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The Effect of the Energy Dependence of the Neutron Widths on the Calculation of Average Reaction Cross Sections

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THE EFFECT OF THE ENERGY DEPENDENCE OF THE NEUTRON WIDTHS ON
THE CALCULATION OF AVERAGE REACTION CROSS SECTIONS

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ABSTRACT

We study the validity of neglecting the energy dependence of the neutron width in the calculation of average reaction cross sections.

I. INTRODUCTION

Energy averaging of neutron reaction cross sections is widely used for the determinations of average resonance parameters [1]. Conversely in nuclear reactor calculations, one obtains group cross sections from "local" average resonance parameters as provided for example by the ENDF/B file 2 system [2]. In both instances the average reaction cross section is parameterized in the form [3]

$$\langle \sigma_{nr} \sqrt{E} \rangle = \frac{2\pi C}{\langle D \rangle} \left\langle \frac{\Gamma_{on} \Gamma_r}{\Gamma} \right\rangle, \quad (1)$$

where σ_{nr} is the neutron-reaction cross section at energy E ,

$$C = \frac{\pi \hbar^2}{2m} g, \quad (2)$$

m the neutron mass, g the spin factor, Γ_{on} the reduced neutron width, Γ_r the reaction width and Γ the total width.

The brackets in the right-hand side of equation (1) indicate an ensemble average over the nuclear resonances in the energy region of interest.

For the purpose of computing average cross sections the above expression can be utilized in two different ways:

- (i) Starting from resonance "ladders," obtained from the known statistical distributions of the level parameters by Monte Carlo techniques, one performs the indicated ensemble average, computing the neutron width at some average energy in each energy interval.
- (ii) Equation (1) is rewritten in the form

$$\langle \sigma_{nr} \sqrt{E} \rangle = \frac{2\pi C}{\langle D \rangle} \frac{\langle \Gamma_{on} \rangle \langle \Gamma_r \rangle}{\langle \Gamma \rangle} R, \quad (3)$$

where R is the so-called statistical fluctuation factor [1]. Then one utilizes the average value of the level parameters, with the neutron width again computed at the average energy in each energy interval.

It is somewhat amusing to review how Eq. (1) has been derived and used. To this end we start with the single-level formalism for the reaction cross section, which can be written as

$$\sigma_{nr}(E) \sqrt{E} = C \sum_{\lambda} \frac{\Gamma_{o\lambda n} \Gamma_{\lambda r}}{(E_{\lambda} - E)^2 + \Gamma_{\lambda}^2/4}, \quad (4)$$

where E_{λ} is the resonant energy.

Integration between the energy limits E_1 and E_2 yields

$$\langle \sigma_{nr}(E) \sqrt{E} \rangle = \frac{2C}{E_2 - E_1} \sum_{\lambda} \frac{\Gamma_{o\lambda n} \Gamma_{\lambda r}}{\Gamma_{\lambda}} \left\{ \operatorname{tg}^{-1} \left(\frac{E_{\lambda} - E}{\Gamma_{\lambda}/2} \right) \right\}_{E_1}^{E_2}, \quad (5)$$

where we have neglected the energy dependence of the neutron width entering in the expression of the total level width Γ_{λ} :

$$\Gamma_{\lambda} = \Gamma_{\lambda t} + \sqrt{E} \Gamma_{o\lambda n}, \quad (6)$$

where $\Gamma_{\lambda t}$ is the total reaction width.

In Eqs. (4) and (5) the sum is to be extended over all nuclear resonances both inside and outside the energy interval E_1, E_2 . Those resonances belonging to this interval and far away from its limits will make a contribution proportional to $\pi \Gamma_{o\lambda n} \Gamma_{\lambda r} / \Gamma_{\lambda}$. This is due to the fact that for these resonances Γ_{λ} is much smaller than either $|E_{\lambda} - E_2|$ or $E_{\lambda} - E_1$. Conversely the resonances either near to or outside of the interval limits will contribute terms of the form $f_{\lambda} \Gamma_{o\lambda n} \Gamma_{\lambda r} / \Gamma_{\lambda}$ where $f_{\lambda} < \pi$.

In consequence, to arrive at the result shown in equation (1) one has to:

- (a) neglect the influence of those resonances near to or outside of the interval limits, i.e., the energy interval is wide enough to neglect "end-effect."
- (b) neglect the energy dependence of the total width Γ_λ .

The purpose of the present work is to investigate the implications of the approximation (b).

II. EXACT CALCULATION OF THE AVERAGE REACTION CROSS SECTION WITH THE SINGLE-LEVEL BREIT-WIGNER FORMULA

The contribution of each level λ to the resonant reaction cross section σ_{nr} at energy E can be written as

$$\sqrt{E} \sigma_{nr} = C \sum_{\lambda} \frac{\Gamma_{o\lambda n} \Gamma_{\lambda r}}{(E_{\lambda} - E)^2 + \Gamma_{\lambda}^2/4} . \quad (7)$$

The average of $\sqrt{E} \sigma_{nr}$ between two energies E_2 and E_1 is then

$$\langle \sigma_{nr} \sqrt{E} \rangle = \frac{C}{E_2 - E_1} \sum_{\lambda} \Gamma_{o\lambda n} \Gamma_{\lambda r} \int_{E_1}^{E_2} \frac{dE}{(E_{\lambda} - E)^2 + \Gamma_{\lambda}^2/4} . \quad (8)$$

Our intermediate goal is the calculation of the integral

$$I_{\lambda} = \int_{E_1}^{E_2} \frac{dE}{(E_{\lambda} - E)^2 + (\Gamma_{\lambda t} + \sqrt{E} \Gamma_{o\lambda n})^2/4} , \quad (9)$$

where, according to approximation (a) in the introduction, E_λ belongs to the energy interval E_1, E_2 .

With

$$x = \sqrt{E} , \quad (10)$$

Eq. (9) is transformed into

$$I_\lambda = \int_{\sqrt{E_1}}^{\sqrt{E_2}} \frac{2x \, dx}{(E_\lambda - E^2)^2 + (\Gamma_{\lambda t} + x\Gamma_{o\lambda n})^2/4} . \quad (11)$$

The zeros of the denominator in Eq. (11) are given by the equation

$$(E_\lambda - x^2)^2 = - (\Gamma_{\lambda t} + x\Gamma_{o\lambda n})^2/4 . \quad (12)$$

or, after taking the square root in both terms,

$$E_\lambda - x^2 = \pm i (\Gamma_{\lambda t} + x\Gamma_{o\lambda n})/2 . \quad (13)$$

From Eq. (13) we obtain two quadratic equations for x , namely

$$E_\lambda - x^2 = i (\Gamma_{\lambda t} + x\Gamma_{o\lambda n})/2 \quad (14)$$

and

$$E_\lambda - x^2 = -i (\Gamma_{\lambda t} + x\Gamma_{o\lambda n})/2 . \quad (15)$$

Then, the four zeros are given by:

$$x_1 = a + (b - c) i , \quad (16)$$

$$x_2 = -a - (b + c) i , \quad (17)$$

$$x_3 = a - (b - c) i , \quad (18)$$

$$x_4 = -a + (b + c) i , \quad (19)$$

where

$$a = \sqrt{\frac{\sqrt{(E_\lambda - \frac{\Gamma_{0\lambda n}^2}{16})^2 + \frac{\Gamma_{\lambda t}^2}{4}} + (E_\lambda - \frac{\Gamma_{0\lambda n}^2}{16})}{2}} , \quad (20)$$

$$b = -\sqrt{\frac{\sqrt{(E_\lambda - \frac{\Gamma_{0\lambda n}^2}{16})^2 + \frac{\Gamma_{\lambda t}^2}{4}} - (E_\lambda - \frac{\Gamma_{0\lambda n}^2}{16})}{2}} , \quad (21)$$

$$c = \frac{\Gamma_{0\lambda n}}{4} , \quad (22)$$

As can be seen directly, the following relations are valid between the roots of Eq. (12):

$$2ab = -\frac{\Gamma_{\lambda t}}{2} , \quad (23)$$

$$x_1 = x_3^* , \quad (24)$$

and

$$x_2 = x_4^* . \quad (25)$$

Equations (20) and (21) for a and b , respectively, can be greatly simplified in view of the fact that both the reduced neutron width and the total reaction width are much smaller than E_λ in the region of interest:

$$a \cong \sqrt{E_\lambda} \quad (26)$$

and

$$b \cong - \frac{\Gamma_{\lambda} t}{4\sqrt{E_{\lambda}}} . \quad (27)$$

The integral I_{λ} can be calculated in a straightforward manner, yielding

$$\begin{aligned} \frac{I_{\lambda}}{2} = & [Ax_1 \ln(x - x_1) + Bx_2 \ln(x - x_2) + Cx_3 \ln(x - x_3) \\ & + Dx_4 \ln(x - x_4)] \frac{\sqrt{E_2}}{\sqrt{E_1}} , \end{aligned} \quad (28)$$

where

$$A = \frac{1}{8(a + bi)[(b-c)i](a - ci)} , \quad (29)$$

$$B = \frac{-1}{8(a + bi)[(b+c)i](a + ci)} , \quad (30)$$

$$C = A^*, \text{ and} \quad (31)$$

$$D = B^* . \quad (32)$$

By virtue of the relations between x_1 and x_3 , x_2 , and x_4 , and C and A , D and B , we obtain:

$$\frac{I_{\lambda}}{4} = \{ \text{Re}[Ax_1 \ln(x - x_1) + \text{Re}[Bx_2 \ln(x - x_2)] \} \frac{\sqrt{E_2}}{\sqrt{E_1}} , \quad (33)$$

where Re denotes real part.

Then I_{λ} is given by

$$\begin{aligned} \frac{I_\lambda}{4} = & \alpha \ln \frac{|\sqrt{E_2} - x_1| |\sqrt{E_1} - x_2|}{|\sqrt{E_1} - x_1| |\sqrt{E_2} - x_2|} - \beta [\arg(\sqrt{E_2} - x_1) - \arg(\sqrt{E_1} - x_1)] \\ & - \delta [\arg(E_2 - x_2) - \arg(E_1 - x_2)] , \end{aligned} \quad (34)$$

where $\arg(z)$ denotes the argument of the complex number Z , and α , β , and δ are given by

$$\alpha = \frac{bc}{8(a^2 + b^2)(a^2 + c^2)} , \quad (35)$$

$$\beta = - \frac{a}{8(a^2 + c^2)(a^2 + b^2)} \left(b - c + \frac{a^2 + bc}{b - c} \right), \text{ and} \quad (36)$$

$$\delta = - \frac{a}{8(a^2 + b^2)(a^2 + c^2)} \left(b + c + \frac{a^2 - bc}{b + c} \right) . \quad (37)$$

To put Eq. (34) in a more convenient form, we define

$$\eta \equiv \frac{\beta + \delta}{2} \quad (38)$$

and

$$\epsilon \equiv \frac{\beta - \delta}{2} . \quad (39)$$

Then Eq. (34) transforms into

$$\begin{aligned} \frac{I_\lambda}{4} = & \alpha \ln \frac{|\sqrt{E_2} - x_1| |\sqrt{E_1} - x_2|}{|\sqrt{E_1} - x_1| |\sqrt{E_2} - x_2|} - \eta \arg(\sqrt{E_2} - x_1)(\sqrt{E_2} - x_2) \\ & - \arg(\sqrt{E_1} - x_1)(\sqrt{E_1} - x_2)] - \epsilon [\arg(\sqrt{E_2} - x_1)(\sqrt{E_2} - x_2^*) \\ & - \arg(\sqrt{E_1} - x_1)(\sqrt{E_1} - x_2^*)] , \end{aligned} \quad (40)$$

where

$$\eta = - \frac{ab}{8(a^2 + c^2)(b^2 - c^2)}, \quad (41)$$

$$\epsilon = - \frac{ac}{8(a^2 + b^2)(b^2 - c^2)}, \quad (42)$$

$$\arg(\sqrt{E} - x_1)(\sqrt{E} - x_2) = \arctg \frac{(\Gamma_{0\lambda n}/2) \sqrt{E} + (\Gamma_{\lambda t}/2)}{E - E_\lambda}, \quad (43)$$

and

$$\arg(\sqrt{E} - x_1)(\sqrt{E} - x_2^*) = \arctg \frac{2ac - 2b\sqrt{E}}{E + c^2 - (a^2 + b^2)}. \quad (44)$$

Then the exact value of the average cross section is given by

$$\langle \sigma_{nr} \sqrt{E} \rangle = \frac{C}{E_2 - E_1} \sum_{\lambda} \Gamma_{0\lambda n} \Gamma_{\lambda r} I_{\lambda}, \quad (45)$$

where I_{λ} is calculated by Eq. (40).

III. APPROXIMATIONS TO THE EXACT INTEGRAL I_{λ}

In what follows we discuss various approximations to the exact result [Eq. (40)]. From Eqs. (26), (27), (35), (41), (42) we obtain

$$\alpha \approx \frac{\Gamma_{\lambda t} \Gamma_{0\lambda n}}{128} \frac{1}{F^{5/2}}, \quad (46)$$

$$\eta \approx \frac{\Gamma_{\lambda t}}{2(\Gamma_{\lambda t}^2 - \Gamma_{0\lambda n}^2 E_{\lambda})}, \quad (47)$$

$$\epsilon \approx \frac{\Gamma_{0\lambda n} \sqrt{E_{\lambda}}}{2(\Gamma_{\lambda t}^2 - \Gamma_{0\lambda n}^2 E_{\lambda})}. \quad (48)$$

In view of the smallness of the resonance partial widths in comparison with E_λ , one can always neglect α . However, one cannot neglect ϵ in comparison with η except when the neutron width, $\Gamma_{\lambda n}$, is much smaller than the total reaction width $\Gamma_{\lambda t}$.

In view of the smallness of α , one can neglect in Eq. (40) the contribution of the logarithmic term. Next we discuss the terms depending on the argument of the complex logarithm function.

Equation (40) can be written in the form

$$\frac{I_\lambda}{4} = -\eta[\phi_2 - \phi_1] - \epsilon[\psi_2 - \psi_1], \quad (49)$$

where

$$\phi_i = \arctg \frac{(\Gamma_{0\lambda n}/2)\sqrt{E_i} + (\Gamma_{\lambda t}/2)}{E_i - E_\lambda} \quad (i = 1, 2), \quad (50)$$

$$\psi_i = \arctg \frac{2ac - 2b\sqrt{E_i}}{E_i + c^2 - (a^2 + b^2)} \quad (i = 1, 2), \quad (51)$$

or with the approximate expressions for a and b [Eqs. (27) and (28)]

$$\psi_i = \arctg \frac{(\sqrt{E_\lambda} \Gamma_{0\lambda n}/2) + (\Gamma_{\lambda t}/2\sqrt{E_\lambda})\sqrt{E_i}}{E_i + (\Gamma_{0\lambda n}^2/16) - [E_\lambda + (\Gamma_{\lambda t}^2/4E_\lambda)]}. \quad (52)$$

Taking into account that $E_\lambda \gg (\Gamma_{0\lambda n}^2/16)$ and $E_\lambda \gg (\Gamma_{\lambda t}^2/4E_\lambda)$, one can write

$$\psi_i = \arctg \frac{(\Gamma_{0\lambda n}/2) \sqrt{E_\lambda} + (\Gamma_{\lambda t}/2\sqrt{E_\lambda}) \sqrt{E_i}}{E_i - E_\lambda}. \quad (53)$$

Now if $E_2 - E_\lambda$ (which is always positive) is substantially greater than the numerator of Eqs. (50) and (53) we get

$$\phi_2 \longrightarrow 0 \quad (54)$$

and

$$\psi_2 \longrightarrow 0 . \quad (55)$$

Conversely in the lower limit, $E_1 - E_\lambda$ (which is always negative) is substantially greater than the numerator of Eqs. (50) and (53). In this case,

$$\phi_1 \longrightarrow -\pi \quad (56)$$

$$\psi_2 \longrightarrow -\pi . \quad (57)$$

These approximations become invalid for those resonances close to the energy limits E_1 and E_2 . However the approximations so far discussed still apply when averaging a large number of resonances.

Then we obtain

$$I_\lambda = 4\pi[\eta + \epsilon] , \quad (58)$$

or with the values of η and ϵ given by Eqs. (41) and (42),

$$I_\lambda = -4\pi \frac{a^3 + a[(b-c)^2 + bc]}{8(b-c)(a^2 + c^2)(a^2 + b^2)} . \quad (59)$$

By definition

$$c = \frac{\Gamma_{0\lambda n}}{4} ,$$

and to a very good approximation,

$$b \cong \frac{-\Gamma_{\lambda} t}{4\sqrt{E_{\lambda}}}$$

and

$$a \cong \sqrt{E_{\lambda}}.$$

Then we have

$$a^3 \gg a[(b - c)^2 - bc], \quad (60)$$

$$a^2 \gg c^2, \quad (61)$$

$$a^2 \gg b^2, \quad (62)$$

and Eq. (59) reduces to

$$I_{\lambda} = \frac{-4\pi}{8ab - 8ac}, \quad (63)$$

but

$$8ab = -2\Gamma_{\lambda} t,$$

and

$$8ac \cong 2\sqrt{E_{\lambda}} \Gamma_{0\lambda n}.$$

Then Eq. (63) is finally reduced to

$$I_{\lambda} = \frac{2\pi}{\Gamma_{\lambda}(E_{\lambda})}, \quad (64)$$

where $\Gamma_{\lambda}(E_{\lambda})$ is the total width given by Eq. (6) evaluated at the resonant energy E_{λ} .

Upon introduction of the results, Eq. (64), for I_λ , into Eq. (45), one obtains

$$\langle \sigma_{nr} \sqrt{E} \rangle = \frac{C}{E_2 - E_1} 2\pi \sum_{\lambda} \frac{\Gamma_{o\lambda n} \Gamma_{\lambda r}}{\Gamma_{\lambda}(E_{\lambda})}, \quad (65)$$

which can be rewritten in the form:

$$\langle \sigma_{nr} \sqrt{E} \rangle = \frac{2\pi C}{(E_2 - E_1)/N} \frac{1}{N} \sum_{\lambda=1}^N \frac{\Gamma_{o\lambda n} \Gamma_{\lambda r}}{\Gamma_{\lambda}(E_{\lambda})}, \quad (66)$$

where N is the number of levels within the energy limits. We now introduce the average level spacing $\langle D \rangle$ in Eq. (66), to obtain

$$\langle \sigma_{nr} \sqrt{E} \rangle = \frac{2\pi C}{\langle D \rangle} \left\langle \frac{\Gamma_{o\lambda n} \Gamma_{\lambda r}}{\Gamma_{\lambda}(E_{\lambda})} \right\rangle, \quad (67)$$

where the bracket in the right-hand side denotes an ensemble average. In Eq. (67) we have used the approximations (54) through (57) for the arguments of the logarithmic terms and the approximations (59) through (64).

When the energy interval $E_2 - E_1$ is narrow we can substitute E_{λ} in Eq. (67) by an average value $\bar{E} = (E_1 + E_2)/2$. With this approximation Eq. (67) takes the form

$$\langle \sigma_{nr} \sqrt{E} \rangle = \frac{2\pi C}{\langle D \rangle} \left\langle \frac{\Gamma_{o\lambda n} \Gamma_{\lambda r}}{\Gamma_{\lambda t} + \Gamma_{o\lambda n} \sqrt{E}} \right\rangle. \quad (68)$$

The result (68) is the usual expression utilized in the calculation of average cross sections.

IV. A NUMERICAL EXAMPLE

To test the various approximations discussed previously, the program POLLA [4] was utilized to generate a ladder of resonance parameters by Monte Carlo techniques. Table I shows the average parameters utilized in the energy region between 5020.5 eV up to 7182.5 eV.

Table I

Material	²³⁸ U
Average Spacing	20 eV
Average Radiation Width	0.024 eV
Average Reduced Neutron Width	0.0021 eV

The results of the various tests are shown in Table II. The first approximation used was to neglect the logarithmic term in Eq. (40). Neglecting this term did not alter the exact results within the accuracy of the calculation. This is indeed a good approximation because in the region of interest (unresolved resonance energy region) the level widths are always much smaller than the resonance energy.

Table II

	$\langle \sigma_{nr} \sqrt{E} \rangle$ [barn·(eV) ^{1/2}]	Deviation (%)
Exact	30.71	-
Approximation 1(a)	30.71	0
Approximation 2(b)	30.98	0.88
Approximation 3(c)	30.98	0.88
Approximation 4(d)	31.07	1.2

^aEquation (40) without the logarithmic term.

^bEquation (40) without the logarithmic term and with the argument of the complex logarithmic approximated by Eqs. (54) through (57).

^cEquation (67).

^dEquation (68).

The second approximation tried was to approximate the arguments of the complex logarithmic term in Eq. (40) by the expressions (54), (55), (56), and (57). This approximation introduced an error less than 1%. The third approximation based on the approximate results in Eq. (64) yields for Eq. (67) again an error of less than 1%. Finally the result, Eq. (68), was compared with the exact Eq. (40), also with small error.

V. CONCLUSIONS

As far as the modulus of the logarithmic term, the effect of the integration limits, E_1 and E_2 , is negligible whenever $\Gamma_{\lambda t} \Gamma_{o\lambda n} \ll 128 E_{\lambda}^{5/2}$. This condition is satisfied even in the resolved low energy region. This relation allows dropping the modulus of the complex logarithm in Eq. (34). The argument of the complex logarithm term can be simplified to the expressions (54) through (57) provided that the partial reaction widths are small compared with the interval of integration. In this manner one obtains the result (67) in which the total level widths are computed at their respective level energies. Up to this step the different approximations take into account rigorously the energy dependence of the neutron widths. In so far that the energy-dependent neutron widths are not much larger than the reaction widths, the usual recipe of computing the neutron widths at an average energy produces only a small error. Hence, the use of Eq. (68) for the calculation of average cross sections appears to be a good approximation at least for the case studied here.

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