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COMPARISON OF NUMERICAL TECHNIQUES FOR THE EVALUATION OF THE DOPPLER BROADENING FUNCTIONS $\psi(x,\theta)$ AND $\chi(x,\theta)$

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16. Abstract

Several approximations to the Doppler broadening functions $\psi(x, \theta)$ and $\chi(x, \theta)$ are compared with respect to accuracy and speed of evaluation. A technique due to A. M. Turning (1943) is shown to be at least as accurate as direct numerical quadrature and somewhat faster than Gaussian quadrature. FORTRAN IV listings are included.

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COMPARISON OF NUMERICAL TECHNIQUES FOR THE EVALUATION OF THE DOPPLER BROADENING FUNCTIONS $\psi(x, \theta)$ AND $\chi(x, \theta)$

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SUMMARY

The two Doppler broadening functions, $\psi(x, \theta)$ and $\chi(x, \theta)$, are necessary for the computation of accurate temperature dependent resonance neutron cross sections. With the present use of many resonances and ever increasing resonance energies for reactor physics calculations in support of fast reactor development, the direct numerical quadrature evaluation of these functions has become prohibitively expensive in terms of computer time.

In this report direct numerical quadrature is compared with the techniques of Gaussian quadrature, contour integrations, and cubic spline interpolation in terms of both accuracy and ease of computation. A form of contour integration due to A. M. Turing (1943) is found to be much faster than (approximately six times) and as accurate as direct numerical quadrature.

Execution times for the evaluation of these functions on the IBM 7094-II computer and FORTRAN IV listings are included.

INTRODUCTION

It was noted early in the study of neutron physics that the neutron cross section, or interaction probability, of materials is dependent on the temperature of the material. Thus, a rapid variation of cross section with respect to neutron energy could be inferred (refs. 1 and 2). It was then pointed out by Breit and Wigner (ref. 3) that the nuclear cross sections for the formation of the compound nucleus, or target nucleus plus neutron, should exhibit a resonance structure. For the reaction, neutron in and gamma out, the cross section $\sigma_{n\gamma}$ should vary as a function of neutron energy E as shown in the following equation (ref. 4):

$$\sigma_{n\gamma}(E) = \frac{\pi}{k^2} g_J \frac{\Gamma_n \Gamma_\gamma}{(E - E_o)^2 + \left(\frac{\Gamma}{2}\right)^2} \tag{1}$$

where k is the wave number of the neutron in the center of the mass system, g_J is the spin factor $(2J + 1)/2(2I + 1)$, J is the spin quantum number of the compound system and I that of the nucleus, Γ_n is the scattering width, Γ_γ is the radiative width, E_o is the energy of resonance, and Γ is the total width. Equation (1) is correct for stationary nuclei. However, since the nuclei of all materials are in thermal agitation, equation (1) must be modified to account for the effect of thermal motion. Briefly, the nuclei are assumed to have a Maxwellian velocity distribution and the cross section is folded into this velocity distribution. The resulting cross section is then a function of temperature as well as neutron energy; this cross section is the Doppler broadened cross section. Two functions arise from the derivation of the Doppler broadening of the cross section; they are $\psi(x, \theta)$ and $\chi(x, \theta)$. The derivation of the function $\psi(x, \theta)$ is shown in detail in appendix A. The respective definitions are as follows:

$$\psi(x, \theta) \equiv \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp\left[-\frac{1}{4}\theta^2(x - y)^2\right]}{1 + y^2} dy \tag{2}$$

$$\chi(x, \theta) \equiv \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp\left[-\frac{1}{4}\theta^2(x - y)^2\right]}{1 + y^2} 2y\, dy \tag{3}$$

Here $x = (2/\Gamma)(E - E_o)$, $\theta = \Gamma(4mTE_o/M)^{-1/2}$, m is the neutron mass, M is the nuclear mass, and T is the effective temperature in eV's.

Plots of $\psi(x, \theta)$ and $\chi(x, \theta)$ are shown for selected values of θ and a range of x from 0 to 10 in figures 1 and 2. Detailed plots of the regions of interest are shown in figures 3 and 4.

In the past various forms of "brute force" direct numerical quadrature have been used to evaluate ψ and χ (ref. 5). However, with the present use of many resonances and ever increasing resonance energies for reactor physics calculations in support of fast reactor development direct numerical quadrature has become prohibitively expensive in terms of computer time. The following report evaluates various techniques which might avoid the excessively long computer runs needed to calculate the Doppler

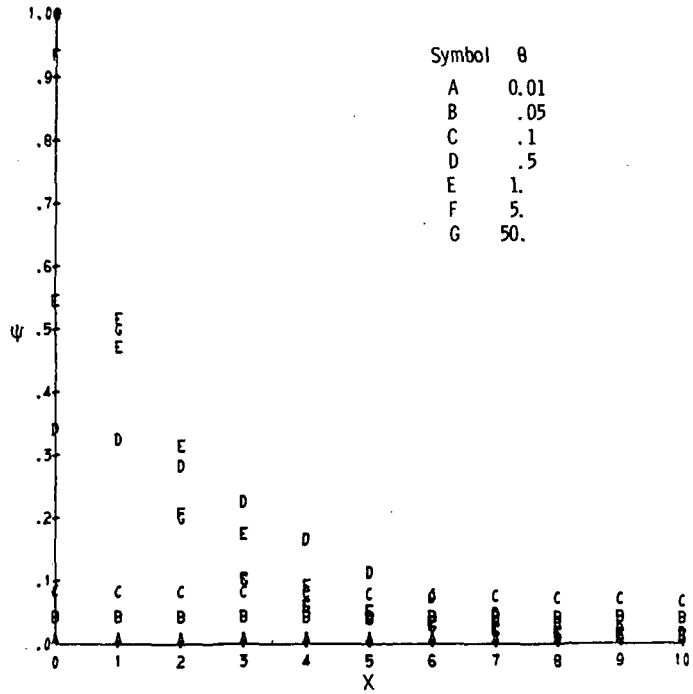

Figure 1. - Values of ψ for selected values of θ.

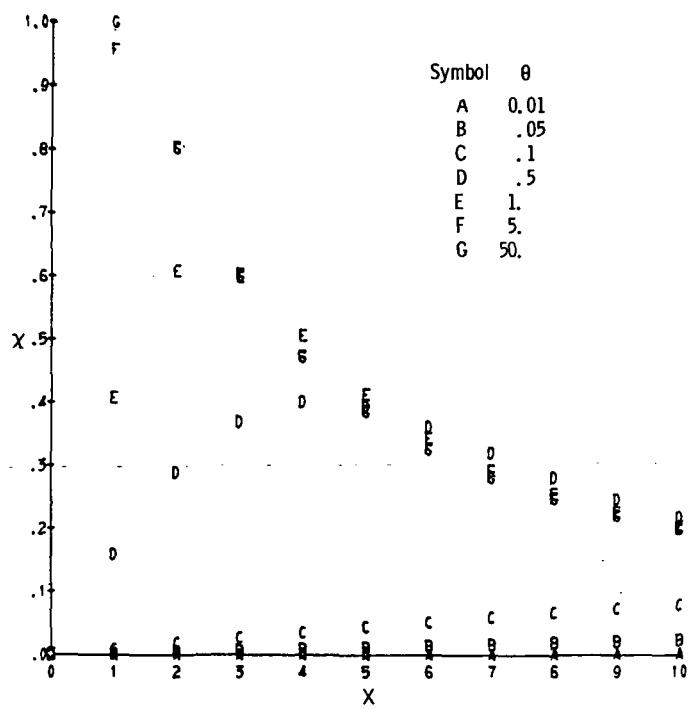

Figure 2. - Values of χ for selected values of θ.

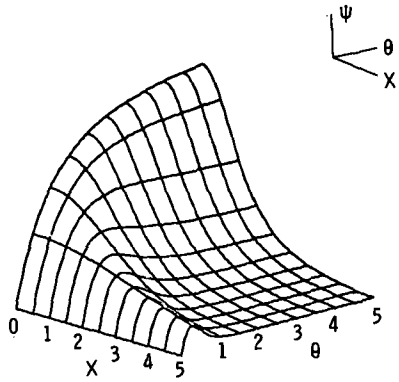

Figure 3. - Portion of (ψ, X, θ) surface.

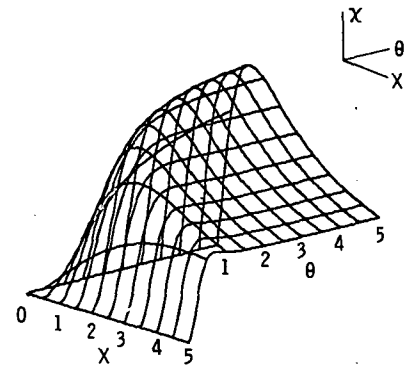

Figure 4. - Portion of (χ, X, θ) surface.

broadened cross sections by direct numerical quadrature. Such an evaluation is valuable because of present widespread interest in such fast reactors, and because "lengthy and involved routines giving wrong values for the (Doppler broadening) functions are prevalent" (ref. 6).

It should be noted that, although these integrals have been extensively studied (refs. 6 to 12), there is virtually no standard notation for either the Doppler broadening functions or the independent variables. We follow the notation of Dresner (ref. 4). Here θ is proportional to $T^{-1/2}$ and x is proportional to the energy distance from the resonance peak. Typical transformations for comparing our notation to others include

Dresner		Bhat and Lee-Whiting		Matta and Reichel	
$\psi(x, \theta)$	$=$	$\frac{\theta\sqrt{\Pi}}{2}\, u\left(\frac{x\theta}{2}, \frac{\theta}{2}\right)$	$=$	$U_o\left(x, \frac{1}{\theta^2}\right)$	(4)
$\chi(x, \theta)$	$=$	$\theta\sqrt{\Pi}\, v\left(\frac{x\theta}{2}, \frac{\theta}{2}\right)$	$=$	$2V_o\left(x, \frac{1}{\theta^2}\right)$	(5)

NUMERICAL TECHNIQUES

In order to evaluate temperature dependent continuous neutron cross sections, one must evaluate ψ and χ many times; therefore, both accuracy and as much speed in computation as possible are required. Special series methods, numerical quadrature, contour integration techniques, and interpolation have been considered for their evaluation; these studies indicate that a specialized quadrature and contour integration yield the accuracy required.

Asymptotic Series and Limiting Cases

Several special forms for ψ and χ are known which are simple to evaluate, but taken all together, do not cover much of the physically meaningful range of x and θ. For most work $|x| < 1000$, $0.001 < \theta < 100$. For this reason such special forms are used only as boundary check values for the other more general methods.

For example, for $x\theta >> 1$

$$\psi(x, \theta) = \frac{1}{1 + x^2}\left(1 + \frac{2}{\theta^2}\frac{3x^2 - 1}{(1 + x^2)2} + \ldots\right) \qquad \text{(ref. 4)}$$

Also,

$$\psi(x, \infty) = \frac{1}{1 + x^2} \qquad \chi(x, \infty) = \frac{2x}{1 + x^2} \qquad \text{(ref. 4)}$$

$$\psi(0, \theta) = \frac{1}{2}\sqrt{\pi\theta}\,\exp\left(\frac{\theta^2}{4}\right)\operatorname{erfc}\left(\frac{\theta}{2}\right) \qquad \chi(0, \theta) = 0 \qquad \text{(ref. 4)}$$

Direct Numerical Quadrature

For large-scale problems, several hundred resonances and several thousand energy points, the standard quadrature techniques in use at Lewis Research Center are too slow by at least two orders of magnitude. Because of the form of the integrand, programs using a Gaussian quadrature and also a Simpson's rule quadrature containing step modification logic were tried. This adaptive Simpson's rule quadrature, called method A, is coded in FORTRAN in appendix B as function SIMPS1. Both programs produced large errors for some values of x and θ; the critical parameter is the product $x\theta$. Both the shape of the integrands and the choice of limits of integration depend on this product. Let us transform the integrands and examine their behavior. Let

$$t = \frac{\theta}{2}(y - x) \tag{6}$$

Then

$$\psi(x,\theta) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-t^2}\,dt}{1 + \left(\frac{2t}{\theta} + x\right)^2} \tag{7}$$

$$\chi(x,\theta) = \frac{2}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-t^2}\left(\frac{2t}{\theta} + x\right)dt}{1 + \left(\frac{2t}{\theta} + x\right)^2} \tag{8}$$

The damping factor e^{-t^2} in these integrands is now independent of x and θ both (with a maximum at $t = 0$) and the remaining terms are

$$f \equiv \frac{1}{1 + \left(\frac{2t}{\theta} + x\right)^2} \tag{9}$$

$$g \equiv \frac{\left(\frac{2t}{\theta} + x\right)}{1 + \left(\frac{2t}{\theta} + x\right)^2} \tag{10}$$

These terms are sketched in figures 5 and 6. Note that both f and g have critical points which depend on $-x\theta/2$.

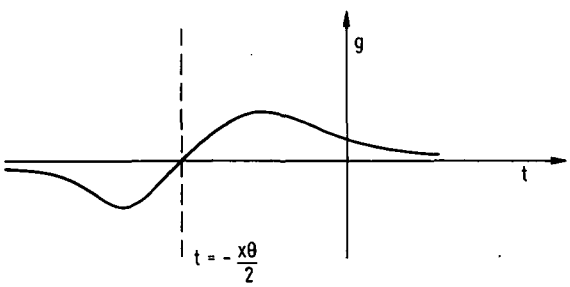

Figure 6. - Integrand g.

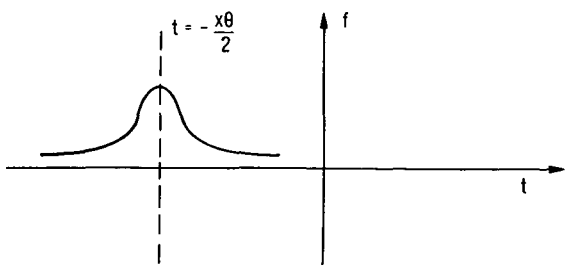

Figure 5. - Integrand f.

The integrals for ψ and χ are now in convenient form for application of Gauss-Hermite quadrature (ref. 13). That is,

$$\psi = \int_{-\infty}^{\infty} e^{-t^2} f(t)\, dt \doteq \sum_{i=1}^{N} A_i f(t_i) \tag{11}$$

$$\chi = \int_{-\infty}^{\infty} e^{-t^2} g(t)\, dt \doteq \sum_{i=1}^{N} A_i g(t_i) \tag{12}$$

where the t_i and A_i are tabulated for many N; for example, we chose $N = 16$ and $N = 32$.

However, it can be seen from figures 5 and 6 that, for Gauss-Hermite quadrature, no matter what t_i are picked, there will be both x and θ such that much of the area under f and g is far from any of the t_i. For example, for $N = 16$, the maximum $t_i = \pm 4.689$ - meaning f and g are sampled only in this range; typical values of $x = 20$, $\theta = 2$ place the critical points at $t = -20$. This inability to sample from significant values of f(t) and g(t) explains why Gauss-Hermite quadrature fails to give accurate results.

On examining figure 6 from the point of view of using a Simpson's rule quadrature, it can be seen that, for some values of x and θ, the χ integrand has a positive portion and a negative portion. To achieve and maintain accuracy, χ must be broken into positive and negative portions and evaluated separately. With these modifications, the adaptive Simpson's rule was successfully applied to ψ and χ; this shall be referred to as method A. One should note that the two parts $-\infty < t < -x\theta/2$ and $-x\theta/2 < t < +\infty$ of χ sometimes agree in magnitude to 12 significant figures. For comparison, another quadrature method in use at this center called method D was also studied.

Contour Integration

Integrals of the form $\int_{-\infty}^{\infty} f(t)\, e^{-t^2}\, dt$, as we see in equations (7) and (8) can sometimes be evaluated by contour integration in the complex plane (ref. 14). A. M. Turing first suggested this method for evaluating ψ and χ in 1943 (ref. 15). The Turing method is attractive because it should require much less arithmetic than numerical quadrature. This method has been formulated independently by Bhat and Lee-

Whiting, and by Matta and Reichel. We have applied the method of Bhat and Lee-Whiting (ref. 6), called method B and the similar method of Matta and Reichel (ref. 12), which we call method C. These methods are very useful for many related integrals as well (ref. 12). Methods B and C use series with a parameter h (and corresponding error estimate E(h)) which can be varied to achieve desired accuracy. In addition to the series contribution, both methods have a contribution from the poles (places where the denominator of the integrands is zero) which depends on whether θ is inside, on, or outside the contour chosen for integration. The formulas are the following: For method B let $a \equiv x\theta/2$, $b \equiv \theta/2$, and recall transformations (4) and (5). Then

$$\psi(a, b) = \frac{hb}{\sqrt{\pi}}\left[\sum_{-\infty}^{\infty} \frac{e^{-n^2h^2}}{(a - nh)^2 + b^2}\right] + 2P(h)e^{(b^2-a^2)} \frac{\cos(2ab) - e^{2\pi b/h}\cos\left(\frac{2\pi a}{h} - 2ab\right)}{D}$$

$$+ \text{ real part of } E(h) \qquad (13)$$

$$\chi(a, b) = \frac{2h}{\sqrt{\pi}}\left[\sum_{-\infty}^{\infty} \frac{e^{-n^2h^2}(a - nh)}{(a - nh)^2 + b^2}\right] - 4P(h)e^{(b^2-a^2)} \frac{\sin(2ab) + e^{2\pi b/h}\sin\left(\frac{2\pi a}{h} - 2ab\right)}{D}$$

$$+ \text{ imaginary part of } E(h) \qquad (14)$$

where

$$D = 1 - 2e^{2\pi b/h}\cos\frac{2\pi a}{h} + e^{4\pi b/h}$$

and

$$\left.\begin{array}{lll} P = 0 & \text{for} & 2\pi/h < \theta \\ P = 1/2 & \text{for} & 2\pi/h = \theta \\ P = 1 & \text{for} & 2\pi/h > \theta \end{array}\right\} \quad \text{(ref. 6)}$$

Finally,

$$|E(h)| \sim \frac{\sqrt{a^2 + b^2}\, e^{-\pi 2/h}}{\left|\frac{\pi^2}{h^2} - b^2\right|} \tag{15}$$

This method is coded in FORTRAN in appendix C, as subroutine PSCH.

Similarly, for method C, let $t \equiv 1/\theta^2$. Then

$$\psi(x, t) = \frac{h}{\sqrt{\pi}\,(1 + x^2)} + \frac{2h}{\sqrt{\pi}} \sum_{n=1}^{\infty} \frac{e^{-n^2h^2}(1 + x^2 + 4tn^2h^2)}{\left(1 - x^2 + 4tn^2h^2\right)^2 + 4x^2} + PP_1 - \frac{E(h)}{t} \tag{16}$$

$$\chi(x, t) = \frac{2hx}{\sqrt{\pi}(1 + x^2)} + \frac{4hx}{\sqrt{\pi}} \sum_{n=1}^{\infty} \frac{e^{-n^2h^2}(1 + x^2 - 4tn^2h^2)}{\left(1 - x^2 + 4tn^2h^2\right)^2 + 4x^2} - 2\left[PQ_1 + \frac{x}{t} E(h)\right] \tag{17}$$

where

$$P = 0 \quad \text{for} \quad 2\pi/h < \theta \quad \text{or} \quad t < h^2/4\pi^2$$

$$P = 1/2 \quad \text{for} \quad 2\pi/h = \theta \quad \text{or} \quad t = h^2/4\pi^2$$

$$P = 1 \quad \text{for} \quad 2\pi/h > \theta \quad \text{or} \quad t > h^2/4\pi^2$$

Also,

$$P_1 = \alpha\left(\frac{AC - BD}{C^2 + D^2}\right), \quad Q_1 = \alpha\left(\frac{BC + AD}{C^2 + D^2}\right)$$

and

$$\alpha = \sqrt{\frac{\pi}{t}}\, e^{-(x^2/4t + \pi/h\sqrt{t} - 1/4t)}$$

$$A = \cos \frac{x}{2t}$$

$$B = \sin \frac{x}{2t}$$

$$C = e^{-\pi/h\sqrt{t}} - \cos \frac{\pi x}{h\sqrt{t}}$$

$$D = \sin \frac{\pi x}{h\sqrt{t}}$$

Finally,

$$\left|E(h)\right| \leq \frac{e^{-\pi^2/h^2}}{2\left(1 - e^{-\pi^2/h^2}\right)} \tag{18}$$

This method is coded in FORTRAN in appendix C, as subroutine PSIPHI.

Using these estimates for the error, and knowing the accuracy desired, one can choose the largest possible h which will achieve this accuracy. For method B, h = 1.0 was used; for method C, h = 0.75. The series of each method was truncated at nine terms. The same number of terms is used in order to make comparisons of execution times.

Interpolation

Using methods A, B, and C tables were built of ψ and χ for various x and θ in hopes that interpolation would be possible. These tables were fit with cubic splines (refs. 16 and 17). Briefly, cubic splines are cubic polynomials passed piecewise through each pair of adjacent data points. The coefficients of these cubics are chosen so as to match first and second derivatives at the data points; this is usually called the spline property. These points were used to generate contour plots as shown in figures 7 and 8. This method of interpolation has not yet achieved the accuracy of methods A, B, or C. Interpolation remains attractive and is a subject for future work.

Contour label	Contour value
A	0.050
B	.100
C	.200
D	.300
E	.400
F	.500
G	.600
H	.800

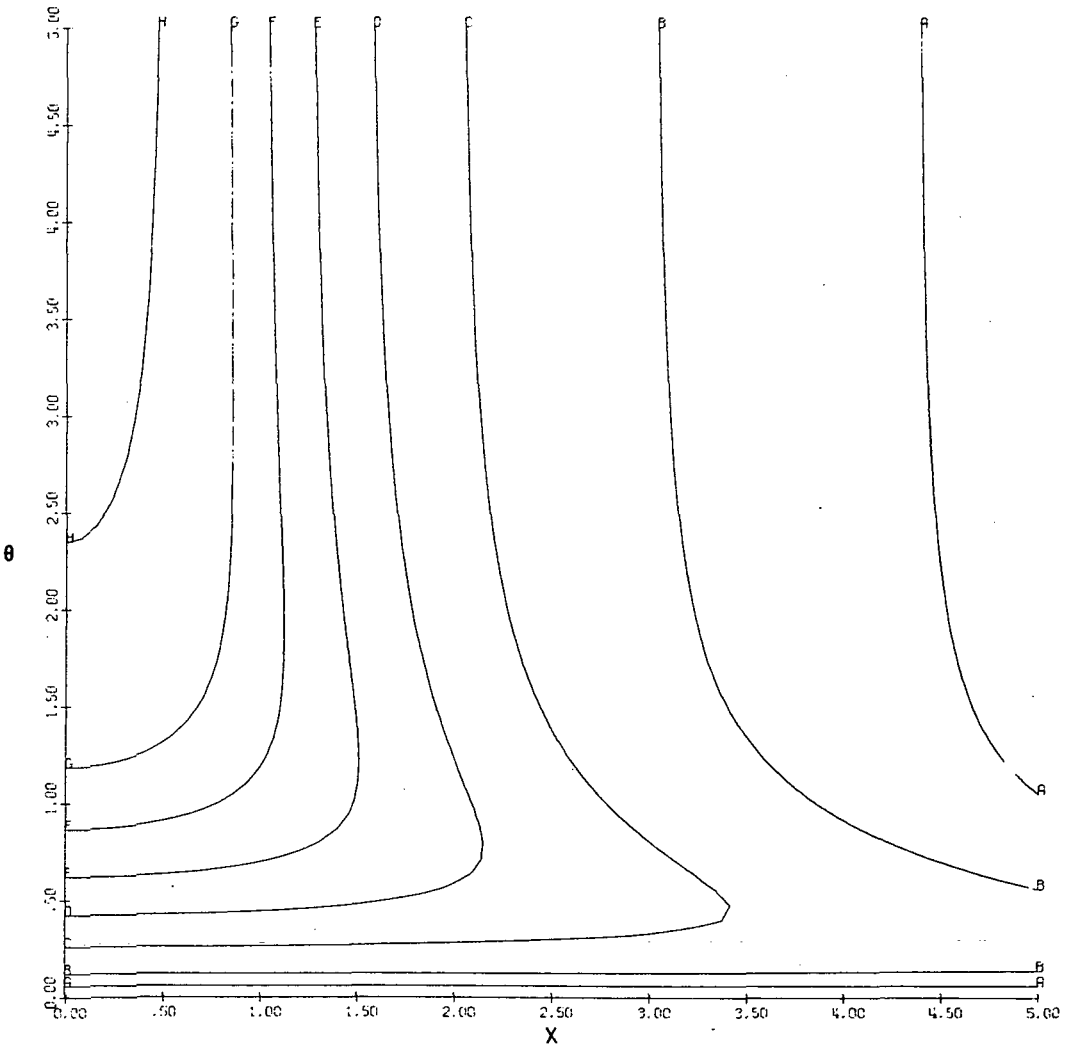

Figure 7. - Contour plot of ψ.

Contour label	Contour value
A	0.050
B	.100
C	.200
D	.300
E	.400
F	.500
G	.600
H	.800

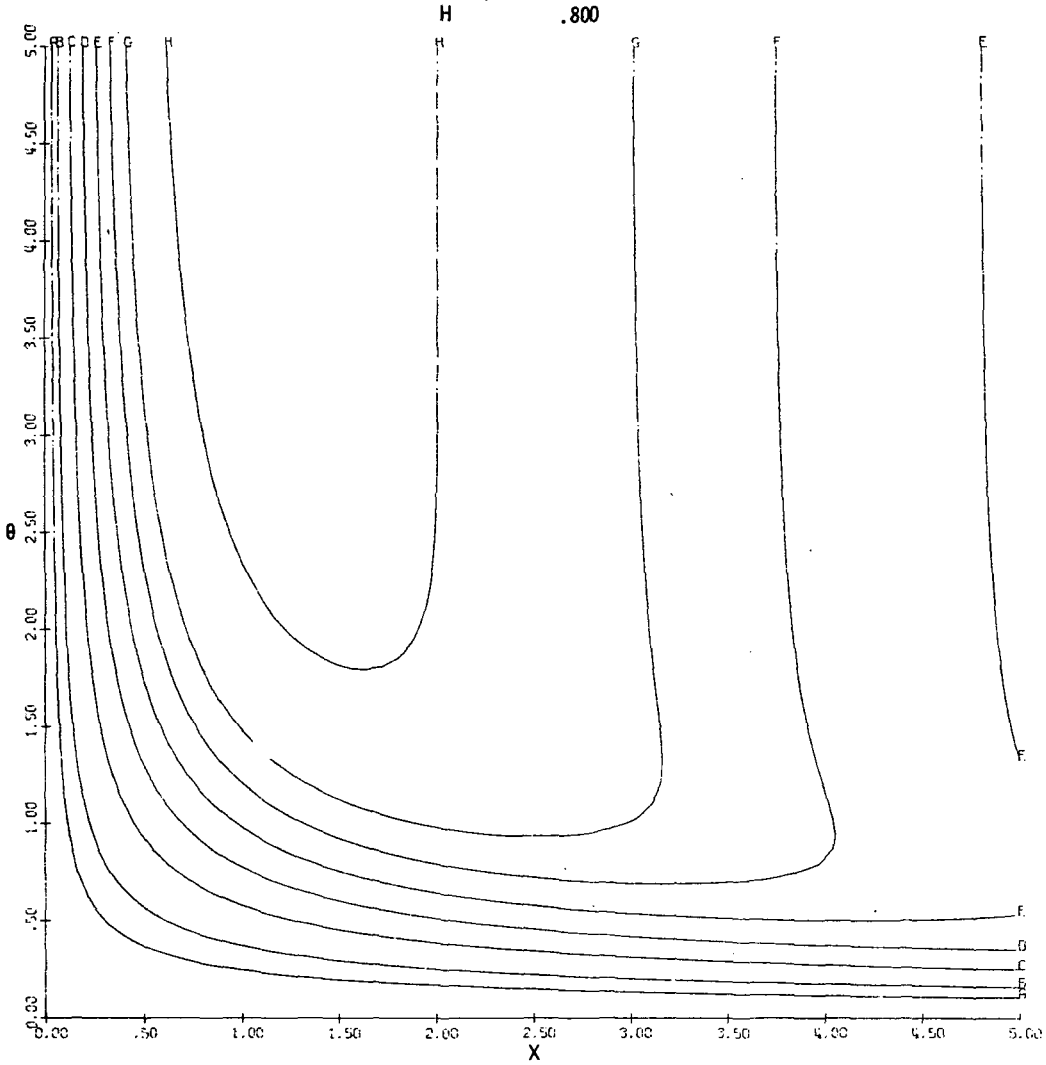

Figure 8. - Contour plot of χ.

RESULTS

Accuracy Comparisons

The Gaussian quadrature techniques as used herein do not give satisfactory relative accuracy in computing ψ and χ. This is true whether or not the weighting function e^{-t^2} is removed from the integrand. For most values of x and θ this method is satisfactory, but wrong results occur in an unpredictable fashion. Since the error estimate associated with Gaussian quadrature assumes the use of functionals not readily obtainable, it has not been used. The results are in error because this quadrature uses fixed abscissas, while, as discussed in the section Direct Numerical Quadrature, the peaks of the integrands for ψ and χ vary as the product $x\theta$.

The adaptive Simpson's rule method (method A), with numerical results given in table I, yields satisfactory accuracy for our work, four significant figures. This method was the first one found to be sufficiently accurate; it was used as a check against published values and against other methods discussed in this report.

The contour integration methods, methods B and C, have accuracies controllable by choice of a parameter h. See tables II and III. They both have corresponding error estimates $E(h)$. For a given fixed h, methods B and C give much the same results, and speed becomes the deciding factor. However, there is one region where method B

TABLE I. - TYPICAL VALUES OBTAINED BY METHOD A

(a) Values of ψ

x	θ			
	0.01	0.5	1	2
0.001	0.00881246	0.341353	0.545648	0.757895
.1	.00881246	.341191	.544852	.755166
1	.00881224	.325577	.472498	.540149
4	.00880896	.164687	.0915975	.0643058

(b) Values of χ

x	θ			
	0.01	0.5	1	2
0.001	0.991191×10^{-7}	0.164663×10^{-3}	0.454362×10^{-3}	0.968510×10^{-3}
.1	$.991191\times10^{-5}$	.0164612	.0453743	.0965705
1	$.991175\times10^{-4}$	.159261	.408498	.738117
4	$.396371\times10^{-3}$	.400753	.504762	.481550

TABLE II. - TYPICAL VALUES OBTAINED BY METHOD B

(a) Values of ψ

x	θ			
	0.01	0.5	1	2
0.001	0.00881269	0.341350	0.545639	0.757862
.1	.00881239	.341189	.544844	.755133
1	.00881233	.325574	.472496	.540137
4	.00880900	.164686	.0915985	.0643081

(b) Values of χ

x	θ			
	0.001	0.5	1	2
0.001	0.995718×10^{-7}	0.164663×10^{-3}	0.454363×10^{-3}	0.968537×10^{-3}
.1	$.988693\times10^{-5}$	.0164608	.0453872	.0965732
1	$.992042\times10^{-4}$	.159267	.408535	.738138
4	$.396523\times10^{-3}$	.400761	.504784	.481569

TABLE III. - TYPICAL VALUES OBTAINED BY METHOD C

(a) Values of ψ

x	θ			
	0.01	0.5	1	2
0.001	0.00881246	0.341351	0.545641	0.757872
.1	.00881249	.341189	.544846	.755143
1	.00881225	.325575	.472498	.540145
4	.00880898	.164687	.0915994	.0643072

(b) Values of χ

x	θ			
	0.01	0.5	1	2
0.001	0.990694×10^{-7}	0.164662×10^{-3}	0.454359×10^{-3}	0.968511×10^{-3}
.1	$.991765\times10^{-5}$	.0164607	.0453867	.0965709
1	$.990592\times10^{-4}$	.159265	.408530	.738117
4	$.396352\times10^{-3}$	.400756	.504770	.481536

TABLE IV. - TYPICAL VALUES OBTAINED BY METHOD D

(a) Values of ψ

x	θ			
	0.01	0.5	1	2
0.001	0.00881212	0.341334	0.545639	0.757872
.1	.00881228	.341179	.544870	.755142
1	.00881233	.325574	.472496	.540137
4	.00880896	.164684	.0916000	.0643058

(b) Values of χ

x	θ			
	0.01	0.5	1	2
0.001	0.951862×10^{-7}	0.164369×10^{-3}	0.455154×10^{-3}	0.968535×10^{-3}
.1	$.941018\times10^{-5}$	.0164325	.0454529	.0965704
1	$.994859\times10^{-4}$	.159274	.408537	.738117
4	$.395791\times10^{-3}$	.400745	.504769	.481550

loses all accuracy, while method C remains stable. For $\theta \sim 0.001$ (high energies >1 eV) method B failed, even with $h = 0.5$ and 20 terms in the series. In this region method C, with $h = 0.75$ and nine terms as before, gives four significant figures for ψ and one for χ. We conclude that, for small θ, method B should be used with caution.

Some sample results obtained by methods A, B, C, and D are given in tables I to IV.

Speed Comparisons

Because the numerical quadrature of method A requires far more arithmetic operations than methods B and C, method A has been modified to split the argument ranges into two regions and to use an asymptotic expansion when possible. Values for x were chosen uniformly in the range $0 < x < 1000$. (Note that $\psi(-x) = \psi(x)$ and $\chi(-x) = -\chi(x)$.) Two sets of θ ranges were used: in the range $0 < \theta < 1$, the pole contributions are always present; while in the range $0 \lesssim \theta < 100$, these contributions are usually zero. Execution times on an IBM 7094 for 2000 evaluations are given in table V. An example of a Doppler broadening resonance cross section code which may be used with the subroutines herein is shown in appendix D.

TABLE V. - COMPARISON OF EXECUTION TIMES

θ range	Method				
	A (integrals only)	A (integrals + series)	B	C	D
	Time, sec				
$0 < \theta < 100$	[a]5.30	2.17	0.77	1.87	2.16
$0 < \theta < 1$	----	11.5	2.05	2.20	----

[a]Run for comparison only--it was known that this method would not be fast enough to be practicable.

Discussion of Execution Times

Several conclusions can be drawn from table I. First, even the slow numerical quadrature method is accurate, and as mentioned earlier "lengthy and involved routines giving wrong values for the ψ and χ functions are prevalent" (ref. 6). Study of these integrals began because an existing routine was very slow, about six times slower than our quadrature. Note that adding a test and an asymptotic expansion to method A increases the speed nearly $2\frac{1}{2}$ times. Most important for this study, method B is nearly $2\frac{1}{2}$ times faster than method C for the distribution $0 < \theta < 100$. This is because terms in the series of method B can be written more compactly than those of method C; and only for small θ is the pole contribution needed; that is, the series is the only calculation required. Fourth, for $0 < \theta < 1$ most of this speed advantage is gone. Now the pole calculations are always needed. Method B, coded as subroutine PSCH listed in appendix C, is still to be preferred, for methods B and C are about equally accurate.

CONCLUDING REMARKS

Direct numerical quadrature using an adaptive Simpson's rule technique yields results accurate to four significant figures for both $\psi(x, \theta)$ and $\chi(x, \theta)$. However, this method is quite slow and expensive in terms of computer time.

The method of Gaussian quadrature used herein was evaluated and found to be erratic in terms of error and somewhat slower than the techniques of contour integration. Error estimation for the Gaussian quadrature proved to be incapable of rapid calculation.

Both contour integration methods, method B using subroutine PSCH, and method C using subroutine PSIPHI gave very rapid and accurate results. The accuracy is comparable with that of direct numerical quadrature.

The method of cubic spline interpolation failed to achieve the accuracy of the other methods evaluated.

Of the numerical methods considered and evaluated contour integration, subroutines PSCH and PSIPHI, achieved the greatest speed of computation combined with quite satisfactory accuracy.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, April 10, 1972,
132-80.

APPENDIX A

DERIVATION OF $\psi(x, \theta)$ - THE DOPPLER BROADENING FUNCTION

If a beam of neutrons with velocity $\vec{v}$ impinges upon a group of nuclei at rest, the reaction rate for process x is proportional to $v\sigma_x(v)$, where $\sigma_x(v)$ is the nuclear cross section for process x as a function of velocity. However, the nuclei are not stationary but are in thermal motion. We may assume the nuclei have a Maxwellian velocity distribution characterized by a temperature T; then the three-dimensional Maxwell velocity distribution may be written as

$$P(\vec{V})\, d\vec{V} = \left(\frac{M}{2\pi kT}\right)^{3/2} e^{-MV^2/2kT}\, dV_x\, dV_y\, dV_z$$

where T is the effective temperature, M is the nuclear mass, and $\vec{V}$ is the nuclear velocity.

The value of the velocity of the neutron, of mass m, relative to the nucleus is then the magnitude of the difference of the velocity vectors. That is,

$$v_r = |\vec{V} - \vec{v}|$$

The corresponding energy is then $E_r = \frac{1}{2} m v_r^2$. Since $P(\vec{v})\, d\vec{v}$ is the probability of a nucleus having a velocity within $d\vec{v}$ about $\vec{v}$, the probable number of reactions to type x per second is

$$v_r \sigma_x(E_r) P(\vec{v})\, d\vec{v}$$

The total probability is then

$$\sigma_x(E) = \frac{1}{v} \int v_r \sigma_x(E_r) P(\vec{V})\, d\vec{V}$$

If a coordinate system is chosen such that the z-direction is parallel to the neutron velocity, then

$$E_r = \frac{1}{2} m(\vec{v} - \vec{V})^2 = \frac{1}{2} m\left[(v - V_z)^2 + V_x^2 + V_y^2\right]$$

Since the neutron velocity is quite high compared to the thermal motion of the nuclei, the V_z^2, V_x^2, and V_y^2 terms may be neglected. Hence,

$$E_r = \frac{1}{2} m(v^2 - 2vV_z)$$

Thus

$$v_r = \sqrt{\frac{2E_r}{m}}$$

Integrating out the V_x and V_y velocity components from the Maxwellian results on the following distribution for the z-component:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} P(\vec{V})\, dV_x\, dV_y = \left(\frac{M}{2\pi kT}\right)^{1/2} e^{-MV_z^2/2kT}$$

The Breit-Wigner expression for a single-level resonance cross section for absorption is

$$\sigma_\gamma(E) = \sigma_o \frac{\Gamma_\gamma}{\Gamma} \sqrt{\frac{E_o}{E}} \frac{\Gamma^2}{4(E - E_o)^2 + \Gamma^2}$$

where $\sigma_o = 4\pi \lambda\!\!\!^{-}{}_g^2 (\Gamma_n/\Gamma)$, $\lambda\!\!\!^{-}$ is neutron wave length over 2π, g is the statistical weighting factor, Γ_n is the scattering width, Γ is the total width, Γ_γ is the radiative width, and E_o is the resonance energy. Substituting into the previous equation gives

$$\sigma_\gamma(E) = \sigma_o \frac{\Gamma_\gamma}{\Gamma} \sqrt{\frac{E_o}{E}} \left(\frac{M}{2\pi kT}\right)^{1/2} \int_{-\infty}^{\infty} e^{-MV_z^2/2kT} \frac{\Gamma^2\, dV_z}{4(E_r - E_o)^2 + \Gamma^2}$$

If one defines

$$x \equiv \frac{2}{\Gamma} (E - E_o)$$

$$y \equiv \frac{2}{\Gamma}(E_r - E_o)$$

$$\Delta \equiv \sqrt{\frac{4mkTE}{M}} \doteq \sqrt{\frac{4kTE_o}{M}} \qquad m \doteq 1$$

(a very good approximation for large E_o) and

$$\theta \equiv \frac{\Gamma}{\Delta}$$

then

$$\sigma_\gamma(E) = \sigma_o \frac{\Gamma_\gamma}{\Gamma} \sqrt{\frac{E_o}{E}} \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp\left[-\frac{1}{4}\theta^2(y - x)^2\right] dy}{1 + y^2}$$

or

$$\sigma_\gamma(E) = \sigma_o \frac{\Gamma_\gamma}{\Gamma} \sqrt{\frac{E_o}{E}} \psi(x, \theta)$$

where

$$\psi(x, \theta) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp\left[-\frac{1}{4}\theta^2(y - x)^2\right] dy}{1 + y^2}$$

The function

$$\chi(x, \theta) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{2y \exp\left[-\frac{1}{4}\theta^2(y - x)^2\right] dy}{1 + y^2}$$

may be derived in the same manner using the same assumptions.

APPENDIX B

FORTRAN IV LISTING OF SIMPS1

This function SIMPS1 is a Simpson's rule integrating routine, which integrates the external function FUNC1 from XMIN to XMAX. When sufficient accuracy is not attained, the flag KER is incremented by 1.

```
      FUNCTION SIMPS1(XMIN,XMAX,FUNC1,KER)
      DIMENSION V(200),H(200),A(200),B(200),C(200),P(200),E(200)
      DATA T/3.0E-4/
      IF(XMIN.EQ.XMAX)  GO TO 18
      V(1)=XMIN
      H(1)=0.5*(XMAX-XMIN)
      A(1)=FUNC1(XMIN)
      B(1)=FUNC1(XMIN+H(1))
      C(1)=FUNC1(XMAX)
      P(1)=H(1)*(A(1)+4.0*B(1)+C(1))
      E(1)=P(1)
      ANS=P(1)
      N=1
      FRAC=2.0*T
    1 FRAC=0.5*FRAC
    2 TEST=ABS(FRAC*ANS)
      K=N
    3 DO 7 I=1,K
    4 IF(ABS(E(I)).LE.TEST)  GO TO 7
    5 N = N+1
      V(N)=V(I)+H(I)
      H(N)=0.5*H(I)
      A(N)=B(I)
      B(N)=FUNC1(V(N)+H(N))
      C(N)=C(I)
      P(N)=H(N)*(A(N)+4.0*B(N)+C(N))
      Q=P(I)
      H(I)=H(N)
      B(I)=FUNC1(V(I)+H(I))
      C(I)=A(N)
      P(I)=H(I)*(A(I)+4.0*B(I)+C(I))
      Q=P(I)+P(N)-Q
      ANS=ANS+Q
      E(I)=Q
      E(N)=Q
    6 IF(N-200) 7,13,13
    7 CONTINUE
    8 IF (N-K) 9,9,2
    9 Q = 0.0
   10 DO 11 I=1,N
   11 Q=Q+E(I)
   12 IF (ABS(Q)-T*ABS(ANS)) 14,14,1
13    KER=KER+1
   14 ANS=0.0
   15 DO 16 I=1,N
   16 ANS=ANS+P(I)
```

APPENDIX C

FORTRAN IV LISTINGS OF METHODS B AND C

Subroutine PSCH uses the technique of Bhat and Lee-Whiting (ref. 6). The arguments are XX and TT where

XX natural distance X

TT temperature parameter

The values U and V are returned where

U first Doppler broadening integral

V second Doppler broadening integral

```
$IBFTC PSCHBL

C         FROM BHAT AND LEE-WHITING, P.278
C         H=1.
      SUBROUTINE PSCH(XX,TT,U,V)
      DIMENSION EMN(5),EN2(10)
      DATA PI22/12.566371/
      DATA RTPI/1.7724539/ , PIH/1.5707963/
      DATA PI,PI2,N /3.1415927,6.2831854,5/
      DATA (EMN(I),I=2,5) /.11709966E0,.58300489E-2,.39282561E-4,
     1  .35821059E-7 /
      DATA (EN2(I),I=2,10) /.24789999,.11709966,.33549615E-1,.58300489E-
     *2,.61448264E-3,.39282561E-4,.15231502E-5,.35821059E-7,.51095996E-9
     */
C
      XD=ABS(XX)
      THETA=ABS(TT)
      Y=THETA/2.
      X=XD*Y
C         ARE WE IN DANGER
      XTEST=X-AINT(X)
      IF((XTEST.LT..01 .OR. XTEST.GT..99) .AND. ABS(Y).LT..01) GO TO 40
      IF(XD.GT.75.*SQRT(1.+1./(Y*Y))) GO TO 30
      IF(Y.LT..001) GO TO 40
C         BEGIN SERIES SUMATION
      Y2=Y*Y
C         SET N=0 TERM -- NOTE PI IS IN THIS ONE
      D=PI*(X*X+Y2)
      SU=Y/D
      SV=X/D
      DO 10 I=2,N
      AM=I-1
      XNP=X-AM
      XNM=X+AM
      DP=XNP*XNP+Y2
      DM=XNM*XNM+Y2
```

```
      SU = SU + EMN(I)*Y*(1./DP+1./DM)
      SV = SV + EMN(I)*(XNP/DP+XNM/DM)
   1C CONTINUE
      IF(Y.GT.PI) GO TO 20
      P=2.
      IF(Y.EQ.PI) P=1.
C        BEGIN POLE CONTRIBUTION
      XP2=X*PI2
      EYP2=EXP(Y*PI2)
   15 CONTINUE
      XY2=X*Y*2.
      SXY2=SIN(XY2)
      CXY2=COS(XY2)
      SXP2=SIN(XP2)
      CXP2=COS(XP2)
      EYX=EXP(Y2-X*X)
      D = 1. - EYP2*(2.*CXP2-EYP2)
      SU = SU + P*EYX*(CXY2-EYP2*(CXP2*CXY2+SXP2*SXY2))/D
      SV = SV - P*EYX*(SXY2+EYP2*(SXP2*CXY2-CXP2*SXY2))/D
   2C U=SU*Y*RTPI
      V=SV*THETA*RTPI
      IF(XX.LT.0.) V=-V
      GO TO 5C
   3C F=RTPI*Y
      SU=1./((1.+XD*XD)*F)
      SV=SU*XD
      GO TO 2C
   4C CONTINUE
      IF(XD.LT.4. .AND. THETA.LE..009) WRITE(6,1C1) XD,THETA
  1C1 FORMAT(4H BAD,2G14.6)
C        THIS IS EXPANSION WITH H=C.5
      Y2=Y*Y
      D=PI*(X*X+Y2)
      SU=Y/D
      SV=X/D
      DO 45 I=2,10
      AM=0.5*FLOAT(I-1)
      XNP=X-AM
      XNM=X+AM
      DP=XNP*XNP+Y2
      DM=XNM*XNM+Y2
      SU = SU + EN2(I)*Y*(1./DP+1./DM)
      SV = SV + EN2(I)*(XNP/DP+XNM/DM)
   45 CONTINUE
      SU=SU*0.5
      SV=SV*0.5
      IF(Y.GT.PIH) GO TO 20
      P=2.
      IF(Y.EQ.PIH) P=1.
      XP2=X*PI22
      EYP2=EXP(Y*PI22)
      GO TO 15
   5C RETURN
      END
```

Subroutine PSIPHI uses the technique of Matta and Reichel (ref. 12). The arguments and values are the same as for routine PSCH.

```
$IBFTC MATTA
C
C         FROM MATTA+REICHEL  MATH. COMP. P.340 APRIL 1971
C         H=1. , 11 TERMS (FOR COMPARISON)
C
      SUBROUTINE PSIPHI(XX,TT,U,V)
      DATA H/0.75/
      DATA PI/3.14159265/ , RTPI/1.7724539/
      DIMENSION ENH(9),FNH(9)
      DATA FNH/2.25,9.,20.25,36.,56.25,81.,110.25,144.,182.25/
      DATA ENH / .56978283,.10539922,.63297154E-2,.12340981E-3,
     * .78114894E-6,.16052281E-8,.10709232E-11,.23195228E-15,
     * .16310139E-19 /
      DATA BOUND/.14248292E-1/
      X=ABS(XX)
      TH=ABS(TT)
      T=1.0/TH**2
      X2=X*X
C
C         START SERIES -- SET N=0 TERM
C
      XP=1.0+X2
      XN=1.0-X2
      SU=0.5/XP
      SV=SU
      X24=4.0*X2
C
      DO 10 N=1,9
      FNHT=FNH(N)*T
      DENOM=X24+(XN+FNHT)**2
      TERM=ENH(N)/DENOM
      SU = SU + TERM*(XP+FNHT)
      SV = SV + TERM*(XP-FNHT)
   10 CONTINUE
C
      SU=SU*2.0*H/RTPI
      SV=SV*2.0*H/RTPI*X
C
C         START POLE TESTS
C
      IF(T.LT.BOUND) GOTO 30
      RTT=SQRT(T)
      EXPON=XN*0.25/T - PI/H/RTT
      IF(EXPON.LT. (-34.)) GO TO 30
      ARG1=X*0.5/T
      ARG2=PI*X/(H*RTT)
      A=COS(ARG1)
      B=SIN(ARG1)
      C=EXP(-PI/(H*RTT)) - COS(ARG2)
      D=SIN(ARG2)
      TERM=RTPI/RTT*EXP(EXPON)/(C*C+D*D)
```

```
      P1=TERM*(A*C-B*D)
      Q1=TERM*(B*C+A*D)
      IF(T.NE.ECUND) GOTO 20
      P1=P1*0.5
      Q1=Q1*0.5
   20 CONTINUE
      SU=SU+P1
      SV=SV-Q1
   30 CONTINUE
      U=SU
      V=SV*2.0
      RETURN
      END
```

APPENDIX D

A SAMPLE DOPPLER BROADENING CROSS SECTION CODE WHICH REQUIRES VALUES OF ψ AND χ

```
$IBFTC RP3TAP
C
      LOGICAL START
      DIMENSION DATUM(12003)
      DIMENSION DATUMS(4001,3)
      EQUIVALENCE (DATUM(1),DATUMS(1,1))
      DIMENSION TITLE(24), UG(150), DU(150)
      DIMENSION GG(20)
      DIMENSION EO(300),GAMN(300),GAMG(300),GAM(300),GAME(300)
      DIMENSION SIGCO(300),SIGFO(300),SIGSO(300),SIGTO(300),CON3(300)
      DIMENSION A(300),SIG1(300),SIG2(300),SIG3(300)
      DIMENSION   X (300) , THETA(300) , PSI(300) , PHI(300)
C
C
      COMMON NRES,X,THETA,PSI,PHI
C
C
C
C
      START=.TRUE.
      NUNIT=1
      REWIND NUNIT
      CALL SKFILE(NUNIT)
      BACKSPACE NUNIT
    1 CONTINUE
      IF(START) GO TO 111
C        FIND END OF THIS TAPE
C        PUT ON ID RECORD
      WRITE(NUNIT) ID
C        WRITE GOOD STUFF
      JWORDS=3*NWORDS
      WRITE(NUNIT)DATUM
   75 FORMAT(A6,4X,I10)
   76 FORMAT(1H1,A6)
   77 FORMAT(10X,3F13.4)
  111 CONTINUE
      START=.FALSE.
      READ (5,50) (TITLE(M),M=1,24)
      READ(5,75) ID,NWORDS
      READ (5,51) T,ANU,UKT,SIGOT,SIGFT,USTART,NRES,NDU
      READ (5,53) SIGMAT,SIGPOT,G
      READ (5,52) (UG(K),DU(K),K=1,NDU)
      READ (5,67) (A(I),EO(I),GAMN(I),GAMG(I),GAME(I),I=1,NRES)
      READ (5,71) NUMBG
      READ (5,53) (GG(I),I=1,NUMBG)
      READ(5,72) I2,I4,I6,I8
      WRITE (6,54)
      WRITE (6,50) (TITLE(M),M=1,24)
```

```
      WRITE (6,55)
      WRITE (6,56) T,ANU,UKT,SIGCT,SIGFT,SIGMAT,SIGPOT
      DO 2 K=1,NDU,52
      IHI=MINO(NDU,K+51)
C        NEW PAGE
      WRITE (6,54)
      WRITE (6,57)
      WRITE (6,58) (J,UG(J),DU(J),J=K,IHI)
2     CONTINUE
      DO 3 I=1,NRES
      GAM(I)=GAMN(I)+GAMG(I)+GAME(I)
      CON1=(2.607E06/(GAM(I)**2))*G*GAMN(I)
      CON2   =(A(I)+1.0)/A(I)
      CON3(I)=1.0/CON2
      AEO   =ABS(EO(I))
      SIGCO(I)=(CON1*GAMG(I)*CON2   **1.5)/SQRT(AEO   )
      SIGFO(I)=(GAME(I)*SIGCO(I))/GAMG(I)
      SIGSO(I)=(CON1*GAMN(I)*CON2   **2)/AEO
      SIGTO(I)=2.607E06*G*GAMN(I)/(AEO   *GAM(I))
3     CONTINUE
      DO 4 I=1,NRES,52
      IHI=MINO(NRES,I+51)
C        NEW PAGE
      WRITE (6,54)
      WRITE (6,59)
      WRITE (6,60) (J,A(J),EO(J),GAMN(J),GAMG(J),GAME(J),J=I,IHI)
4     CONTINUE
      DO 5 I=1,NRES,52
      IHI=MINO(NRES,I+51)
C        NEW PAGE
      WRITE (6,54)
      WRITE (6,61)
      WRITE (6,62) (J,EO(J),SIGCO(J),SIGFO(J),SIGSO(J),SIGTO(J),J=I,IHI)
5     CONTINUE
      WRITE (6,55)
C
      NCOUNT=0
      NTALLY=1
      KKK=0
      JJJ=0
C
      ET=EXP(-UKT)*1.0E07
6     DO 13 I=1,NRES
      IF (KKK) 7,7,10
7     X(I)=(2.0*(ET-EO(I))*CON3(I))/GAM(I)
      IF (T) 8,8,9
8     TDOP=0.0
      GO TO 11
9     TDOP=293.0
      GO TO 11
10    TDOP=T
   11 THETA(I) = GAM(I)/CON3(I)*SQRT(A(I)/(TDOP*ABS(EO(I))*3.446E-04))
13    CONTINUE
14    CALL PSIPHI
      IF (KKK) 25,15,25
15    SIGCTP=0.0
      SIGFTP=0.0
      ZEC1=SQRT(ET)
      DO 16 I=1,NRES
```

```
      SIGCTP=SIGCTP+SIGCO(I)*PSI(I)
      SIGFTP=SIGFTP+SIGFO(I)*PSI(I)
16    CONTINUE
      SCV=SIGCT-SIGCTP/ZED1
      SFV=SIGFT-SIGFTP/ZED1
      AKC=SCV*ZED1
      AKF=SFV*ZED1
      WRITE (6,64) SCV,SFV
      ABN=0.0
      DO 17 I=1,NRES
      ABN=ABN+A(I)
17    CONTINUE
      SIGP=.27154671*(ABN/FLOAT(NRES))**.66666667
      IF (SCV.LT.0.0.AND.SFV.LT.0.0) GO TO 1
      IF(I2)  19,19,18
18    SIGP=SIGFCT
      GO TO 20
19    CONTINUE
      WRITE (6,65) SIGP
      IF (SIGP) 1,20,20
   20 WRITE( 6,54)
      WRITE( 6,66)
      LA=1
      IF(I6)  22,22,21
21    E=USTART
      U=16.118096-ALOG(E)
      GO TO 23
22    U=USTART
      E=1.0E07*EXP(-U)
23    DO 24 I=1,NRES
   24 X(I) = (2.0*CON3(I)/GAM(I))*(E-EO(I))
      KKK=KKK+1
      GO TO 6
C
25    SIGCN=0.0
      SIGFN=0.0
      SIGSN=0.0
      ZED1=SQRT(E)
      DO 26 I=1,NRES
      ZILCH1=SQRT(SIGSO(I))
      ZILCH2=PHI(I)*SQRT(G*SIGP*SIGSO(I))
      ZILCH3=PSI(I)
      SIG1(I)=PHI(I)*ZILCH1
      SIG2(I)=ZILCH2
      SIG3(I)=ZILCH3*ZILCH1
      WORK = ZILCH2/CON3(I)
      TEMP=SIGSO(I)*PSI(I)
      SIGCN=SIGCN+SIGCO(I)*ZILCH3
      SIGFN=SIGFN+SIGFO(I)*ZILCH3
      SIGSN=SIGSN+TEMP+WORK
26    CONTINUE
      SIGCN=(SIGCN+AKC)/ZED1
      SIGFN=(SIGFN+AKF)/ZED1
      SIGSN=SIGSN+SIGP
      IF(I8)  30,30,27
27    SIGSN=SIGP
```

```
      DO 29 I=1,NUMBG
      SIGY1=0.
      SIGY2=0.
      SIGY3=0.
      DO 28 J=1,NRES
      IF (ABS(G-GG(I)).GT.0.00001) GO TO 28
      SIGY1=SIGY1+SIG1(J)
      SIGY2=SIGY2+SIG2(J)
      SIGY3=SIGY3+SIG3(J)
28    CONTINUE
      SIGSN=SIGSN+0.25*SIGY1**2+SIGY2+SIGY3**2
29    CONTINUE
30    IF (SIGSN) 31,32,32
31    JJJ=1
32    SIGA=SIGCN+SIGFN
      ANUSIG=ANU*SIGFN
C
      IF (NCOUNT-54) 34,34,33
   33 WRITE( 6,54)
      WRITE( 6,66)
      NCOUNT=0
   34 WRITE( 6,68) NTALLY,U,E,SIGA,SIGSN,ANUSIG
      IWORD = NWORDS-NTALLY + 1
      NTALLY=NTALLY+1
      NCOUNT=NCOUNT+1
      DATUMS(IWORD,1) = E
      DATUMS(IWORD,2) = SIGA
      DATUMS(IWORD,3) = SIGSN
C
      IF(I6)  44,44,37
37    IF ((UG(LA)-E)+0.00001) 38,40,40
38    E=E-DU(LA)
      U=16.118096-ALOG(E)
      GO TO 43
40    E=UG(LA)
      LA=LA+1
      IF ((UG(NDU)-E)+.000001) 38,41,41
   41 CONTINUE
      IF(JJJ)  1,1,42
42    WRITE (6,54)
      WRITE (6,70)
      WRITE(18,70)
      GO TO 1
C
44    IF ((UG(LA)-U)-0.00001) 47,47,45
45    U=U+DU(LA)
      E=1.0E07*EXP(-U)
   43 CONTINUE
      DO 46 I=1,NRES
   46 X(I) = (2.0*CON3(I)/GAM(I))*(E-EO(I))
      GO TO 14
47    U=UG(LA)
      LA=LA+1
      IF ((UG(NDU)-U)-.00001) 48,48,45
   48 CONTINUE
      IF (JJJ) 1,1,49
```

```
49    WRITE (6,54)
      WRITE (6,70)
      GO TO 1
C
50    FORMAT (12A6)
51    FORMAT (6F10.5,2I5)
52    FORMAT (2F10.6)
53    FORMAT (7F10.7)
54    FORMAT (1H1)
55    FORMAT (1HK)
56    FORMAT (3X,6HTEMP =F12.2,3X,4HNU =F6.3,3X,6HU KT =F8.4,3X,12HSIG C
     1AP KT =F10.4,3X,10HSIG F KT =F10.4,3X,9HSIG TOT =F10.4/3X,9HSIG PO
     2T =F9.3)
57    FORMAT (10X,2H K,7X,3H UG,11X,3H DU)
58    FORMAT (I12,2F13.5)
59    FORMAT (1HJ/3X,1HI,15H  ATOMIC WEIGHT,3X,10HRES ENERGY,6X,7HGAMMA
     1N,7X,7HGAMMA G,7X,7HGAMMA F)
60    FORMAT (I4,F14.3,F18.4,3F14.8)
61    FORMAT (4X,1HI,3X,10HRES ENERGY,5X,5HSIGCO,9X,5HSIGFO,9X,5HSIGSO,9
     1X,5HSIGTO)
62    FORMAT (I5,F13.4,4F14.4)
64    FORMAT (10X,10HSIG C /V =,F12.4,5X,10HSIG F /V =,F12.4)
65    FORMAT (1H /10X,10HSIG POT  =F12.4)
66    FORMAT (6X,1HK,6X,1HU,11X,1HE,11X,5HSIG A,8X,6HSIG ES,7X,8HNU SIG
     1F)
67    FORMAT (10X,F10.7,10X,4F10.7)
68    FORMAT (I7,2X,F8.5,F13.5,6F13.4)
70    FORMAT (10X,22HSIG S IS NEG AT SOME E)
71    FORMAT (I5)
   72 FORMAT(1X,I1,1X,I1,1X,I1,1X,I1)
      END
```

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