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PEAS – A RESONANCE ABSORPTION PROGRAMME

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ABSTRACT

Details are given of a 7090 FORTRAN computer programme to calculate the neutron absorption in individual symmetric, single level, Doppler broadened Breit Wigner resonances for a homogeneous system of two nuclides. The flux used in determining the resonance absorption is calculated from the numerical solution of the slowing down integral equation.

A listing of the programme is provided.

CONTENTS

1. INTRODUCTION

The reasonably accurate calculation of resonance absorption is essential in a reactor system breeding fuel, as a large fraction of the neutrons undergo resonance reactions. One of the formulae which have been proposed for calculation of effective resonance integrals is the "intermediate-resonance (IR)" formula of Goldstein and Cohen (1962) which interpolates between two simple approximations in general use; the "narrow-resonance (NR)" and "infinite-mass (IM)" formulae. The programme PEAS was written to calculate the resonance absorption accurately to enable comparison to be made with the IR result. It is not recommended that PEAS should be used for everyday calculation of resonance absorption, but rather its main use is to indicate possible inaccuracies caused by using the IR method for systems under study.

The accurate calculation of resonance reaction rates is based on the accurate calculation of the neutron flux through a resonance, taking into account the flux depression caused by the resonance itself. The programme PEAS is based on an infinite homogeneous system composed of two nuclides. The flux derived from a neutron source distributed with equal intensity throughout this system is space-independent and may be calculated as the solution of the slowing down integral equation provided the cross sections are known. Neglecting interference between resonance and potential scattering and assuming that the resonances are isolated with symmetric single level Doppler broadened Breit Wigner contours, the resonance cross sections may be calculated from the resonance line shape function differential equation.

The approximate calculation, based on the IR method, may be readily expressed in terms of simple functions and integrals involving the resonance line shape function.

2. FUNDAMENTAL EQUATIONS

A balance of neutron collisions derived from a unit source in an infinite homogeneous system of two nuclides yields the slowing down integral equation:

$$F(E) = Y_1(E) + Y_2(E) \quad , \qquad (1)$$

where

$$F(E) = \xi\, \Sigma_t(E)\, \phi(E) \, ,$$

$$Y_i(E) = \frac{1}{1-\alpha_i} \int_E^{E/\alpha_i} R_i(E')\, \frac{dE'}{E'} \quad ,$$

and

$$R_i(E) = \frac{\Sigma_{si}(E)}{\Sigma_t(E)}\, F(E) \quad .$$

It is convenient to change the variable in the above integral to lethargy, that is,

$$u = \ln(10^7/E) \; .$$

Then

$$Y_i(u) = \frac{1}{1-\alpha_i} \int_{u-\mathfrak{U}_i}^{u} R_i(u')\, du' \quad ,$$

where

$$R_i(u') = R_i(E') \quad .$$

Considering the resonance to be cut off at u_1 and u_M then within the resonance the probability of a neutron escaping resonance absorption is related to the collision density through the equation:

$$p(u) = 1 - \frac{1}{\xi} \int_{u_1}^{u} \frac{\Sigma_a(u')}{\Sigma_t(u')}\, F(u')\, du' \quad , \qquad (2)$$

where

$$F(u) = EF(E) \tag{3}$$

is the normalized collision density per unit lethargy.

Outside the resonance, further analysis gives the equations:

$$\left.\begin{aligned} F(u) &= 1 \quad (4a) \\ p(u) &= 1 \quad (4b) \end{aligned}\right\} , \; u \leqslant u_1 ,$$

and

$$\left.\begin{aligned} F(u) &= p \quad (5a) \\ p(u) &= p \quad (5b) \end{aligned}\right\} , \; u >> u_M ,$$

where

$$p = 1 - \frac{1}{\bar{\xi}} \int_{u_1}^{u_M} \frac{\Sigma_a(u')}{\Sigma_t(u')} F(u')\, du' \quad . \tag{6}$$

Equation 4a may be considered the initial condition necessary for the solution of Equation 1.

Although not necessary for the solution of Equation 1, it is convenient to define the function:

$$W(u) = \frac{F(u)}{p(u)} \quad , \tag{7}$$

which has the property:

$$W(u) = 1 \text{ for } u \leqslant u_1 \text{ and } u >> u_M \quad . \tag{8}$$

The effective resonance integral is defined as:

$$I_{ex}(u) = -\bar{\xi}\, \sigma_p \ln p(u) \quad , \tag{9a}$$

and hence

$$I_{ex}(u) = \sigma_p \int_{u_1}^{u} \frac{\Sigma_a(u')}{\Sigma_t(u')} W(u')\, du' \quad . \tag{9b}$$

The various formulae proposed for calculating the effective resonance integral may be thought of as giving approximations for the function $W(u)$ within the resonance; $W(u) = 1$ gives the NR result, $I_{(1)}(u)$, while $W(u) = \Sigma_t(u)/\Sigma_t^*(u)$ gives the IM result, $I_{(0)}(u)$. Goldstein and Cohen (1962) have proposed the IR formula for the complete resonance:

$$I_\mu = \frac{(I_{(0)} + \mu I_{(1)})}{(1+\mu)} \quad . \tag{10}$$

From Equation 10, the interpolation parameter which gives the exact effective resonance integral, I_{ex}, is therefore:

$$\mu_{ex} = \frac{I_{(0)} - I_{ex}}{I_{ex} - I_{(1)}} \quad . \tag{11}$$

This may be compared with the value calculated using the theory of Goldstein and Cohen (1962), modified slightly by McKay and Pollard (1963):

$$\mu = \frac{\frac{\Gamma}{\Gamma_a}\frac{\sigma_m}{\sigma_{p2}} J_0 - \left(\frac{\sigma_m}{\sigma_{p2}} + \frac{1}{\alpha_2}\right) J_1 - K_0}{\left(\frac{1-\alpha_2}{\alpha_2}\right) J_1 + K_1} \quad ; \tag{12}$$

where $J_\lambda = J(\infty, a_\lambda)$ – the J–function tabulated by Dresner (1960) and others,

$$a_\lambda = \Gamma(\sigma_m + \lambda\sigma_{p2})/(\sigma_o(\Gamma_a + \lambda\Gamma_n)) \quad ,$$

$$K_\lambda = \left(\frac{a_\lambda - a_\infty}{x_r \; a_\infty}\right) J_\lambda \; J_1 \left(\frac{2}{\pi}\right) \text{artan}\left(\frac{x_r}{c_\lambda + c_1}\right) \quad ,$$

$$c_\lambda = \left(1 - \frac{1}{a_\lambda}\right)^{\frac{1}{2}} \quad ,$$

and

$$x_r = (1-\alpha_2)\, E_r \Big/ \left(\frac{\Gamma}{2}\right) \quad .$$

The IR effective resonance integral I_μ may be calculated from Equation 10 and should compare favourably with I_{ex} calculated from the solution of the slowing down equation.

Neglecting the variation of the reciprocal of energy over a resonance, the NR and IM approximations may be written:

$$I_{(\lambda)} = \frac{\Gamma_a \sigma_o}{E_r} \; a_\lambda \; J(\theta, a_\lambda) \quad . \tag{13}$$

3. RESONANCE CROSS SECTIONS

Neglecting 1/v absorption and assuming that the resonances are isolated with symmetric single level Doppler broadened Breit Wigner contours, the resonance cross sections may be represented:

$$\sigma_a(E) = \frac{\Gamma_a}{\Gamma} \sigma_o \; \psi(\theta, x) \quad , \tag{14a}$$

and

$$\sigma_s(E) = \frac{\Gamma_n}{\Gamma} \sigma_o \; \psi(\theta, x) \quad , \tag{14b}$$

where no account has been taken of interference between resonance and potential scattering. The resonance line shape function is given by:

$$\psi(\theta, x) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-\frac{1}{4}\theta^2 (x-y)^2}}{1+y^2} \, dy \quad ,$$

although it may be obtained more readily as the solution of the differential equation:

$$\psi''(\theta, x) = \frac{1}{4}\theta^4 - \theta^2 x \, \psi'(\theta, x) - \frac{1}{4}\theta^2 (2 + \theta^2 + \theta^2 x^2)\, \psi(\theta, x), \tag{15}$$

$$\psi(\theta, 0) = \frac{1}{2}\sqrt{\pi}\, \theta \, e^{\frac{\theta^2}{4}} \, \text{erfc}\left(\frac{1}{2}\theta\right) \quad ,$$

$$\psi'(\theta, 0) = 0 \quad ,$$

where primes denote differentiation with respect to the variable x .

4. NUMERICAL PROCEDURE

The numerical procedure follows closely the method used by McKay and Pollard (1963).

4.1 Choice of Grid

The input information on the second input record (see Appendix A) gives the order of magnitude of the step length, δx , and cut-off, $x = a$, of the desired grid. The constant lethargy grid spacing, δu , is given approximately by:

$$\delta u = \frac{\Gamma}{2} \frac{\delta x}{E_r} ,$$

and is modified slightly so that the number of lethargy steps for a collision range of the heavy absorber, N, is an even integer.

The centre of the resonance is located and the grid is labelled J ($= a/\delta x$ — except for a slight adjustment to make J an odd integer). The number of grid steps for the cut-off resonance is then simply

$$M = 2J - 1 .$$

The high energy cut-off of the resonance is

$$E_1 = E_r \, e^{+(J-1)\,\delta u} ,$$

the low energy cut-off is

$$E_M = E_r \, e^{-(J-1)\,\delta u} .$$

In general

$$E_K = E_{K-1} \, e^{-\delta u} ,$$

and

$$x_K = x_{K-1} - dE_{K-1} ,$$

where

$$d = \frac{2}{\Gamma} \delta u \left(1 - \frac{\delta u}{2} + \frac{\delta u^2}{6} - \frac{\delta u^3}{24}\right) .$$

Note that the step length is not constant in δx and that the resonance cut-off only approximately agrees with the quantity used as input, that is:

$$x_1 \approx - x_M \approx a .$$

4.2 Generation of $\psi(\theta, x)$

The differential equation (15) is solved numerically for x values corresponding to the grid.

The initial conditions are :

$$E_J = E_r ,$$

$$x_J = 0 ,$$

$$\psi_J = \theta \, \mathrm{erc}\left(\frac{\theta}{2}\right) ,$$

and

$$\psi_J' = 0 ,$$

where $$\operatorname{erc}(y) = \frac{1}{2}\sqrt{\pi}\; e^{y^2} \operatorname{erfc}(y)$$

$$\approx \sum_{l=1}^{5} a_l \, \eta^l \text{ provided } y \leqslant 1.5$$

$$\eta = \frac{1}{(1 + p\,y)} ,$$

and the constants p and a_l $(l = 1, 2, \ldots, 5)$ have been given by Hastings (1955), page 169.

If $|x_K| < \frac{b}{\theta}$, $\psi(\theta, x_K)$ is obtained as the solution of the differential equation (15) using the method:

$$\delta x_K = - d E_{K-1} ,$$

$$x_K = x_{K-1} + \delta x_K ,$$

$$E_K = E_{K-1} + \frac{\Gamma}{2}\, \delta x_K ,$$

$$\psi_K = \psi_{K-1} + \delta x_K \, \psi'_{K-1} + \frac{\delta x_K^2}{2}\, \psi''_{K-1} + \frac{\delta x_K^3}{6}\, \psi'''_{K-1} ,$$

$$\psi'_K = \psi'_{K-1} + \delta x_K \, \psi''_{K-1} + \frac{\delta x_K^2}{2}\, \psi'''_{K-1} ,$$

$$\psi''_K = \frac{1}{4}\,\theta^4 - \theta^2 x_K \psi'_K - \frac{1}{4}\,\theta^2 (2 + \theta^2 + \theta^2 x_K^2)\, \psi_K ,$$

and $$\psi'''_K = -\theta^2 x_K \psi''_K - \frac{1}{4}\,\theta^2 (6 + \theta^2 + \theta^2 x_K^2)\, \psi'_K - \frac{1}{2}\,\theta^4 x_K \psi_K .$$

If $|x_K| \geqslant \frac{b}{\theta}$, $\psi(\theta, x_K)$ is obtained from three terms of the asymptotic series:

$$\psi_K = \frac{1}{1 + x_K^2} \left\{ 1 + \left[(3 x_K^2 - 1) + \left(15\, x_K^2 \,(x_K^2 - 2) + 3\right) v_K \right] v_K \right\} ,$$

where $$v_K = \frac{1}{(1 + x_K^2)^2} \quad \frac{2}{\theta^2} .$$

When $|x_K|$ increases and the value of $\left[(3 x_K^2 - 1) + \left(15 x_K^2 (x_K^2 - 2) + 3\right) v_K \right] v_K$ decreases to less than 10^{-4}, the simple expression:

$$\psi_K = \frac{1}{1 + x_K^2}$$

is used.

The preceding equations are used for both $K < J$ and $K > J$ over the range $K = 1$ to M, as the symmetric property of the function $\psi(\theta, x)$ cannot be used with the chosen grid.

4.3 Calculation of the J-functions

The J-functions are obtained using Simpson's rule, with an allowance for the truncated resonance range.

$$J(\theta, a_\lambda) = \int_0^\infty \frac{\psi(\theta, x)}{\psi(\theta, x) + a_\lambda} \, dx$$

$$= \frac{1}{2} \{ d' \sum_{K=1}^{M} (S_K \, r_K^{(\lambda)} \, E_K) + c_{\lambda,1} + c_{\lambda,M} \} ,$$

where $(S_K) = \frac{1}{3} (1, 4, 2, 4, \ldots, 2, 4, 1)$,

$$r_K^{(\lambda)} = \frac{\psi_K}{\psi_K + a_\lambda} ,$$

$$c_{\lambda,K} = \frac{1}{a_\lambda c_\lambda} \arctan \left| \frac{c_\lambda}{x_K} \right| ,$$

and $d' = 2 \frac{\delta u}{\Gamma}$.

4.4 Solution of the Slowing Down Equation for F(E)

The initial condition given by Equation 4a gives

$$R_{iK} = R_i(E_K) = \frac{\Sigma_{si}}{\Sigma_t} \frac{1}{E_K} , \quad K \leqslant 1 , \tag{16}$$

where $E_K = E_1 e^{-(K-1)\delta u}$,

hence

$$Y_{i1} = Y_i(E_1) = R_{i1} . \tag{17}$$

Within the resonance a recurrence relation for Y_{iK} can be obtained in terms of a previously calculated Y_{iK} and either previously calculated R_{iK}'s, or R_{iK}'s with negative indices which can be calculated from Equation 16. The procedure thus amounts to "marching" from high energies, starting at $E = E_1$ and continuing in equal lethargy steps of the grid until $E = E_M$. Fitting cubics through the R_{iK}'s at four points around $u' = u$ and $u' = u - \mathfrak{U}_i$, the following recurrence relation can be obtained:

$$Y_{iK} = Y_{i,K-1} + \frac{\delta u}{1-\alpha_i} \cdot \frac{1}{24} \{ 9 R_{iK} + 19 R_{i,K-1} - 5 R_{i,K-2} + R_{i,K-3} - Q_{iK} \} \tag{18a}$$

$$Q_{iK} = \omega_{i1} R_{i,K-n_i-1} + \omega_{i2} R_{i,K-n_i} + \omega_{i3} R_{i,K-n_i+1} + \omega_{i4} R_{i,K-n_i+2} , \tag{18b}$$

where the ω_{il}'s are constants which depend only on the lack of coincidence of the end of a collision range and the grid, and $n_i = \left[\text{integer just smaller than} \left(\frac{\mathfrak{U}_i}{\delta u} \right) \right] + 1$.

Not all of the terms of Equation 18 are known for the K^{th} grid, as $F(E_K)$ is unknown. However, separating off the unknown quantity and writing:

$$Y'_{iK} = \frac{\delta u}{1-\alpha_i} \cdot \frac{1}{24} \left\{ 19 R_{i,K-1} - 5 R_{i,K-2} + R_{i,K-3} - Q_{iK} \right\} ,$$

Equation 1 may be written:

$$F(E_K) = \frac{9}{24} \, \delta u \left(\frac{1}{1-\alpha_1} \, \frac{\Sigma_{s1}(E_K)}{\Sigma_t(E_K)} + \frac{1}{1-\alpha_2} \, \frac{\Sigma_{s2}(E_K)}{\Sigma_t(E_K)} \right) F(E_K) + Y'_{1K} + Y'_{2K} \quad . \qquad (19)$$

This can be readily rearranged to give $F(E_K)$, the required solution of the slowing down equation.

4.5 Calculation of Resonance Absorption

The resonance capture probability is calculated using Simpson's rule:

$$I = \frac{1}{\xi} \int_{u_1}^{u_M} \frac{\Sigma_a(u')}{\Sigma_t(u')} \, F(u') \, du'$$

$$= \frac{\delta u}{\xi} \sum_{K=1}^{M} S_K \, \frac{\Sigma_a(u_K)}{\Sigma_t(u_K)} \, F(u_K) \quad . \qquad (20a)$$

This is then corrected for the truncated resonance range, assuming that

$$\psi(\theta, x) = \frac{1}{1+x^2} ,$$

$$F(u) = 1 \text{ for } u \leqslant u_1 ,$$

and

$$F(u) = p \text{ for } u \geqslant u_M .$$

Hence

$$I_c = \frac{(c'_{1,1} + I + c'_{1,M})}{(1 + c'_{1,M})} , \qquad (20b)$$

where

$$c'_{\lambda,K} = \frac{\Gamma_a}{2\xi E_r} \, c_{\lambda,K} .$$

4.6 Calculation of p

The resonance escape probability is simply:

$$p = 1 - I_c , \qquad (21)$$

and the effective resonance integral is given by:

$$I_{ex} = -\xi \, \sigma_p \ln p , \text{ for } I_c > 10^{-4}$$

or

$$I_{ex} = \xi \, \sigma_p \, I_c , \text{ for } I_c \leqslant 10^{-4} .$$

5. TYPICAL RESULTS

Some typical results from PEAS for resonances of U238 are collected in the tables. For convenience $\sigma_m = \zeta \sigma_{p1}$ (the microscopic potential scattering cross section of the light scatterer per heavy absorber atom) has been introduced.

Tables 1-2 are for H and Be systems and are derived from data compiled from the A.A.E.C. Data Library (Doherty 1964) except for the 192eV resonance parameters which were chosen to agree with the resonance studied by Goldstein and Cohen (1962). A value of 10 barns for σ_{pU238} was used in the programme and the expression used for the resonance peak height was $\sigma_o = 2.62 \times 10^6 g\ \Gamma_n/(\Gamma E_r)$ barns.

Tables 3-5 are for a C system and are derived from the data given by Sumner (1963), except that by mistake the value of σ_{pU238} used was 10.8 barns instead of 10.64. As a result the NR results are slightly different. The expression used for the resonance peak height was

$$\sigma_o = 2.60 \times 10^6 g\ \Gamma_n /(\Gamma E_r) \text{ barns.}$$

An approximation for the J-function suggested by Doherty (1963) was used in preparing the approximate IR (AIR) results of Tables 3-5, which otherwise are based on the IR method. The advantage of the AIR method is its great speed (approximately 1/50 sec per resonance on the IBM 7090). A 7090 FORTRAN subroutine for this called RESON (Pollard 1964) has been written.

Table 6 gives the variation of the IR interpolation parameter, μ, with E_r and σ_m for a C system.

The temperature variation of μ recorded in Table 1 should be compared with the results of McKay and Pollard (1963), and the effective resonance integrals for a C system based on the μ method should be compared with the λ method results of Sumner (1963).

The layout of a sample problem and the output from "PEAS" are presented in Appendices B and D.

6. CONCLUSIONS

The results recorded in the tables suggest the following:

(i) The temperature variation of μ is considerable in some instances. However, as observed by McKay and Pollard (1963), the variation has only a small effect on the estimate of the effective resonance integral. The present results are in qualitative agreement with those of McKay and Pollard.

(ii) For the same scattering cross section, H and Be systems have different effective resonance integrals - a result which is not predicted by the IR method used. As the ratio of light scatterer to U decreases, the difference becomes more pronounced and the Be system gives an effective resonance integral which is further from the IR result than that given by the equivalent H system.

(iii) The μ method used in this work and the λ method used by Sumner (1963) give substantially the same estimate of the effective resonance integral.

(iv) For most of the resonances the IR method is a considerable improvement over the NR and IM methods.

(v) The improvement of the IM method over the NR and IM methods is not pronounced for the low energy resonances except for the H system.

(vi) The AIR method, using the J-function of Doherty (1963), gives a fairly good estimate of the effective resonance integral although, as noted by Doherty, the method may not be satisfactory for estimating Doppler coefficients.

(vii) Although not recorded in the tables it has been observed that to give p the IR result must be used in an equation which is in exponential form (similar to 9a) and not in the linear form

$$p = 1 - \frac{I\mu}{(\xi \sigma_p)} \quad .$$

The latter gives reasonable results only when $\frac{I\mu}{\xi\sigma_p}$ is small.

7. FURTHER STUDY

It was observed in the last section that differences exist between hydrogen and other scatterers, particularly for low energy resonances in low ratios of scatterer to absorber. The IR method must be further developed to give a quantitive explanation of this effect. A suggestion by McKay (1963) promises to give a good quantitative explanation.

The programme PEAS should be extended to include more than two nuclides and should allow for overlapping of resonances and the effect of interference between resonance and potential scattering, although since the writing of PEAS the author's attention has been drawn to the programme RESLOW (Collins 1963) which already takes account of these features.

8. ACKNOWLEDGMENTS

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10. NOTATION

The following notation is used in the report. Subscript i = 1 indicates a light scatterer, for example Be. Subscript i = 2 indicates a heavy absorber, for example U238. Nuclide properties without energy dependence indicated are to be calculated for an energy well away from the resonance energy.

E_r	=	resonance energy in eV
Γ_n	=	resonance level width for scattering in eV
Γ_γ	=	resonance level width for γ–emission in eV
Γ_f	=	resonance level width for fission in eV

Γ_a	=	$\Gamma_\gamma + \Gamma_f$
Γ	=	$\Gamma_n + \Gamma_a$
g	=	resonance spin factor
σ_o	=	$2.6 \times 10^6 g \, \Gamma_n/(\Gamma E_r)$
E	=	energy in eV
x	=	$(E-E_r)/(\Gamma/2)$
u	=	lethargy
	=	$\ln(10^7/E)$
$\Sigma_{si}(E)$	=	macroscopic scattering cross section for the i^{th} nuclide
$\Sigma_t(E)$	=	total macroscopic cross section
$\Sigma_t^*(E)$	=	infinite mass cross section
	=	$\Sigma_t(E) - \Sigma_{s2}(E)$
σ_{pi}	=	potential scattering cross section of the i^{th} nuclide
ζ	=	atomic ratio of the light scatterer to the heavy absorber
σ_m	=	$\zeta \sigma_{p1}$
σ_p	=	$\sigma_m + \sigma_{p2}$
$\bar{\xi}$	=	average logarithmic energy decrement for the mixture
$\phi(E)$	=	flux per unit energy derived from a source emitting 1n cm^{-3} s^{-1}
F(E)	=	normalized collision density per unit energy
	=	$\bar{\xi} \Sigma_t(E) \phi(E)$
F(u)	=	normalized collision density per unit lethargy
	=	EF(E)
p(u)	=	resonance escape probability
μ	=	interpolation parameter recommended by Goldstein and Cohen (1962)
μ_{ex}	=	interpolation parameter required to give correct absorption based on F(E)
$I_{(0)}$	=	IM approximation for the effective resonance integral
$I_{(1)}$	=	NR approximation for the effective resonance integral
I_μ	=	IR approximation for the effective resonance integral
I_{ex}	=	calculated effective resonance integral based on F(E)
A_i	=	atomic number of the i^{th} nuclide

α_i = maximum possible fraction of energy loss for elastic collisions with the i^{th} nuclide

$$= \left(\frac{A_i - 1}{A_i + 1}\right)^2$$

$\mathfrak{U}_i$ = $\ln(1/\alpha_i)$

T = temperature in degrees Kelvin

k = Boltzmann constant

(kT = temperature in eV)

$$\theta = \frac{1}{2}\,\Gamma\,\sqrt{\frac{A_2}{E_r\,kT}}$$

$\psi(\theta,x)$ = resonance line shape function

$$= \frac{\theta}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{e^{-\frac{1}{4}\theta^2(x-y)^2}}{1+y^2}\,dy$$

$J(\theta, a_\lambda)$ = J-function of Dresner (1960), and others

$$= \int_{0}^{\infty}\frac{\psi(\theta,x)}{\psi(\theta,x)+a_\lambda}\,dx \quad .$$

APPENDIX A

INPUT DATA FOR PEAS ON TAPE 2

Each problem requires 4 data records which should be in the following form.

The first record must contain a 1 in column 1, which may be followed by 49 Hollerith characters forming an output label. The 1 is required in case an incorrect number of data cards is used as input. A fresh problem will start from the next data card containing a 1 in the first column. Normal data should not therefore have the first field of each record left-justified.

The second record should comprise:

(i) (E10.3, the temperature T in degrees Kelvin (if $T = 0$ then θ is set to 9.999×10^5 and b is set to zero).

(ii) E10.3, the resonance cut-off, $a = \sqrt{-x_1 x_M}$.

(iii) E10.3, the resonance line shape function changeover point b, such that for $|x| \geqslant b/\theta$ the line shape function is obtained from three terms of its asymptotic expansion (for example $b = 12$).

(iv) E10.3, the integration step length, δx, for the middle of the resonance (for example $\delta x = 0.1875$). Note that $a/\delta x \ngtr 10001$.

(v) 5X15, the frequency of output of F(u) for the middle of the resonance (for example use 5 for liberal output, a few pages, and 25 for restricted output, one page). Note that only every second step is available for output in the middle of the resonance, and every fortieth step in the wings.

(vi) 5X15, the required minimum number of integration steps between peaks before classification of a new peak in F(u)/p(u) (for example 20).

(vii) 7X15), the option, ID, required for the cut-off and over-shoot on the low energy side of the resonance.

If $ID = -i$, i integration steps are used before exit from the resonance.

If $ID = 0$ (blank), the calculation will overshoot the low energy cut-off to enable F(u) to become asymptotic and $F(u)/p(u) \to 1$. (This may be considered a rough criterion for deciding that the step length was not excessive, as deviations from 1 give a measure of the numerical inaccuracies).

If $ID = i$, the calculation is terminated at the low energy cut-off.

The third record should comprise:

(i) (E10.3, the atomic ratio of the light scatterer to the heavy absorber, ζ (for example N_{Be} / N_{Th}).

(ii) 1X6HbbbbbbI3, the chemical symbol and atomic number of the light scatterer (for example bbbbBEbb9).

(iii) E10.3, the potential scattering cross section of the light scatterer, σ_{p1}, in barns.

(iv) 1X6HbbbbbbI3, the chemical symbol and atomic number of the heavy absorber (for example bbbbTH232).

(v) E10.3), the potential scattering cross section of the heavy absorber, σ_{p2}, in barns.

APPENDIX A (continued)

The fourth record should contain the standard A.A.E.C. library resonance information (Doherty, 1964):

(i) (F7.3, u = $\ln(10^7/E)$.

(ii) 1PE11.3, E(eV).

(iii) 4E10.2, Γ_n (eV), Γ_γ (eV), Γ_f (eV), g(spin factor).

(iv) I7, the number 17.

(v) I3, the number of protons for the resonance absorber.

(vi) I4), the atomic number of the resonance absorber (which must agree with the data for (iv) of the third record).

Control is returned to the FORTRAN monitor if an input record containing a negative temperature ((i) of second record) is detected.

Appendix B is a listing of sample input data.

APPENDIX B

SAMPLE INPUT FOR PEAS

```
1     PROBLEM 260   GRAPHITE SIGM =     25. BARNS.
        300.       840.          12.   0.1875            25          20
 5.319E+00        C 12 4.700E+00     U 238 1.080E+01
 8.943    1.306E+03  1.00E-02  2.60E-02  0.0           1.00E+00       17 92 23
```

APPENDIX C

OUTPUT DATA FROM PEAS ON TAPE 3

The output data uses normal FORTRAN output column 1 control and, when listed, each problem will start on a fresh page. The output is of variable length depending on the input data ((v) of second input record) and has the following meaning:

The first record is the problem label, which is a copy of the first 50 columns of the first input record.

The second record is a copy of the composition record used as input (third record, Appendix A).

The third record is a copy of the resonance record used as input (fourth record, Appendix A).

The fourth record comprises:

(i) The temperature, T, in degrees Kelvin.

(ii) The number of integration steps, M, for the cut-off resonance.

(iii) The number of integration steps, N, per collision range of the heavy absorber.

The fifth record comprises:

(i) The value of x at which the resonance line shape function is to be obtained from the asymptotic expansion instead of as the solution of the differential equation.

(ii) The x value of the high energy cut-off of the resonance.

(iii) The x value of the low energy cut-off of the resonance.

(iv) The integration step length, δx, for the middle of the resonance used as input (iv) of second input record).

(v) $\bar{\xi}$.

The sixth and seventh records comprise:

θ, a_0, $J(\theta, a_0)$ (IM),
and θ, a_1, $J(\theta, a_1)$ (NR),
where the J-functions have been evaluated using the resonance line shape function generated in the programme.

Then follows a variable length of output relating to the collision density through the resonance. It consists of

$$x,\ 1-p(u),\ F(u),\ W(u) = F(u)/p(u),\ E(eV)$$

interspersed with output indicating the maxima and minima (peaks) in W(u).

The final block of output is self explanatory and consists of p, u_{ex}, μ (following Goldstein and Cohen, 1962 - G. and C.), I_{ex}, I_{μ} (G. and C.), $I_{(0)}$ (IM), and $I_{(1)}$ (NR) (all the I's in barns), and the percentage errors in the approximations compared with the exact values.

APPENDIX C (continued)

The accuracy depends on the choice of cut-off, a, and the integration step, δx. Using the values recommended for input data (bracketed quantities) a few chosen resonances gave accuracies of better than 0.1 per cent. for the J-functions, and when F(u)/p(u) was calculated well beyond the resonance cut-off the ratio was within 10^{-4} of unity.

A comparison was made between the results of PEAS and the results of the programme RESLOW (Collins, 1963) for two resonances. In both cases the capture probability, 1-p(u), agreed to better than 0.01 per cent. although both programmes use different methods for obtaining $\psi(\theta, x)$ and have different accuracies for the integration procedure.

The actual 7090 machine time depends on the input option ((vii) of second input record), the choice of light scatterer, and the temperature. A typical time for a problem is half a minute.

Appendix D is a listing of sample output.

APPENDIX D

SAMPLE OUTPUT FROM PEAS

```
PROBLEM 260  GRAPHITE SIGM =    25. BARNS.

5.319E 00        C 12 4.700E 00       U 238 1.080E 01
 8.943  1.306E 03 10.00E-03  2.60E-02  0.          1.00E 00       17 92 238
          ER    T=  300.0 M= 8961 N= 6504
  2.511E 02  8.448E 02 -8.351E 02  1.875E-01  1.127E-01
J  4.7783E-02, 6.2594E-02 = 1.7509E 01
J  4.7783E-02, 6.4736E-02 = 1.7092E 01
```

X	CAP PROB	FU	FU/P	E
0.844832E 03	0.1199106E-09	10.000000E-01	10.000000E-01	1.321207E 03
0.750055E 03	0.2026953E-06	9.999925E-01	9.999927E-01	1.319498E 03
0.655401E 03	0.4642898E-06	9.999835E-01	9.999840E-01	1.317789E 03
0.560869E 03	0.8147609E-06	9.999740E-01	9.999748E-01	1.316083E 03
0.466461E 03	0.1308658E-05	9.999650E-01	9.999664E-01	1.314382E 03
0.372175E 03	0.2056958E-05	9.999528E-01	9.999548E-01	1.312681E 03
0.278011E 03	0.3326599E-05	9.999373E-01	9.999407E-01	1.310979E 03
0.183969E 03	0.5977361E-05	9.999278E-01	9.999338E-01	1.309285E 03
0.103941E 03			9.999295E-01	PEAK
0.844175E 02	0.2686475E-04	9.999054E-01	9.999322E-01	1.307490E 03
0.750329E 02	0.4447752E-04	9.998935E-01	9.999380E-01	1.307320E 03
0.656496E 02	0.7947319E-04	9.998710E-01	9.999504E-01	1.307151E 03
0.562674E 02	0.1436931E-03	9.998306E-01	9.999743E-01	1.306982E 03
0.468865E 02	0.2503674E-03	9.997643E-01	1.000015E 00	1.306812E 03
0.375068E 02	0.4096560E-03	9.996659E-01	1.000076E 00	1.306643E 03
0.281284E 02	0.6242836E-03	9.995335E-01	1.000158E 00	1.306473E 03
0.187511E 02	0.8881204E-03	9.993708E-01	1.000259E 00	1.306304E 03
0.937507E 01	0.1187988E-02	9.991857E-01	1.000374E 00	1.306135E 03
0.252420E-03	0.1506654E-02	9.989887E-01	1.000496E 00	1.305965E 03
-0.937335E 01	0.1825258E-02	9.987913E-01	1.000618E 00	1.305796E 03
-0.187457E 02	0.2124960E-02	9.986048E-01	1.000731E 00	1.305627E 03
-0.281169E 02	0.2388587E-02	9.984399E-01	1.000830E 00	1.305457E 03
-0.374868E 02	0.2603037E-02	9.983044E-01	1.000910E 00	1.305288E 03
-0.468556E 02	0.2762237E-02	9.982021E-01	1.000967E 00	1.305118E 03
-0.562231E 02	0.2868926E-02	9.981317E-01	1.001003E 00	1.304949E 03
-0.655894E 02	0.2933228E-02	9.980872E-01	1.001023E 00	1.304781E 03
-0.749545E 02	0.2968324E-02	9.980605E-01	1.001032E 00	1.304612E 03
-0.835693E 02			1.001033E 00	PEAK
-0.843183E 02	0.2986019E-02	9.980442E-01	1.001033E 00	1.304443E 03
-0.936810E 02	0.2994577E-02	9.980334E-01	1.001031E 00	1.304275E 03
-0.187241E 03	0.3007188E-02	9.979684E-01	1.000978E 00	1.302589E 03
-0.280679E 03	0.3009750E-02	9.979078E-01	1.000920E 00	1.300903E 03
-0.373997E 03	0.3010991E-02	9.978434E-01	1.000857E 00	1.299217E 03
-0.467193E 03	0.3011726E-02	9.977836E-01	1.000798E 00	1.297538E 03
-0.560269E 03	0.3012211E-02	9.977191E-01	1.000734E 00	1.295859E 03
-0.653223E 03	0.3012555E-02	9.976487E-01	1.000663E 00	1.294181E 03
-0.746057E 03	0.3012811E-02	9.975802E-01	1.000595E 00	1.292505E 03
-0.835065E 03	0.3013001E-02	9.975146E-01	1.000529E 00	1.290901E 03

```
5.319E 00        C 12 4.700E 00       U 238 1.080E 01
ER= 1.306E 03     T=  300.0
0.9969838E 00  0.3016245E-02 P AND CAPTURE PROB.,O/OEND CORR.= 1.1E-01
MU=-2.014E 01 IEX= 1.219E-02 BARNS   1.207E-02  1.218E-02 10 AND I1
MU=-4.133E 00 IMU= 1.222E-02 BARNS                        (G.AND C.)
     7.95E 01        -2.54E-01          1.00E 00    4.97E-02 O/OERRORS
```

APPENDIX E

LISTING OF PEAS SOURCE DECK

```
C     RP009/08-PEAS 7090 VERSION-NOV. 1962.
C     USES TAPES 2(A2)-INPUT AND 3(A3)-OUTPUT.
      DIMENSION R(10001),V(10001),WW(4),WL(4),AA(2),FJ(2),FJ0(2),FKL(2),
     1CC(2)
    1 FORMAT(E10.3,E10.3,E10.3,E10.3,5XI5,5XI5,7XI5)
    2 FORMAT(1PE10.3,1X6H    BEI3,E10.3,1X6H    THI3,E10.3)
    3 FORMAT(/14H CHECK DATA,M=I6)
    4 FORMAT(19H                  ER    T=F7.1,3H M=I5,3H N=I5)
    5 FORMAT(1P1X5E11.3)
    6 FORMAT(E14.7,E15.7,34H P AND CAPTURE PROB.,O/OEND CORR.=1PE8.1)
    7 FORMAT(1P3H J E11.4,1H,E11.4,2H =E11.4)
    8 FORMAT(1H E13.6,29X1PE14.6,11X4HPEAK)
    9 FORMAT(F7.3,1PE11.3,4E10.2,I7,I3,I4)
   10 FORMAT(1H E13.6,E15.7,1P3E14.6)
   11 FORMAT(1P4H MU=E10.3,5H IEX=E10.3,7H BARNS  E10.3,1XE10.3,10H 10 A
     1ND I1)
   12 FORMAT(1H )
  813 FORMAT(I1,49H                                                  )
  814 FORMAT(1P4H MU=E10.3,5H IMU=E10.3,6H BARNS 23X 10H(G.AND C.))
  815 FORMAT(1PE14.2,E15.2,E17.2,E11.2,10H O/OERRORS)
  816 FORMAT(55H1 RP009/08-PEAS-CALCULATES RESONANCE ESCAPE PROBABILITY)
  817 FORMAT(1P3H J E11.4,1H,E11.4,2H =E11.4,10H,O/OERROR=E8.1)
  818 FORMAT(/23H THETA EXCEEDS 3.,I.E.=1PE11.4)
  819 FORMAT(1P4H ER=E10.3,0P5H    T=F7.1/)
  820 FORMAT(/7X1HX10X8HCAP PROB9X2HFU11X4HFU/P11X1HE/)
  825 FORMAT(22H1 DATA PHASE ERROR OF I5,8H RECORDS)
  950 FORMAT(55H0 SOLVES THE SLOWING DOWN INTEGRAL EQN.                  )
  951 FORMAT(55H0    F(E)=Y1(E)+Y2(E) ,WHERE                             )
  952 FORMAT(55H0    F(E)=XI*SIGMAT(E)*PHI(E) ,                          )
  953 FORMAT(55H0              U                                         )
  954 FORMAT(55H              S                                          )
  955 FORMAT(55H    YI(E)=I DU*RI(E)/(1-ALPHAI) ,                        )
  956 FORMAT(55H              S                                          )
  957 FORMAT(55H               U-UI                                      )
  958 FORMAT(55H0   RI(E)=F(E)*SIGMASI(E)/SIGMAT(E) ,                    )
  959 FORMAT(55H0 AND OBTAINS THE RESONANCE ESCAPE PROBABILITY FROM      )
  960 FORMAT(55H0              U                                         )
  961 FORMAT(55H              S                                          )
  962 FORMAT(55H  1-P(E)=I DU*E*F(E)*SIGMAA(E)/(XI*SIGMAT(E)) .          )
  963 FORMAT(55H              S                                          )
  964 FORMAT(55H               U1                                        )
  965 FORMAT(55H0 THE CROSS SECTIONS ARE GENERATED FROM THE  LINE SHAPE)
  966 FORMAT(55H0 FUNCTION D.E.  D2PSI(THETA,X)/DX2=ETC.                 )
      TAPE ASSIGNMENTS
```

APPENDIX E (continued)

```
      IN=2
      NOUT=3
      WL(1)=9.
      WL(2)=19.
      WL(3)=-5.
      WL(4)=1.
      WRITE OUTPUT TAPENOUT,816
      WRITE OUTPUT TAPE NOUT,950
      WRITE OUTPUT TAPE NOUT,951
      WRITE OUTPUT TAPE NOUT,952
      WRITE OUTPUT TAPE NOUT,953
      WRITE OUTPUT TAPE NOUT,954
      WRITE OUTPUT TAPE NOUT,955
      WRITE OUTPUT TAPE NOUT,956
      WRITE OUTPUT TAPE NOUT,957
      WRITE OUTPUT TAPE NOUT,958
      WRITE OUTPUT TAPE NOUT,959
      WRITE OUTPUT TAPE NOUT,960
      WRITE OUTPUT TAPE NOUT,961
      WRITE OUTPUT TAPE NOUT,962
      WRITE OUTPUT TAPE NOUT,963
      WRITE OUTPUT TAPE NOUT,964
      WRITE OUTPUT TAPE NOUT,965
      WRITE OUTPUT TAPE NOUT,966
  110 NPHAS=0
  510 READ INPUT TAPEIN,813,IPHAS
      IF(IPHAS-1)512,511,512
  512 NPHAS=NPHAS+1
      GO TO 510
  511 IF(NPHAS)513,513,514
  514 WRITE OUTPUT TAPENOUT,825,NPHAS
  513 READ INPUT TAPEIN,1,T,A,B,DX,NPCH,NPEAK,ID
      IF(T)720,721,721
  720 WRITE OUTPUT TAPENOUT,816
      GO TO 730
  721 READ INPUT TAPEIN,2,ZN,MBE,SPBE,MTH,SPTH
      READ INPUT TAPEIN,9,U,ER,GN,GG,GF,GS,I,K,M
      WRITE OUTPUT TAPENOUT,813,IPHAS
      WRITE OUTPUT TAPENOUT,12
      WRITE OUTPUT TAPENOUT,2,ZN,MBE,SPBE,MTH,SPTH
      WRITE OUTPUT TAPENOUT,9,U,ER,GN,GG,GF,GS,I,K,M
      IF(M-MTH)111,112,111
  111 WRITE OUTPUT TAPENOUT,3,M
      GO TO 110
```

APPENDIX E (continued)

```
112 IF(I-17)111,775,111
775 NPCH=NPCH*20
    I50=500
    IPCH=0
    GG=GG+GF
    G=GN+GG
    G2=0.5*G
    SO=(2.60E+6*GS*GN)/(ER*G)
    SCON=GN*SO/G
    ACON=GG*SO/G
    SBE=ZN*SPBE
    SP=SPTH+SBE
    HBE=SBE/SP
    HTH=1.-HBE
    AA(2)=(G*SBE)/(GG*SO)
    AA(1)=SP/SO
    W=MTH
    ABE=MBE
    ATH=(W-1.)/(W+1.)
    ATH=ATH*ATH
    ABE=(ABE-1.)/(ABE+1.)
    ABE=ABE*ABE
    UTH=-LOGF(ATH)
    SITH=1.-ATH*UTH/(1.-ATH)
    IF(MBE-1)14,14,13
 14 UBE=9.999E+5
    SIBE=1.
    KBE=0
    NBE2=0
    GO TO 15
 13 UBE=-LOGF(ABE)
    SIBE=1.-ABE*UBE/(1.-ABE)
    KBE=1
 15 SI=HTH*SITH+HBE*SIBE
    XR=(1.-ATH)*ER/G2
    AA8=G*SPTH/(GN*SO)
    RCON=HTH/SI
    VCON=HBE/SI
    TE=8.62E-5*T
    IF(T)16,16,17
 16 THETA=9.999E+5
    B=0.
    GO TO 18
 17 THETA=G2*SQRTF(W/(ER*TE))
```

APPENDIX E (continued)

```
      IF(THETA-3.)18,18,901
  901 WRITE OUTPUT TAPENOUT,818,THETA
      GO TO 110
   18 TH2=THETA*THETA
      TH4=TH2*TH2*0.25
      THX=1.+2./TH2
      CX=B/THETA
      DU=G2*DX/ER
      N=UTH/DU
      M=N/2
      M=M*2
      IF(N-M)21,22,21
   21 N=N+1
   22 N2=N+2
      W=N
      DU=UTH/W
      DU13=DU*0.33333333
      DU43=DU*1.3333333
      EDU=EXPF(-DU)
      CTH=DU/((1.-ATH)*24.)
      CTH9=CTH*9.
      CBE=DU/((1.-ABE)*24.)
      CBE9=CBE*9.
      IF(KBE)23,23,24
   24 W=UBE/DU
      TRBE=0.
      IF(W-1.E+4)501,501,504
  504 KBE=-1
  502 IF(W-1.E+5)501,501,503
  503 W=W-1.E+5
      TRBE=TRBE+1.E+5
      GO TO 502
  501 NBE=W
      NBE=NBE+1
      NBE2=NBE+2
      D=NBE
      D=D-W
      W1D=D-0.5
      W2D=(D-1.)*D
      W3D=W1D*(W2D+0.5)
      W2D=W2D+0.33333333
      WW(1)=4.*(-2.*W1D+3.*W2D-W3D)
      WW(2)=12.*(2.-W1D-2.*W2D+W3D)
      WW(3)=12.*(2.*W1D+W2D-W3D)
```

APPENDIX E (continued)

```
      WW(4)=4.*(-W1D+W3D)
   23 J=A/DX
      M=J/2
      M=M*2
      IF(J-M)25,26,25
   26 J=J+1
   25 E1=J-1
      E1=E1*DU
      E1=EXPF(E1)
      EM=ER/E1
      E1=ER*E1
      X1=(E1-ER)/G2
      XM=(EM-ER)/G2
      M=2*J-1
      IF(M-10001)27,27,111
   27 WRITE OUTPUT TAPENOUT,4,T,M,N
      WRITE OUTPUT TAPENOUT,5,CX,X1,XM,DX,SI
      LL=-1
      AL=1.
      DO 30 L=1,2
      IAS=0
      CXW=CX
      DU=-DU
      C=DU*(((-DU+4.)*DU-12.)*DU+24.)/(G2*24.)
      E=ER
      X=0.
      DO 31 K=1,J
      I=J+LL*(K-1)
      W=AL*X-CXW
      IF(W)39,38,38
   38 X2=X*X
      VI=1./(1.+X2)
      IF(IAS)770,770,45
  770 VITH2=VI*VI*2./TH2
      W=((3.*X2-1.)+(15.*X2*(X2-2.)+3.)*VITH2)*VITH2
      IF(W-1.E-4)771,772,772
  771 IAS=1
      GO TO 45
  772 VI=VI*(1.+W)
      GO TO 45
   39 IF(K-1)36,36,35
   36 W=THETA*0.5
      W=1./(1.+0.3275911*W)
      ERC=((0.94064607*W-1.2878225)*W+1.2596951)*W
```

```
      ERC=((ERC-0.25212867)*W+0.22583685)*W
      VI=THETA*ERC
      VI1=0.
      GO TO 33
   35 DX2=DX*DX*0.5
      DX3=DX2*DX*0.33333333
      VI=VI+VI1*DX+VI2*DX2+VI3*DX3
      VI1=VI1+VI2*DX+VI3*DX2
   33 W=THX+X*X
      VI2=TH4-TH2*X*VI1-TH4*W*VI
      VI3=-TH2*(X*VI2+VI1)-TH4*(W*VI1+2.*X*VI)
   37 IF(VI)138,138,45
  138 WRITE OUTPUT TAPENOUT,10,X,VI
      CXW=0.
      GO TO 38
   45 V(I)=VI
      DX=-C*E
      X=X+DX
   31 E=E+G2*DX
      LL=1
   30 AL=-1.
      L=3
      DO 40 I=1,2
      L=L-1
      AL=AA(L)
      FJL=0.
      S=1.
      SA=2.
      IE=0
      E=E1
      DO 41 K=1,M
      VI=V(K)
      W=(VI*E)/(VI+AL)
      FJL=FJL+W*S
      IF(K-IE)51,52,53
   53 IE=M-1
      S=4.
      GO TO 41
   52 S=1.
      GO TO 41
   51 S=S-SA
      SA=-SA
   41 E=E*EDU
      FJL=FJL*DU*0.33333333/G
```

```
      VI=SQRTF(1.+1./AL)
      CC(L)=VI
      C1=ATANF(VI/X1)
      CM=ATANF(-VI/XM)
      C1=C1/(AL*VI)
      CM=CM/(AL*VI)
      W=0.5*(C1+CM)
      FJL=FJL+W
      FJ(L)=FJL
      FJLO=1.5707963/(AL*VI)
      FJO(L)=FJLO
      IF(T)700,700,701
  700 PERJ=(1.-FJLO/FJL)*100.
      WRITE OUTPUT TAPENOUT,817,THETA,AL,FJL,PERJ
      GO TO 40
  701 WRITE OUTPUT TAPENOUT,7,THETA,AL,FJL
   40 CONTINUE
      WRITE OUTPUT TAPENOUT,820
      E=E1
      X=X1
      Y=RCON/E1
      Z=VCON/E1
      FIX=0.
      RO=Y*EDU
      R1=RO*EDU
      VO=Z*EDU
      V1=VO*EDU
      IF(J-1)58,58,59
   58 IODD=0
      GO TO 57
   59 IODD=-2
   57 FP1=0.
      SIGN=0.
      IPEAK=0
      P=1.
      IF(ID)161,162,163
  161 ID=-ID
      ID=ID/2
      ID=ID*2+1
      GO TO 160
  162 ID=10001
      GO TO 160
  163 ID=M
  160 DO 60 I=1,ID
```

APPENDIX E (continued)

```
      IPEAK=IPEAK+1
      IODD=IODD+1
      IF(IODD)68,68,167
   68 SAE=ACON*V(I)
      SSE=SCON*V(I)
      STE=SAE+SSE+SP
      HTHE=(SSE+SPTH)/STE
      HBEE=SBE/STE
      GE=SAE/STE
      DEN=1.-CTH9*HTHE-CBE9*HBEE
  167 IF(I-4)61,67,63
   61 IF(I-2)64,65,62
   65 ODD=0.
      YI=19.*R(1)-5.*R0+R1
      ZI=19.*V(1)-5.*V0+V1
      GO TO 66
   62 YI=19.*R(2)-5.*R(1)+R0
      ZI=19.*V(2)-5.*V(1)+V0
      GO TO 66
   67 SIGN=DFP
   63 YI=19.*R(I-1)-5.*R(I-2)+R(I-3)
      ZI=19.*V(I-1)-5.*V(I-2)+V(I-3)
   66 DO 70 K=1,4
      L=I+K-N2
      IF(L)71,71,72
   71 IF(K-1)73,73,74
   73 EL=L-1
      EL=E1*EXPF(-EL*DU)
      RL=RCON/EL
      GO TO 75
   74 RL=RL/EDU
      GO TO 75
   72 RL=R(L)
   75 YI=YI-WL(K)*RL
      L=I+K-NBE2
      IF(KBE)81,70,76
   76 IF(L)81,81,82
   81 IF(K-1)83,83,84
   83 EL=L-1
      EL=EL-TRBE
      EL=E1*EXPF(-EL*DU)
      VL=VCON/EL
      GO TO 85
   84 VL=VL/EDU
```

```
      GO TO 85
   82 VL=V(L)
   85 ZI=ZI-WW(K)*VL
   70 CONTINUE
      YI=YI*CTH
      ZI=ZI*CBE
      Y=Y+YI
      Z=Z+ZI
      FE=(Y +Z )/DEN
      Y =Y +CTH9*HTHE*FE
      Z =Z +CBE9*HBEE*FE
      GO TO 90
   64 FE=1./(SI*E)
   90 FU=E*FE
      IF(IODD)91,92,99
   91 ODD=DU13*GE*FU
      FIX=FIX+ODD
  199 P=1.-FIX
   99 FU=FU*SI
      FP=FU/P
      DFP=FP-FP1
      FP1=FP
      IF(SIGN*DFP)94,101,101
   94 IF(IPEAK-NPEAK)98,97,97
   97 WRITE OUTPUT TAPENOUT,8,X,FP
   98 SIGN=-SIGN
      IPEAK=0
  101 IF(I-IPCH)103,102,102
  102 WRITE OUTPUT TAPENOUT,10,X,FIX,FU,FP,E
   93 IPCH=I+NPCH
  103 IF(I-J+I50)743,744,745
  744 NPCH=NPCH/10
      I50=20001
      GO TO 93
  745 IF(I-J-500)743,746,743
  746 NPCH=NPCH*10
      I50=-20001
      GO TO 93
  743 IF(I-M)69,105,69
  105 IODD=0
      HTHE=HTH
      HBEE=HBE
      DEN=1.-CTH9*HTH-CBE9*HBE
      GO TO 69
```

APPENDIX E (continued)

```
 92 IODD=-2
    FIX=FIX+ODD+DU43*GE*FU
 69 R(I)=HTHE*FE
    V(I)=HBEE*FE
    DX=-C*E
    X=X+DX
    E=E+G2*DX
 60 CONTINUE
    X=X-DX
    E=E-G2*DX
    WRITE OUTPUT TAPENOUT,10,X,FIX,FU,FP,E
    WRITE OUTPUT TAPENOUT,12
    WRITE OUTPUT TAPENOUT,2,ZN,MBE,SPBE,MTH,SPTH
    WRITE OUTPUT TAPENOUT,819,ER,T
    W=GG/(2.*SI*ER)
    C1=C1*W
    CM=CM*W
    W=FIX
    FIX=(C1+CM+FIX)/(1.+CM)
    P=1.-FIX
    PEND=(1.-W/FIX)*100.
    WRITE OUTPUT TAPENOUT,6,P,FIX,PEND
    W=(GG*SO)/ER
    FI0=AA(2)*FJ(2)*W
    FI1=AA(1)*FJ(1)*W
    IF(P)712,712,713
712 FIX=1.E-10
    GO TO 714
713 IF(FIX-1.E-4)716,716,718
716 FIX=SI*SP*FIX
    GO TO 714
718 FIX=-SI*SP*LOGF(P)
714 FMUX=(FI0-FIX)/(FIX-FI1)
    DO 705 L=1,2
705 FKL(L)=((AA(L)-AA8)*FJ0(L)*FJ0(1)*ATANF(XR/(CC(L)+CC(1))))
   1/(XR*AA8*1.5707963)
    W=SBE/SPTH
    FMUM=G*W*FJ0(2)/GG-(W+1./ATH)*FJ0(1)-FKL(2)
    FMUM=FMUM/((1./ATH-1.)*FJ0(1)+FKL(1))
    FIM=(FI0+FMUM*FI1)/(1.+FMUM)
    PERM=(1.-FMUM/FMUX)*100.
    PERI=(1.-FIM/FIX)*100.
    PER0=(1.-FI0/FIX)*100.
    PER1=(1.-FI1/FIX)*100.
```

APPENDIX E (continued)

```
      WRITE OUTPUT TAPENOUT,11,FMUX,FIX,FIO,FI1
      WRITE OUTPUT TAPENOUT,814,FMUM,FIM
      WRITE OUTPUT TAPENOUT,815,PERM,PERI,PERO,PER1
      GO TO 110
  730 CALL EXIT
      END
```

TABLE 1

COMPARISON OF EXACT AND THEORETICAL EFFECTIVE RESONANCE INTEGRALS FOR U238

H and Be, σ_m = 20.2 barns, T = 0 and 900 °K, Γ_γ = 0.025 eV

E_r Γ_n (eV)	Temp. (°K)		H:U = 1:1 μ	I_1 (barns)	I_μ (barns)	I_0 (barns)	Be:U with same scattering μ	I_1 (barns)	I_μ (barns)	I_0 (barns)
6.68	0	exact	0.223	4.78	4.16	4.02	−10.6		4.86	
		theor.	0.051		4.06					
		% error	77	−14.8	2.4	3.3	100	1.6	16.4	17.2
	900		0.200	5.00	4.30	4.16	−12.9		5.07	
		"			4.20					
0.00149			74	−16.3	2.3	3.3	100	1.4	17.2	18.0
21	0		0.294	1.87	1.80	1.78	−1.99		1.95	
		"	0.262		1.80					
			11	−3.7	0.09	1.1	113	4.4	7.9	8.9
	900		0.266	1.98	1.90	1.88	−2.04		2.08	
		"			1.90					
0.009			1.6	−4.2	0.01	1.1	113	4.6	8.5	9.5
36.8	0		0.111	1.18	1.44	1.47	−0.181		1.53	
		"	0.019		1.46					
			83	18.1	−1.6	−2.0	110	23.1	4.5	4.2
	900		0.121	1.22	1.50	1.54	−0.177		1.61	
		"			1.53					
0.0334			84	19.1	−1.9	−2.3	111	24.3	4.7	4.3
66.3	0		0.555	0.448	0.486	0.507	0.187		0.498	
		"	0.337		0.492					
			39	7.9	−1.3	−4.4	−80	10.1	1.1	−1.9
	900		0.555	0.517	0.573	0.603	0.189		0.590	
		"			0.582					
0.0234			39	9.7	−1.6	−5.4	−78	12.3	1.4	−2.3
103	0		0.939	0.289	0.379	0.464	0.834		0.384	
		"	0.554		0.402					
			41	23.9	−5.9	−22.4	34	24.9	−4.5	−20.8
	900		1.04	0.306	0.414	0.527	0.928		0.421	
		"			0.448					
0.066			47	26.1	−8.2	−27.2	40	27.2	−6.6	−25.3
117	0		1.93	0.177	0.181	0.189	1.03		0.183	
		"	1.28		0.182					
			34	2.3	−0.6	−4.3	−25	3.2	0.4	−3.3
	900		1.53	0.266	0.276	0.292	0.769		0.281	
		"			0.278					
0.019			16	3.6	−0.4	−5.6	−67	5.1	1.2	−3.9
192	0		2.22	0.121	0.162	0.253	2.20		0.162	
		"	1.57		0.172					
			29	25.3	−6.4	−56.2	29	25.4	−6.24	−56.0
	900		2.56	0.128	0.177	0.300	2.53		0.177	
		"			0.195					
0.14			39	27.4	−10.5	−70.1	38	27.6	−10.3	−69.8
209	0		3.48	0.0956	0.106	0.140	3.30		0.106	
		"	3.01		0.107					
			14	9.3	−1.1	−32.4	9	9.7	−0.7	−31.9
	900		3.53	0.125	0.144	0.208	3.35		0.144	
		"			0.146					
0.055			15	12.7	−1.7	−44.8	10	13.1	−1.1	−44.0

TABLE 2

COMPARISON OF EXACT AND THEORETICAL EFFECTIVE RESONANCE INTEGRALS FOR U238

H and Be, σ_m = 240 barns, T = 0 °K

E_r (eV)		H : U with same scattering				Be : U = 40 : 1			
		μ	I_1 (barns)	I_μ (barns)	I_0 (barns)	μ	I_1 (barns)	I_μ (barns)	I_0 (barns)
6.68	exact	−0.521	13.68	13.92	13.80	−0.883		14.66	
	theor.	−0.023		13.80					
	% error	96	1.7	0.9	0.9	98	6.6	5.8	5.9
21	,,	0.342	5.35	5.92	6.11	0.082		6.05	
		0.302		5.93					
		12	9.5	−0.3	−3.3	−267	11.6	2.0	−0.9
36.8	,,	0.647	3.39	4.39	5.03	0.553		4.45	
		0.465		4.51					
		28	22.8	−2. 8	−14.8	16	23.9	−1.4	−13. 2
66.3	,,	2.22	1.28	1.42	1.73	2.10		1.43	
		2.04		1.43					
		8	9.8	−0.6	−21.8	3	10.2	−0.2	−21.3
103	,,	2.94	0.825	1.01	1.57	2.94		1.01	
		2.54		1.04					
		14	18.5	−2.1	−54.5	14	18.6	−2.1	−54.5
117	,,	6.49	0.504	0.522	0.639	6.20		0.523	
		6.16		0.523					
		5	3.46	−0.2	−22.5	0.6	3.6	−0.02	−22.3
192	,,	5.96	0.344	0.413	0.822	6.06		0.412	
		5.33		0.420					
		11	16.6	−1.7	−99.0	12	16.4	−1.9	−99.4
209	,,	9.99	0.272	0.289	0.463	10.04		0.289	
		9.48		0.290					
		5	6.0	−0.3	−60.1	6	6.0	−0.3	−60.2

TABLE 3

COMPARISON OF EXACT AND THEORETICAL EFFECTIVE RESONANCE INTEGRALS FOR U238

C, σ_m = 300 barns, T = 300 °K

E_r (eV)	NR (barns)	IR (barns)	exact (barns)	AIR (barns)	IM (barns)
6.68	16.87	17.08	18.46	17.15	17.08
21.0	6.803	7.665	7.909	7.690	7.980
36.8	4.065	5.584	5.492	5.589	6.423
66.3	1.851	2.108	2.128	2.089	2.704
81.2	0.7339	0.7351	0.7386	0.7123	0.7441
0–100	30.323	33.172	34.728	33.230	34.931
102.8	1.046	1.317	1.290	1.308	2.137
116.8	0.9424	0.9847	1.004	0.9634	1.267
145.8	0.1349	0.1350	0.1350	0.1346	0.1349
165.5	0.3685	0.3692	0.3707	0.3603	0.3800
190.5	0.4339	0.5384	0.5269	0.5360	1.141
100–200	2.926	3.344	3.327	3.302	5.060
Totals	33.249	36.516	38.054	36.533	39.991

TABLE 4

COMPARISON OF EXACT AND THEORETICAL EFFECTIVE RESONANCE INTEGRALS FOR U238

C, σ_m = 700 barns, T = 300 °K

E_r (eV)	NR (barns)	IR (barns)	exact (barns)	AIR (barns)	IM (barns)
6.68	26.98	27.54	29.13	27.39	27.63
21.0	11.12	12.35	12.71	12.25	13.22
36.8	6.474	8.425	8.370	8.378	10.40
66.3	3.045	3.322	3.397	3.251	4.349
81.2	0.9123	0.9130	0.9160	0.8979	0.9231
0–100	48.531	52.550	54.523	52.167	56.522
102.8	1.682	1.963	1.976	1.937	3.271
116.8	1.471	1.507	1.540	1.457	1.867
145.8	0.1424	0.1424	0.1425	0.1426	0.1425
165.5	0.4388	0.4391	0.4403	0.4342	0.4475
190.5	0.6813	0.7789	0.7861	0.7735	1.569
100–200	4.416	4.830	4.885	4.744	7.297
Totals	52.947	57.380	59.408	56.911	63.819

TABLE 5

COMPARISON OF EXACT AND THEORETICAL EFFECTIVE RESONANCE INTEGRALS FOR U238

C, σ_m = 1000 barns, T = 300 °K

E_r (eV)	NR (barns)	IR (barns)	exact (barns)	AIR (barns)	IM (barns)
6.68	32.86	33.56	35.24	33.24	33.72
21.0	13.69	15.04	15.49	14.84	16.26
36.8	7.918	10.01	10.02	9.916	12.67
66.3	3.719	3.988	4.093	3.884	5.185
81.2	0.9695	0.9701	0.9726	0.9618	0.9790
0–100	59.157	63.568	65.816	62.842	68.814
102.8	2.049	2.319	2.359	2.282	3.809
116.8	1.724	1.755	1.791	1.695	2.117
145.8	0.1443	0.1443	0.1443	0.1444	0.1444
165.5	0.4599	0.4601	0.4610	0.4575	0.4669
190.5	0.8190	0.9099	0.9264	0.9024	1.735
100–200	5.196	5.588	5.682	5.481	8.272
Totals	64.353	69.156	71.497	68.323	77.086

TABLE 6

U238 IR INTERPOLATION PARAMETER, μ, FOR C, σ_m = 300 – 1000 BARNS, T = 300 °K

E_r (eV)	σ_m (barns)	300	700	1000
6.68	μ exact μ theor.	−0.8652 0.0214	−0.6956 0.1566	−0.6366 0.2220
21.0	,,	0.0644 0.3658	0.3158 0.7003	0.4257 0.8984
36.8	,,	0.6519 0.5519	1.071 1.012	1.261 1.278
66.3	,,	2.078 2.317	2.707 3.704	2.922 4.452
81.2	,,	1.185 7.651	1.913 13.01	2.081 15.28
102.8	,,	3.475 3.022	4.406 4.671	4.669 5.512
116.8	,,	4.274 6.683	4.789 10.04	4.915 11.76
145.8	,,	−1.641 −3.225	1.071 9.574	1.529 13.32
165.5	,,	4.332 17.88	4.893 27.38	5.038 31.58
190.5	,,	6.607 5.770	7.474 8.094	7.534 9.079