M. J. Pears

UNCLASSIFIED

KAPL-M-JHS-1

PHYSICS & MATHEMATICS

General Electric Company
KNOLLS ATOMIC POWER LABORATORY
Schenectady, New York

SOME FORMULAE FOR AVERAGE SELF-SHIELDING FACTORS

by

J. H. Smith

June 26, 1959

John R Stehn — 7 July 1959

Authorized Classifier — Date

This report was prepared as an account of Government-sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, express or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission to the extent that such employee or contractor prepares, handles or distributes, or provides access to, any information pursuant to his employment or contract with the Commission.

Operated for the
United States Atomic Energy Commission
by the
General Electric Company
Contract No. W-31-109-Eng.-52

UNCLASSIFIED

015-1

Distribution List	No of Copies
D. R. Bach	(1)
E. F. Bohl	(1)
J. J. Bulmer	(1)
G. P. Calame	(1)
R. C. Dahlburg	(1)
D. Dougherty	(1)
R. Ehrlich	(1)
F. D. Federighi	(1)
F. Feiner	(1)
R. T. Frost	(1)
N. C. Francis	(1)
R. G. Luce	(1)
C. R. Mullin	(1)
F. C. Merriman	(1)
W. A. Northrop	(1)
C. Randall	(1)
J. R. Stehn	(1)
M. S. Storm	(1)
W. Skolnik	(1)
J. H. Smith	(5)
W. B. Wright	(1)
Technical Publications/M.J. Sears	(3)
TIG File/C.J. Schmidt	(5)
Document Library	(3)

Distribution List (continued)	No. of Copies
External	
Manager, SNROO Office	(7)
A. Radkowsky	(1)

SOME FORMULAE FOR AVERAGE SELF-SHIELDING FACTORS

ABSTRACT

This memo presents analytic formulae for desk computer calculation of average self-shielding factors for 1/v and resonance absorbers. Validity of the results is discussed and a short table of some lesser known functions for calculations is included.

CONTENTS

I Introduction

The average of a self-shielding factor, $f(E)$, taken with respect to an absorption rate, $\sigma(E)\varphi(E)$, is

$$\langle f \rangle = \frac{\int f(E)\sigma(E)\varphi(E)dE}{\int \sigma(E)\varphi(E)dE} . \qquad (1)$$

For a Maxwellian neutron distribution and an energy dependent f of the form

$$f(E) = \frac{1}{1 + a\xi(E)}, \qquad (2)$$

where "a" is a constant and $\xi(E)$ is the number of absorption mean free paths in the capturing material, $\langle f \rangle$ can be evaluated exactly for a 1/v absorber and approximated for a Breit-Wigner one level system.

Such a form for f(E) has been found reasonable for a slab which absorbs much more strongly then it scatters. Whether f(E) can be described equally well by this form for a strong scatterer is not known quantitatively, but at least within this limitation the formulae to be stated provide simple tools for self-shielding studies of two types of absorber.

Section II contains exact relations for $\langle f \rangle$ and $\frac{d\langle f \rangle}{dT}$ for a 1/v absorber. Section IIIa presents convergent series developments which should be useful principally in dealing with narrow resonances with "not too high" self-shielding at peak cross section. Section IIIb contains an asymptotic development probably best for broad or very high resonances. The foregoing qualitative statements can be made quantitative through consideration of the expansion parameters given in those sections. Section IV is a table of values of functions not widely available but essential to some of the work.

II 1/v Absorber

This case is by far the simpler of the two and, within the framework of the model, $\langle f \rangle$ is given exactly by

$$\langle f \rangle = 1 + 2z - 4z^2 e^{-z} \Phi_1 (1/2, 3/2; z) \tag{3}$$

$$- 2\sqrt{\frac{z}{\pi}} \left[1 - z e^{-z} \, Ei(z) \right], \text{ where}$$

$$z = a^2 \xi^2 / kT$$

Incidentally, the temperature coefficient for this $\langle f \rangle$ is easily found from $\frac{\partial}{\partial T} = \frac{-a^2 \xi^2}{T} \frac{d}{dz}$ and

$$\frac{d\langle f \rangle}{dz} = 2(1-z) - 2z(3-2z) e^{-z} \Phi_1 (1/2, 3/2; z) \tag{4}$$

$$- (1-2z) \sqrt{\pi z} + \sqrt{\frac{z}{\pi}} (3-2z) e^{-z} \, Ei(z).$$

For values of the confluent hypergeometric function, Φ_1, see tables in British Assoc. for Adv. of Sci., Report 9, 283 (1926). Ei(z) is the exponential integral of positive argument in either WPA Tables of Sine, Cosine, and Exponential Integrals (1940) or NBS Tables of the Exponential Integral for Complex Arguments. Note, in using the last-named volume that

$$Ei(x) = -E_1(-x) - \pi i.$$

With $x > 0$, what is desired is the limit of $E_1(\zeta)$ as the complex variable ζ approaches $-x$ on the negative real axis through values in the second quadrant. The NBS tabulation arbitrarily adopted a non-zero imaginary component in defining its analytic function: this definition does not suit our purposes, so the $(-\pi i)$ appears in the conversion above.

IIIa Resonance Absorber: Upper Bound for $\langle f \rangle$

For a Breit-Wigner resonance with

$$\sigma = \frac{\sigma_r \Gamma^2}{4} \sqrt{\frac{E_r}{E}} \frac{1}{(E-E_r)^2 + \frac{\Gamma^2}{4}},$$

The transformation $E = E_r x^2$ and the notation $\beta = E_r/kT$, $\gamma = \Gamma/2E_r$, ξ_r = absorber thickness at resonance, give

$$f = \frac{\displaystyle\int_0^\infty \frac{1}{1 + \frac{a\,\xi_r\,\gamma^2}{x} \frac{1}{(x^2-1)^2+\gamma^2}} \frac{x^2\, e^{-\beta x^2}}{(x^2-1)^2+\gamma^2}\, dx}{\displaystyle\int_0^\infty \frac{x^2\, e^{-\beta x^2}}{(x^2-1)^2+\gamma^2}\, dx}.$$

In N.S.E., Vol. 1 No. 5,* the denominator of $\langle f \rangle$ is evaluated in a form which is convenient for accurate numerical work when $\beta\gamma \lesssim 2$: namely,

$$D = \frac{\pi e^{-\beta}\left[(p_+ + \gamma p_-)\cos\beta\gamma + (\gamma p_+ - p_-)\sin\beta\gamma\right]}{2\gamma\sqrt{1+\gamma^2}}$$

$$+ \pi e^{-\beta}\sqrt{\beta} \sum_{n=0}^{\infty} (-1)^n (\beta\gamma)^{2n} \left[\frac{\beta\Phi(1/2,\, 2n+\frac{5}{2};\beta)}{(2n+\frac{3}{2})!} - \frac{\Phi(1/2,\, 2n+\frac{3}{2};\beta)}{(2n+\frac{1}{2})!}\right]$$

Actually, D results from the form in N.S.E. after some manipulations. The statements therein on accuracy continue to be relevant: one of them is that truncation of the series to $\sum_{n=0}^{3}$ or less provides 1% or better, depending on specific values of β and γ in the computation. That article also describes a method for obtaining the Φ's. Note that equation (6) in it should be multiplied by $(\beta\gamma)^2$ on the right hand side to give $\bar{\sigma}/\sigma_r$: the same error appears in KAPL-1522, from which the NSE material was extracted.

---

* The Calculation of Maxwellian Averaged Cross Sections for Resonance Absorbers

The numerator for $\langle f \rangle$ in equation (5) is less tractable: in this section there will be a given relation that is an approximate upper bound. In most cases which are fairly realistic, the flux peaks where $\frac{E}{Er} = x^2 < 1$ and most of the absorptions will occur for $x < 1$ or near $x = 1$. Thus either an upper bound or a close approximation to f(x) is

$$f_1 = \frac{1}{1 + \frac{a \xi_r^2}{(x^2-1)^2 + \gamma^2}}$$

and the numerator of an average value for f_1 is

$$\int_0^\infty \frac{x^2 e^{-\beta x^2}}{(x^2-1)^2 + \gamma^2(1+a\xi_r)} \, dx \qquad (5')$$

Expression (5') approximates $\sigma(E)$ only within f(E), not in the absorption rate $\sigma\varphi$. Comparison of (5') with the denominator of equation (5) shows that 5') is exactly equal to an expression with the form of D but with γ^2 replaced by

$$\gamma_1^2 = \gamma^2(1+a\xi_r).$$

The utility of (6) with γ_1 replacing γ may be decreased: this certainly will be the case for large values of ξ_r unless the resonance is very narrow. Since the formulae for $\langle f \rangle$ in this section deal only with a bound, it will be left to the user's discretion whether calculating a number of terms in (6) first with γ and then with γ_1 is worthwhile. The "1% criterion" stated earlier is quite a restrictive condition, and experience with the series for D has proved that obtaining numerical results of known accuracy from it is really a very simple and quick procedure.

An even simpler expression for $\langle f_1 \rangle$ is desirable for cases in which a resonance is so narrow as to make $\beta\gamma\sqrt{1+a\xi_r}$ somewhat less than 1. In this event, terms in (6) are expanded in power series in $\gamma, \gamma_1, \beta\gamma$ and $\beta\gamma_1$ to give

015 7

$$\langle f_1 \rangle \approx \frac{1}{\sqrt{1+a\,\xi/r}}\;\frac{g(\beta,\gamma_1)}{g(\beta,\gamma)}\text{, where} \tag{7}$$

$$g = 1 + \gamma\sqrt{\frac{\beta}{\pi}}\left[(2\beta-1)\,{}_1\Phi_1(1/2,3/2;\beta) - e^{\beta}\right] + \frac{\gamma^2}{8}(1+4\beta-4\beta^2). \tag{8}$$

The accuracy of equation (7) is to be judged according to decreasing magnitude of terms in equation (8).

IIIb Resonance Absorber: Asymptotic Development for $\langle f \rangle$

If a resonance has a very high peak cross section or is fairly broad, so that the conditions for utility of section IIIa are not fully satisfied, a different approximation may be useful. It is

$$D\langle f \rangle \sim \frac{1}{2\beta^2\gamma^2 a\,\xi/r}\Bigg\{1 - \frac{3}{8}\,\frac{1}{\beta^2\gamma^2 a\,\xi/r}\sqrt{\frac{\pi}{\beta}}\left[2\beta^2(1+\gamma^2)-20\beta+105\right]$$

$$+\frac{2}{\beta}\,\frac{1}{\beta^4\gamma^4 a^2\,\xi^2/r^2}\Big[360-240\beta+24\beta^2(3+\gamma^2) \tag{9}$$

$$-12\beta^3(1+\gamma^2)+(1+\gamma^2)^2\beta^4\Big]$$

$$-O\left(\frac{1}{\beta^{7/2}\gamma^8 a^4\,\xi^4/r^4}\right)$$

The expansion parameter in this development is $\dfrac{1}{\gamma^2 a\,\xi/r\,\sqrt{\beta}}$: it should of course, be small. It can be shown that the terms in equation (9) strictly alternate in sign, but the series is only asymptotic and terms are to be retained only so long as their magnitude decreases. D depends only on (β,γ) and should be readily calculable from equation (6) provided that largeness of $\beta\gamma$ is not essential for the largeness of $\gamma^2 a\,\xi/r\,\sqrt{\beta}$.

015 8

The temperature coefficient is again available through $\frac{\partial \langle f \rangle}{\partial \beta}$; note that D also depends on β.

IV Short Table of Some Confluent Hypergeometric Functions

Because the Φ function tables are not widely available, there is given below a set of values for different arguments which may be useful. These numbers were obtained either directly from the British work mentioned or by means of so-called contiguity relations satisfied by such functions.

$$\Phi\left(\tfrac{1}{2}, c; x\right)$$

c \ x	1	2	4	8
$\frac{1}{2}$	2.7183	7.3891	54.598	2981.0
$\frac{3}{2}$	1.4627	2.3645	8.2263	201.51
$\frac{5}{2}$	1.2522	1.6624	3.6447	41.691
$\frac{7}{2}$	1.1708	1.4199	2.4083	14.66
$\frac{9}{2}$	1.1284	1.3029	1.9081	7.242
$\frac{11}{2}$	1.102	1.2354	1.6543	4.498
$\frac{13}{2}$	1.08	1.192	1.505	3.250
$\frac{15}{2}$	1.04	1.162	1.409	2.591
$\frac{17}{2}$		1.14	1.34	2.20

015 9