an extension of the statistical theory of treating average cross sections[1,2]. The nature of the problems in the reactor applications is, however, considerably different from that in the analysis of cross section measurements. One convenient quantity commonly used to describe the degree of resonance self-shielding is the self-shielding factor f, defined as the ratio of the flux averaged resonance cross-section of a certain type to its value at infinite dilution. Without loss of generality, it is conceptually more useful to express f in the following form.

$$f_x = \frac{\langle \sigma_x \phi \rangle}{\langle \sigma_x \rangle \langle \phi \rangle} = 1 + \frac{\langle \sigma_x \phi \rangle - \langle \sigma_x \rangle \langle \phi \rangle}{\langle \sigma_x \rangle \langle \phi \rangle} \qquad (1)$$

where the bracket denotes the average over energy, space and appropriate statistical distributions, in the case of unresolved resonances.

Thus, the degree of resonance self-shielding is equivalent to that of correlation between the reaction cross section in question and the neutron flux in energy and space. The functional relationship between the neutron flux and the cross sections at any given point in energy and space is described by the integral transport equation. The energy and temperature dependence of cross sections are defined by appropriate formalisms and the Doppler broadening procedure. The characteristics of the individual resonances are specified by two fundamental parameters; namely, the resonance energy E_{oi} and the reduced width amplitude γ_{ci} for a given channel c[3]. From the statistical theory of spectra the distributions of these parameters are well known. The distribution of the level spacing $E_{oi} - E_{oi+1}$ for a given spin state is characterized by the Wigner distribution and by the long range correlations described by Dyson[4,5]. γ_{ci} are statistically independent and normally distributed with zero means and variance of unity according to Porter and Thomas[4]. Given average

parameters $< E_{oi} - E_{oi+1} >$ and $<\gamma_{ci}^2>$, Eq. 1, in principle, includes all the statistical information and the explicit energy dependence of the cross sections from which, and through the integral transport equation, the expectation values are completely specified, provided that the quantitites under consideration are truely statistical in nature.

From a conceptual point of view, there are two general ways of representing the behavior of the unresolved resonances according to how the joint probability density function (p,d,f) is defined[6]. From a practical point of view, these statistical representation can be carried out either directly at run time or through a parameterization procedure beforehand to provide various degrees of rigor.

The most commonly used methods are based on the explicit use of the p.d.f. of resonance parameters and level correlation functions. Relevant quantities of interest are computed either by the integral method, in which the resonance integral is averaged directly using numerical quadratures[7], or by the ladder method[8], in which discrete resonances are generated so that the problem becomes numerically equivalent to the treatment of resolved resonances. Alternatively, the joint p.d.f can also be defined in terms of the conditional distributions of partial cross sections and the marginal distribution of the total cross section. For reactor problems of interest, it has been shown that only the conditional means of the former as a function of the total cross section, in addition to the latter are required[6,8]. Given the statistical distributions of resonance parameters and level spacing, these functions can be determined explicitly or parameterized implicitly. One direct approach is known as the probability table method, in which the cumulative density function of σ_t and the corresponding conditional means of partial cross section are derived numerically and tabulated as a function of σ_t over various energy range of interest[8]. This method has been used extensively in the VIM Monte Carlo code[8].

The analytical behavior of these functions is being explored[9]. A similar concept can be used through the subgroup/multiband methods[10,11,12] with parameters equivalent to the weights and quadrature points which are determined by matching the relevant cross section moments as obtained by the integral methods.

For practical applications, simplifying assumptions are usually inevitable. Aside from the statistical assumptions, existing methods differ essentially only in how rigorously the neutron flux is treated as a function of energy, composition and space. However, unlike the case of the resolved resonance the impact of fundamental assumptions on the self shielding effect and the Doppler effect is far more difficult to assess due to the conflicting requirements of the statistical theory and the rigor in the treatment of the flux. The statistical treatment of the self-shielding effect is apparently subject to various inherent limitations[6,9]. The potential problems must be addressed not only from the perspectives of the theory but also from those of the data base.

On theoretical grounds, the most obvious inherent limitations of the statistical approach are directly related to the determinisitic and multivariate nature of the neutron flux. Strictly speaking, the neutron slowing down process by elastic-scattering is deterministic in nature since the collision density (or slowing down spectrum) can attenuate and/or fluctuate appreciably as neutrons suffer energy losses in the presence of resonances. The gross attenuation of slowing-down spectrum is, in principle, inevitable even under the asymptotic condition as it approaches a 1/E dependence. Consequently the resonance interals near the top of the energy interval under consideration usually require greater weights than those near the bottom in the averaging process. Unlike the estimation of the cross section moments, the fundamental assumption of stationarity of the resonance samples with respect to energy is

clearly less plausible for the estimation of the reaction rates and greater statistical uncertainties are expected. The dilemma is how much the dynamic nature of the slowing down process can be compromised in the statistical treatment and vice versa. Hence, the expectation value of the reaction rate is not statistically meaningful unless the attenuation of the collision density in the energy interval of interest is insignificant. For this reason, the statistical methods are inherently restrictive if they are extended beyond the evaluation of the cross section moments originally intended. To ensure the plausibility of the statistical methods, three criteria are obviously required: (1) the energy interval ΔE under consideration must be much greater than the average level spacing; (2) ΔE must be much smaller than the mean energy of the interval; (3) the average resonance absorption probability must be small compared to unity.

Since the basic assumptions on the in-group slowing down spectrum can be quite different, these criteria are also believed to be useful in the benchmark calculations especially when the results based on the ladder methods are compared to those based on other methods. For a typical lethargy width of 0.25, questions usually arises in the relatively low energy region for nuclides with high concentration as the absorption probability becomes significant. This is particularly true for cases involving highly enriched fissionable isotopes. Cursory calculations with generated ladders have shown that the overall absorption probabilities for ^{239}Pu and ^{235}U can well exceed 0.5 near the top of their resolved energy regions if σ_p becomes less than 100 barns/atom. On the other hand, the application of statistical theory is far more plausible for large fast reactor systems where the absorption probabilities within the group are usually small in the energy region of interest.

The problem is further complicated by the multivariate nature of the self-shielding effect characterized by the overlap effect, composition and spatial

dependece of the neutron flux. An energy interval under consideration usually consists of many sequences of resonances belonging to different nuclides either in homogeneous mixture or spatially separated. For heavy nuclides, resonances are generally narrow and the unresolved regions begin at relatively low energies. For nuclides with medium weight, the resolved energy regions which are characterized by extremely wide s-wave resonances and sharp p-resonances can extend well beyond 60 keV. The resolved resonances, will impact both the detailed as well as the gross spectrum under consideration and will further enhance the deterministric nature of the problem. Various methods that treat these problems to different degrees of sophistication are available. Qualitative merits and potential limitations of existing methods have been discussed in Ref. 9. From the point of view of accuracy in the flux treatment, the validity of the NR-approximation and rational approximation/equivalence relation assumption, ways of including overlapping resonances, and questions of weighting spectrum have been subjects for discussions. However, meaningful assessments based on both rigor and statistical considerations are not always easy. From a practical point of view, the question of relevant nuclear data is believed to be a more important issue than the choice of the methods in the unresolved resonance treatment.

From the data perspective, there are two major problems concerning the unresolved resoances. First, there does not appear to exist an unique way of determining the average resonance parameters for various J- and ℓ-states on the basis of low resolution measurements. For instance, the s-wave strength functions for ^{238}U in the current ENDF/B-V file are taken to be constant at 1.05×10^{-4} for all energies while the p-wave strength functions are allowed to vary in order to preserve the estimated infinitely dilute cross section values deduced from several experiments. For ^{239}Pu data in ENDF/B-V, on the other hand, the p-wave strengths functions are fixed while the s-wave strength

functions are allowed to vary in different energy regions. In addition, the energy intervals in which the varying strength functions were defined are not much greater than the average level spacings of the $J=0^+$ state. Judging from the sensitivity of the self-shielding effect to the s-wave strength function and from statistical considerations, significant uncertainties are anticipated. The problems is further complicated by the significant uncertainties in the measured data themself, particularly in the energy regions just above the resolved energy range. For instance, the measured data for ^{238}U are generally poor between 4 keV and 30 keV where the self-shielding effect is still important. Secondly, direct or relevant experimental data on the self-shielding effect are still lacking. It is doubtful that the self-shielding effect can be accurately estimated by fixing the first order moments in cross section alone especially when more than one ℓ- and J-states are involved. Apparently, additional data bases are needed.

One obvious solution to the problem is to extend the resolved energy region utilizing the recent high resolution data at ORNL[13,14]. Hopefully, the strong s-wave resonances primarily responsible for the self-shielding effect can be resolved in the higher energy regions[14]. The effort in this area has been focused on ^{238}U in the energy region above 4 keV. Another potentially useful data base are the results of self-indication measurements[15,16]. In these measurements, the neutrons pass through a transmission sample with various thicknesses and are either heated or cooled to various temperatures before impinging on a thin capture sample. Two measured quantities of practical importance are the tranmission ratio, the fraction of neutrons transmitted through the transmission sample of given thickness and temperature, and the self-indication ratio, the ratio of capture rate detected in the capture sample with and without the presence of the transmission sample. If n_1 and n_2 are the thickness in atom/barn, these ratios are defined as

$$\langle TR \rangle = \langle \exp(-n_1 \sigma_t) \rangle \tag{2}$$

$$\langle SIR \rangle = \frac{\left\langle \exp(-n_1\sigma_t) \cdot \frac{\sigma_\gamma}{\sigma_t} [1 - \exp(-n_2\sigma_t)] \right\rangle}{\left\langle \frac{\sigma_\gamma}{\sigma_t} [1 - \exp(-n_2\sigma_t)] \right\rangle} = \frac{\langle TR \cdot ABS \rangle}{\langle ABS \rangle} \tag{3}$$

where <ABS> is the average absorption rate in absence of the transmission sample.

It is interesting to note that there is a striking similarity between the self-shielding factor defined in Eq. 1 and the ratio <SIR>/<TR>.

$$r = \frac{\langle SIR \rangle}{\langle TR \rangle} = 1 + \frac{\langle TR \cdot ABS \rangle - \langle TR \rangle \langle ABS \rangle}{\langle TR \rangle \langle ABS \rangle} \tag{4}$$

The obvious analogy between r and f is important on theoretical grounds. In particular, in the limit of high energy or thin sample thickness (or dilution), Eq. 1 and Eq. 4 become

$$1 - f_\gamma = \frac{\langle \sigma_\gamma \sigma_t \rangle - \langle \sigma_\gamma \rangle \langle \sigma_t \rangle}{\langle \sigma_\gamma \rangle \langle \sigma_t \rangle} \tag{5}$$

and

$$1 - r = n_1 \frac{\langle \sigma_\gamma \sigma_t \rangle - \langle \sigma_\gamma \rangle \langle \sigma_t \rangle}{\langle \sigma_\gamma \rangle \langle \sigma_t \rangle} \tag{6}$$

respectively. Thus, both quantities are characterized by the correlation between the capture and total cross sections under the limiting condition. It is not difficult to deduce that the quantity (1-r) can be considered as a measure of the higher order moments in cross sections which are also essential to the self-shielding effect and the related Doppler effect.

Unfortunately, the analysis of the self-indication measurements is by no means simple. Work has been initiated at ORNL and RPI[15,16]. Some preliminary

analysis, on the ^{238}U measurement, has been carried out at ANL in cooperation with the RPI group. The calculated <SIR> values using ENDF/B-V data appear to be low in the resolved energy region but high in the unresolved energy region as compared to the RPI measurements. It is still unlcear how much impact the time-dependent background correction, the multiple scattering corrections and other experimental corrections may have on the results when they are included in the analysis. Further studies are apparently needed.

Finally, it is worth noting that recent improvements in computer efficiency and numerical techniques have significant impact on the basic philosophy of the current cross-section processing. The effects of heterogeneity due to complex geometries have received increasingly more attention in the core design calculations and in the analysis of ZPR/ZPPR experiments. One direct consequence is that the resonance cross section calculations are usually followed by rather ellaborate cell homogenization procedures either based on collisison probability methods or S_N methods at the "fine" group level. The computing time requirement of various cell treatments may well exceed that of the resonance cross sections. Hence, there is strong motivation to improve the treatment of resonance heterogeneity as well for the complex geometries. Problems which have received much attention are the double heterogeneity effect for the fast reactor fuel subassemblies, the interface effect between core and inner blanket, and the general treatment of the non-repeating finite lattice. One simple method to treat the double heterogeneity which is readily amenable to many existing codes was proposed by Nakagawa and Inoue[17]. It is essentially an extension of the conventional rational approximation and equivalent relations which is suitable for both the resolved and the unresolved resonance treatments. Other alternatives including the Monte-Carlo based two term rational approximation and the extension of the more rigorous transmission probability approach to complex pin geometries are also under examination at ANL. For the unresolved

resonance treatment, the inclusion of the direct ladder approach and the probability table/subgroup methods will also provide more flexibility to estimate the heterogeneity effect of complex cells.

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