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## ABSTRACT

A function $K(\theta, a_1, a_\lambda, x_0^*)$, which occurs in the evaluation of second order approximations to the effective resonance integral, is investigated. Various approximations to this function are given for a range of parameters appropriate to resonance calculations and a description is given of an economic numerical method of evaluating the function accurately.

## CONTENTS

## 1. INTRODUCTION

The conventional form of the effective resonance integral for an isolated resonance at energy $E_r$ of an absorber in an infinite homogeneous mixture may be written in the form:

$$I_r = \int_{E_r^-}^{E_r^+} \sigma_a(E)\ \phi_r(E)\, dE \ , \qquad (1)$$

where $E_r^+$ and $E_r^-$ are respectively the upper and lower bounds of the energy range over which the resonance takes effect, $\sigma_a(E)$ is the microscopic absorption cross section of the absorber at energy E, and $\phi_r(E)$ is the neutron flux per unit energy, normalised to unit source, so that its asymptotic value above the resonance is 1/E. In the vicinity of the resonance, $\phi_r(E)$ is given by the equation:

$$\sigma_t(E)\ \phi_r(E) = \sum_k \int_E^{E/\alpha_k} \frac{\sigma_{pk} + \delta_{0k}\,\sigma_{rs}(E')}{(1-\alpha_k)E'}\ \phi_r(E')\, dE' \ , \qquad (2)$$

where $\sigma_t(E)$ is the total cross section of the mixture per absorber atom, $\sigma_{pk}$ is the potential scattering cross section of the k th constituent of the mixture per absorber atom, $\sigma_{rs}(E)$ is the microscopic resonance scattering cross section of the absorber, and $\alpha_k$ is the minimum fraction of the neutron's energy which may be retained after collision with a nucleus of the k th species. The subscript 0 has been used to specify the absorber and $\delta_{0k}$ is the Kronecker delta.

First order approximations to the normalised flux $\phi_r(E)$ may be written in the form:

$$\phi_{r\lambda}^{(1)}(E) = \frac{\sigma_{p\lambda}}{E\{\sigma_a(E) + \sigma_{s\lambda}(E)\}} \ , \qquad (3)$$

where $\sigma_{p\lambda} = \sum_k \lambda_k\, \sigma_{pk}$

and $\sigma_{s\lambda}(E) = \sigma_{p\lambda} + \lambda_0 \sigma_{rs}(E)$ ,

$\lambda_k$ being parameters such that $0 \leqslant \lambda_k \leqslant 1$. Equation 3 gives the first order narrow-resonance (NR) approximation to the flux if all the $\lambda_k$ are put equal to unity, and the first order infinite-mass (IM) approximation if $\lambda_0$ is equated to zero and all the other $\lambda_k$ are equated to unity.

The intermediate-resonance (IR) approximation proposed by Goldstein and Cohen (1962) is also given by Equation 3 if all the $\lambda_k$ except $\lambda_0$ are put equal to unity and $\lambda_0$ is determined from the transcendental equation:

$$\lambda_k = 1 - \frac{\alpha_k}{x_k^*}(c_1 + c_\lambda)\ \text{artan}\ \frac{x_k^*}{c_1 + \alpha_k c_\lambda} \ , \qquad (4)$$

where $x_k^* = \frac{2E_r}{\Gamma}(1-\alpha_k)$

and $c_\nu = (1 + \frac{1}{a_\nu})^{\frac{1}{2}}$ , $\quad (\nu = 1, \lambda)$

with $a_1 = \frac{\sigma_p}{\sigma_0}$

and $a_\lambda = \frac{\sigma_{p\lambda}\,\Gamma}{\sigma_0(\Gamma_\gamma + \lambda_0 \Gamma_n)}$ ,

$\sigma_0$ being the peak microscopic resonance cross section for absorption plus resonance scattering, $\sigma_p$ the potential scattering cross section of the mixture per absorber atom, $\Gamma_\gamma$ and $\Gamma_n$ respectively the radiation and neutron partial widths of the resonance, and $\Gamma$ the total level width. In the generalisation of the IR approximation suggested by Hill and Schaefer (1962) each of the $\lambda_k$ is determined from Equation 4.

Both the Goldstein–Cohen IR approximation and the Hill–Schaefer generalised version of it involve interpolation parameters which are appropriate to effective resonance integrals evaluated with unbroadened cross sections corresponding to absolute zero temperature. However, it has been shown by McKay and Pollard (1963) that, while the neglect of temperature dependence in the interpolation parameter leads to an error of no more than about two per cent. in very concentrated mixtures, this error increases considerably for dilute mixtures.

To take account of the effect of temperature variation on the interpolation parameters, it is necessary to evaluate second order effective resonance integrals involving Doppler–broadened cross sections. These result from insertion into Equation 1 of the second order approximations to the flux which may be obtained from Equation 2 by iteration, using the first order flux given by Equation 3.

Neglecting interference scattering and the variation in the reciprocal of the energy over a resonance, we get, for the second order effective resonance integral:

$$I_{r\lambda}^{(2)} = \frac{\Gamma_\gamma [1 + (1-\alpha_0)\sigma_{p0}]}{2\alpha_0 E_r} J(\theta, a_1) + \frac{\Gamma_\gamma \sigma_{p0}(a_\gamma - a_\infty)}{2E_r x_0^* a_\infty} K(\theta, a_1, a_\lambda, x_0^*), \qquad (5a)$$

where $$J(\theta, a_1) = \int_{-\infty}^{\infty} \frac{\psi(\theta,x)}{a_1 + \psi(\theta,x)}\, dx \quad ; \qquad (5b)$$

$$K(\theta, a_1, a_\lambda, x_0^*) = \int_{-\infty}^{\infty} \frac{\psi(\theta,x)}{a_1 + \psi(\theta,x)} \int_{x}^{\frac{x+x_0^*}{\alpha_0}} \frac{\psi(\theta,x')}{a_\lambda + \psi(\theta,x')}\, dx'\, dx, \qquad (5c)$$

and $$a_\infty = \frac{\Gamma \sigma_{p0}}{\Gamma_n \sigma_0} \quad .$$

In the expressions for $J(\theta, a_1)$ and $K(\theta, a_1, a_\lambda, x_0^*)$, $\psi(\theta,x)$ is the well–known line–shape function, given by:

$$\psi(\theta,x) = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp[-\frac{1}{4}\theta^2(x-y)^2]}{1+y^2}\, dy \quad , \qquad (6)$$

where $$\theta = \frac{1}{2}\Gamma \sqrt{\frac{A}{kTE_r}} \quad ,$$

A being the atomic mass of the absorber, k Boltzmann's constant, and T the temperature on the Kelvin scale.

With the aid of the rational approximation, the second order effective resonance integral for a lattice may also be expressed in terms of the functions J and K, as may be seen by inserting Doppler–broadened cross sections into the formulae given by McKay and Schaefer (1961). It has also been shown by Keane (1964) that effective resonance integrals for granular fuel embedded in a moderator may be reduced to the same form.

The function $J(\theta,a_\nu)$, which occurs also in first order effective resonance integrals, has been studied by many authors (for example Roe 1954; Dresner 1956, 1960), and several computer programmes are available for its accurate and approximate evaluation (for example Bell, Buckler, and Pull 1963; Doherty 1963). In this report the function $K(\theta,a_1,a_\lambda,x_0^*)$ and some approximations to it are studied in some detail, and a description is given of a numerical method of evaluating K that is both accurate and economic of computer time.

## 2. ANALYTIC APPROXIMATIONS TO THE FUNCTION K

### 2.1 Zero Temperature Evaluation

Exact analytic evaluation of $K(\theta,a_1,a_\lambda,x_0^*)$ is only possible for absolute zero temperature, when $\theta$ becomes infinite, giving

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

$$J(\infty,a_\nu) = \frac{\pi}{2a_\nu c_\nu} ,$$

and
$$K(\infty,a_1,a_\lambda,x_0^*) = \frac{\pi}{a_1 a_\lambda c_1 c_\lambda} \operatorname{artan} \frac{x_0^* \sqrt{a_1 a_\lambda}}{a_\lambda c_1 + \alpha_0 a_1 c_\lambda} , \tag{7}$$

### 2.2 Approximation for $a_\nu << \theta$

If $a_1$ and $a_\lambda$ are small compared with $\theta$, the integrand of K is approximately unity for small values of x and x', so that we may use the asymptotic expansion:

$$\psi(x,\theta) = \frac{1}{1+x^2} + \frac{6x^2-2}{\theta^2(1+x^2)^3} + \ldots , \tag{8a}$$

which, for large x, reduces to:

$$\psi(x,\theta) \simeq \frac{\theta^2 x^2 + 6}{\theta^2 x^4} . \tag{8b}$$

Under the stated conditions this approximation may be used to give

$$K(\theta,a_1,a_\lambda,x_0^*) \simeq \sum_{j=0}^{1} \sum_{k=0}^{1} A_{1j} A_{\lambda k} \operatorname{artan} \frac{x_0^*}{B_{1j} + \alpha_0 B_{\lambda k}} , \tag{9}$$

where
$$A_{\nu j} = \frac{1}{4a_\nu B_{\nu j}} \left[ 2 + (-1)^j \left( D_\nu + \frac{1}{D_\nu} \right) \right]$$

and
$$B_{\nu j} = \left[ \frac{1 + (-1)^j D_\nu}{2a_\nu} \right]^{\frac{1}{2}} ,$$

with
$$D_\nu = \left( 1 - \frac{24\, a_\nu}{\theta^2} \right)^{\frac{1}{2}} .$$

As the temperature approaches absolute zero, $D_\nu$ approaches unity, so that (9) reduces to:

$$\frac{\pi}{\sqrt{a_1 a_\lambda}} \operatorname{artan} \frac{x_0^* \sqrt{a_1 a_\lambda}}{\sqrt{a_\lambda} + \alpha_0 \sqrt{a_1}} ,$$

which is a good approximation for $K(\infty, a_1, a_\lambda, x_0)$ when $a_1$ and $a_\lambda$ are both very small.

### 2.3 Further Approximations for Small Values of $a_\nu$

It is easy to see that, if $a_\lambda << a_1 << 1$,

$$K(\theta,a_1,a_\lambda,x_0^*) \simeq K(\theta,a_1,0,x_0^*)$$

$$= \frac{2x_0^*}{\alpha_0} J(\theta,a_1) \quad . \tag{10}$$

However, the operation of the above condition is restricted to strongly absorbing resonances with $\Gamma_\gamma >> \Gamma_n$ in very concentrated mixtures. Since it is more usual in practical circumstances that $a_1 < a_\lambda$, the result corresponding to (10) for $a_1 << a_\lambda << 1$ is of more interest. By changing the order of integration we see that, with this condition,

$$K(\theta,a_1,a_\lambda,x_0^*) \simeq K(\theta,0,a_\lambda,x_0^*)$$

$$= \frac{2x_0^*}{\alpha_0} J(\theta,a_\lambda) \, . \tag{11}$$

### 2.4 Approximations for Large and Small $x_0^*$ Respectively

For large $x_0^*$ it may be seen that

$$K(\theta,a_1,a_\lambda,x_0^*) \simeq K(\theta,a_1,a_\lambda,\infty)$$

$$= 2J(\theta,a_1) J(\theta,a_\lambda) \quad . \tag{12}$$

On the other hand, for small $x_0^*$, we find that, provided $a_1 \neq a_\lambda$,

$$K(\theta,a_1,a_\lambda,x_0^*) \simeq \frac{2x_0^*}{\alpha_0(a_\lambda - a_1)} [a_\lambda J(\theta,a_\lambda) - a_1 J(\theta,a_1)] \quad , \tag{13}$$

which reduces to (10) or (11) under the appropriate conditions.

If $a_\lambda = a_1$, we get, for small $x_0^*$,

$$K(\theta,a_1,a_1,x_0^*) = \frac{2x_0^*}{\alpha_0} J_2(\theta,a_1) \quad , \tag{14}$$

where $$J_2(\theta,a_1) = \int_0^\infty \left[\frac{\psi(x,\theta)}{a_1 + \psi(x,\theta)}\right]^2 dx \quad .$$

The function $J_2(\theta,a_1)$, which also occurs elsewhere in the theory of resonance absorption, may be evaluated approximately under certain conditions as indicated below.

#### 2.4.1 The function $J_2(\theta,a_1)$

In the case of absolute zero temperature an exact analytic evaluation of $J_2(\theta,a_1)$ may be obtained, namely:

$$J'_2(\infty,a_1) = \frac{\pi}{4a_1c_1(1 + a_1)} \quad . \tag{15}$$

At working temperatures, the following approximations hold for the stated conditions.

(i) $a_1 > \psi(0,\theta)$:

$$J_2(\theta,a_1) = \frac{1}{2} \sum_{k=0}^{\infty} (-1)^k (k+1) a_1^{-k-2} \psi_{k+2}(\theta) \quad , \tag{16}$$

where $\psi_n(\theta) = \int_{\infty}^{\infty} [\psi(x,\theta)]^n dx.$

$\psi_n(\theta)$ may be evaluated quite accurately for $\theta \ll 1$ by the approximation given by McKay (1965), namely:

$$\psi_n(\theta) \simeq \frac{1}{\sqrt{n}} \left[\frac{\theta}{2\sqrt{\pi}}\right]^{n-1} A_n^n \left[1 + \binom{n}{2} \frac{\theta^4}{8n^2} \left(\frac{B_n}{A_n}\right)^2 + \binom{n}{3} \frac{\theta^6}{8n^3} \left(\frac{B_n}{A_n}\right)^3\right] \quad , \tag{17}$$

where $A_n = \exp\left[\frac{1}{4} \theta^2 \left(\frac{n-1}{n}\right)\right] \operatorname{erfc}\left[\frac{1}{2} \theta \left(\frac{n-1}{n}\right)^{\frac{1}{2}}\right]$

and $B_n = \frac{2}{\theta} \left(\frac{n\pi}{n-1}\right)^{\frac{1}{2}} - A_n \quad .$

Provided $a_1$ is greater than about 0.5, only a few terms of the expansion (16) need be taken to give a good approximation to $J_2(\theta,a_1)$.

(ii) $\theta << 1$ and $a_1 > \frac{1}{2}\sqrt{\pi\theta}$:

$$J_2(\theta,a_1) \simeq \frac{\pi}{2a_1} \sum_{k=0}^{\infty} (-1)^k \frac{k+1}{\sqrt{n+k}} \theta^{*n+k-1} \quad , \tag{18}$$

where $\theta^* = \frac{\sqrt{\pi\theta}}{2a_1} \quad .$

(iii) $\theta << 1$ and $a_1 \simeq \frac{1}{2}\sqrt{\pi\theta}$:

$$J_2(\theta,a_1) \simeq \frac{\pi}{2a_1} \sum_{k=0}^{\infty} \sum_{j=0}^{k} (-1)^j \binom{k}{k-j} \frac{j+1}{\sqrt{j+2}} \left[\frac{\theta^*}{1+\theta^*}\right]^{k+1} \quad . \tag{19}$$

(iv) $6a_1 << \theta^2$ :

$$J_2(\theta,a_1) \simeq 2\,J(\theta,a_1) - \frac{3\pi}{4\sqrt{a_1}} \left(1 + \frac{a_1}{\theta^2}\right) \quad . \tag{20}$$

The above approximations are special cases of the more general results given for $J_n(\theta,a)$ by McKay (1964).

## 2.5 An Approximation for K with Wide Validity

For values of the parameters relevant to the resonances of the fertile nuclei $Th^{232}$, $U^{238}$, and $Pu^{240}$ under practical conditions, it has been found that the function $K(\theta,a_1,a_\lambda,x_0^*)$ is given within a few per cent. by the formula:

$$K(\theta,a_1,a_\lambda,x_0^*) \simeq L(\theta,a_1,a_\lambda,x_0^*) \quad , \tag{21a}$$

where

$$L(\theta,a_1,a_\lambda,x_0^*) = \frac{4}{\pi} J(\theta,a_1)\, J(\theta,a_\lambda) \arctan \frac{x_0^* \sqrt{a_1 a_\lambda}}{a_\lambda c_1 + \alpha_0 a_1 c_\lambda} \quad . \tag{21b}$$

It should be noted that this approximation becomes exact in the limit as $\theta$ tends to infinity and also in the limit as $x_0^*$ tends to infinity.

To demonstrate the extraordinarily wide range of validity of the approximation (21), we present in Table 1 values of the ratio

$$r(\theta,a_1,a_\lambda,x_0^*) = K(\theta,a_1,a_\lambda,x_0^*)\Big/L(\theta,a_1,a_\lambda,x_0^*) \qquad (22)$$

for values of $a_1$ and $a_\lambda$ ranging from 0.001 to 0.1, values of $\theta$ ranging from 0.05 to 1.0, and values of $x_0^*$ ranging from 5 to 200, with $\alpha_0$ having a value appropriate to the fertile nuclei. Details of the method used for the evaluation of the functions $J(\theta,a_1)$ and $K(\theta,a_1,a_\lambda,x_0^*)$ are given in Section 3.

It may be seen that approximation (21) gives reasonable accuracy for the whole range of values considered, except when both $x_0^*$ and $\theta$ are small, which very rarely occurs in practice. For better accuracy we may write:

$$K(\theta,a_1,a_\lambda,x_0^*) = r(\theta,a_1,a_\lambda,x_0^*)\, L(\theta,a_1,a_\lambda,x_0^*) \qquad (23)$$

where values of $r(\theta,a_1,a_\lambda,x_0^*)$ may be obtained from Table 1 or from the empirical formula:

$$r(\theta,a_1,a_\lambda,x_0^*) \simeq 1 + 0.004 \ln\left(\tfrac{1}{2} a_1 a_\lambda\right) \ln\left\{\tfrac{1}{2}(\theta + \theta^{0.4})\right\} \exp(-0.02\, x_0^*\, \theta) \ . \qquad (24)$$

This approximation involves an error of less than 4 per cent. for $x_0^*\,\theta \geq 4$, with a mean absolute error of about ¾ per cent. for the tabulated values in this range.

## 3. NUMERICAL EVALUATION OF $K(\theta,a_1,a_\lambda,x_0^*)$

The evaluation of the K-function (Equation 5c) may be considered in two parts: the generation of the line shape function $\psi(\theta,x)$ (Equation 6) and the actual evaluation of K. In addition the J-function (Equation 5b) is required in the evaluation of second order effective resonance integrals and the ratio function, r (Equation 22). The r-function provides a convenient method for presentation of results of this work (Table 1) as it is only a slowly varying function of its parameters. Details of the numerical analysis are given, following McKay and Pollard (1963), finer points of the method being discussed in this work.

In order to make the computation more manageable, and without any loss in accuracy in practical resonance studies, we may set $\alpha_o = 1$ in the upper limit of the integral defining K. This simplification has been adopted in all numerical studies in this report. The equation defining K thus becomes

$$K(\theta,a_1,a_\lambda,x_0^*) = \int_{-\infty}^{\infty} \frac{\psi(\theta,x)}{a_1 + \psi(\theta,x)} \int_x^{x+x_0^*} \frac{\psi(\theta,x')}{a_\lambda + \psi(\theta,x')}\, dx'\, dx \ . \qquad (25)$$

### 3.1 Generation of $\psi(\theta,x)$

The generation of the line shape function may be divided into two parts: the initial conditions and the solving of the differential equation which the line shape satisfies.

#### 3.1.1 Initial conditions

The initial conditions necessary for the solution of the differential equation given in the next sub-section may be obtained directly from the integral representation of $\psi(\theta,x)$ given as Equation 6. We obtain

$$\psi(\theta,0) = \theta \operatorname{erc} \theta/2$$

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

where $\operatorname{erc} z = \exp(z^2) \int_z^\infty \exp(-t^2)\, dt$

$$= \frac{1}{2} \sqrt{\pi} \exp(z^2) \operatorname{erfc} z \quad .$$

An approximation for erc z may be obtained from Hastings (1955 p.169) and Clenshaw (1962 p.28). This approximation covers the full range of positive z giving a result which has better than 4 figures accuracy. In this work z is never greater than 0.5, but for completeness both approximations are given. We have:

$$\operatorname{erc} z = q \sum_{k=1}^{5} a_k u^{k-1} .$$

For $z \leqslant 2.6$ ,

$q = 3.0525860/(3.0525860 + z)$

$u = q$

$a_1 = 0.22583685$

$a_2 = -0.25212867$

$a_3 = 1.2596951$

$a_4 = -1.2878225$

$a_5 = 0.94064607$ ,

and for $z > 2.6$ ,

$q = 1/z$

$u = 32\, q^2$

$a_1 = 0.5$

$a_2 = -7.8121744 \times 10^{-3}$

$a_3 = 3.6484547 \times 10^{-4}$

$a_4 = -2.6537167 \times 10^{-5}$

$a_5 = 1.7325337 \times 10^{-6}$ .

### 3.1.2 Solution of the differential equation

A very convenient method for calculating the line shape function when the function is required for a range of values is to employ the differential equation

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

$$= f_2(\theta,x) \quad ,$$

and its derivative

$$\psi'''(\theta,x) = -\theta^2 x \psi''(\theta,x) - \frac{1}{4}\theta^2(6 + \theta^2 + \theta^2 x^2)\psi'(\theta,x) - \frac{1}{2}\theta^4 x \psi(\theta,x)$$

$$= f_3(\theta,x) \quad ,$$

in a Taylor's series expansion connecting one step with the next. The initial conditions (Section 3.1.1) provide the starting point.

The infinite range of integration required for the evaluation of J and K is split into five regions consistent with the needs of these integrals. The five regions are (i) $-\infty < x \leqslant -d$, (ii) $-d \leqslant x \leqslant 0$, (iii) $0 \leqslant x \leqslant d$, (iv) $d \leqslant x \leqslant d + x_0^*$, and (v) $d + x_0^* \leqslant x < \infty$. The line shape function is only evaluated numerically by solving the differential equation for regions (ii) to (iv) and then only for $|x| < 12/\theta$ as we may use the asymptotic expansion (Equation 8a):

$$\psi(\theta,x) = \frac{1}{1+x^2}\left\{1 + \frac{2(3x^2-1)}{\theta^2(1+x^2)^2}\right\}$$

$$= \frac{1}{1+x^2}\, f_0(\theta,x) \quad , \tag{26}$$

for $|x| \geqslant 12/\theta$. In order to simplify analysis in obtaining end corrections to J and K for regions (i), (iv), and (v), the above formula is used in these regions with $f_0(\theta,x) = 1$.

A constant step length, h, is chosen to divide region (ii) exactly into an even number of steps j and region (iv) exactly into an even number of steps in n; d must be chosen to make this possible.

Using a subscript to denote the value of parameters at a certain step i, such that i = 1 corresponds to x = -d and increasing i implies increasing x, the initial conditions may be written:

$$x_{j+1} = 0$$

$$\psi_{j+1} = \theta \operatorname{erc} \theta/2$$

$$\psi'_{j+1} = 0$$

$$\psi''_{j+1} = f_2(\theta,x_{j+1})$$

$$\psi'''_{j+1} = f_3(\theta,x_{j+1}) \quad .$$

The calculation is then carried out for increasing x using the following algorithms.

For $j + 1 < i \leqslant 2j + 1 + n$

$$x_i = x_{i-1} + h \quad ,$$

if $x_i < 12/\theta$ ,

$$\psi_i = \psi_{i-1} + h\psi'_{i-1} + \frac{1}{2} h^2 \psi''_{i-1} + \frac{1}{6} h^3 \psi'''_{i-1}$$

$$\psi'_i = \psi'_{i-1} + h\psi''_{i-1} + \frac{1}{2} h^2 \psi'''_{i-1}$$

$$\psi''_i = f_2(\theta,x_i)$$

$$\psi'''_i = f_3(\theta,x_i) \quad ,$$

or, if $x_i \geqslant 12/\theta$ ,

$$\psi_i = \frac{1}{1+x_i^2}\, f_0(\theta,x_i) \quad .$$

Symmetry of the line shape function,

$$\psi(\theta,-x) = \psi(\theta,x) \quad ,$$

is used to provide the values of the function for region (ii). The required algorithm is simply:

for $1 \leqslant i \leqslant j$ ,

$$\psi_i = \psi_{2j+2-i} \ .$$

3.2 Evaluation of Integrals J and K

In this section we consider the evaluation of three integrals $J(\theta,a_1)$, $J(\theta,a_\lambda)$, and $K(\theta,a_1,a_\lambda,x_0^*)$. These integrals may be written in terms of the following four functions:

$$w(\theta,x,a_\nu) = \frac{\psi(\theta,x)}{a_\nu + \psi(\theta,x)} \quad , \quad (\nu = 1 \text{ and } \lambda) \quad , \tag{27}$$

$$s(\theta,x,a_\lambda,x_0^*) = \int_x^{x+x_0^*} w(\theta,x',a_\lambda)\, dx' \quad , \tag{28}$$

$$J(\theta,a\,;d) = \int_0^d w(\theta,x,a_\nu)\, dx \quad , \tag{29}$$

$$K(\theta,a_1,a_\lambda,x_0^*;d) = \int_{-d}^{d} w(\theta,x,a_1)\, s(\theta,x,a_\lambda,x_0^*)\, dx \quad . \tag{30}$$

Then

$$J(\theta,a_\nu) = J(\theta,a_\nu;\infty)$$

$$= J(\theta,a_\nu\,;d) + \{J(\theta,a_\nu;\infty) - J(\theta,a_\nu;d)\} \quad , \tag{31}$$

and

$$K(\theta,a_1,a_\lambda,x_0^*) = K(\theta,a_1,a_\lambda,x_0^*;\infty)$$

$$= K(\theta,a_1,a_\lambda,x_0^*;d) + \{K(\theta,a_1,a_\lambda x_0^*;\infty) - K(\theta,a_1,a_\lambda,x_0^*;d)\} \ . \tag{32}$$

The evaluation of the infinite range integrals is thus decomposed into two parts: the numerical integration over the finite range (regions (ii) and (iii) ) and the estimation of end corrections, given above in braces { }, based on asymptotic properties of the integrands.

3.2.1 End corrections

Based on the asymptotic formula for the line shape function (Equation 26 with $f_0 = 1$), which is equivalent to the situation when $\theta$ is infinite for the full range of x , Equation 27 becomes:

$$w(\infty,x,a_\nu) = 1/a_\nu\,(x^2 + c_\nu^2) \quad , \tag{33}$$

where $c_\nu$ is given by Equation 4. Hence we obtain

$$\{J(\theta,a_\nu\,;\infty) - J(\theta,a_\nu\,;d)\} = \int_d^\infty w(\infty,x,a_\nu)\, dx$$

$$= \frac{1}{a_\nu c_\nu}\left(\frac{\pi}{2} - \tan^{-1}\frac{d}{c_\nu}\right) \ . \tag{34}$$

The asymptotic Equation 33 also simplifies considerably the expression for $s(\theta,x,a_\lambda,x_0^*)$, Equation 28, which becomes:

$$s(\infty,x,a_\lambda,x_0^*) = \frac{1}{a_\lambda c_\lambda}\left[\tan^{-1}\left(\frac{x+x_0^*}{c_\lambda}\right) - \tan^{-1}\left(\frac{x}{c_\lambda}\right)\right] .$$

If $x/c_\lambda$ is large we may use the expansion of the inverse tangents,

$$\tan^{-1}y = \frac{\pi}{2}\frac{y}{|y|} - \frac{1}{y} ,$$

to give $s(\infty,x,a_\lambda,x_0^*) = x_0^*/a_\lambda x(x+x_0^*)$ ,

which is valid for either positive or negative $x$, provided $|x| > x_0^*$. From this it follows that $d$ in the equation to follow must also be greater than $x_0^*$. The end correction for the K–function then becomes:

$$\{K(\theta,a_1,a_\lambda,x_0^*;\infty) - K(\theta,a_1,a_\lambda,x_0^*;d)\} = \left(\int_{-\infty}^{-d} + \int_d^{\infty}\right) w(\infty,x,a_1)\, s(\infty,x,a_\lambda,x_0^*)\, dx$$

$$= \frac{x_0^*}{a_1 a_\lambda}\left(\int_{-\infty}^{-d} + \int_d^{\infty}\right) \frac{dx}{x(x+x_0^*)(x^2+c_1^2)} .$$

Carrying out the integration, we obtain:

$$K(\theta,a_1,a_\lambda,x_0^*;\infty) - K(\theta,a_1,a_\lambda,x_0^*;d) = \frac{1}{a_1 a_\lambda (x_0^{*2}+c_1^2)}\left[\ln\left(\frac{d+x_0^*}{d-x_0^*}\right) - \frac{2x_0^*}{c_1}\left(\frac{\pi}{2} - \tan^{-1}\frac{d}{c_1}\right)\right] \quad (35)$$

$$\simeq 2x_0^*/3a_1 a_\lambda d^3 .$$

Equation 35 is used, rather than the above approximation, when applied in practice.

3.2.2 Numerical integration

All numerical integration is carried out to the accuracy of Simpson's rule. If we write

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

then Simpson's integration rule enables the J–function of Equation 29 to be simply calculated thus:

$$J(\theta,a_\nu;d) = h\sum_{i=1}^{j+1} S_i\, w(\theta,x_i,a_\nu) . \quad (36)$$

Similarly we may calculate the quantities given by Equations 28 and 30 :

$$s(\theta,x_i,a_\lambda,x_0^*) = h\sum_{k=i}^{i+n} S_k\, w(\theta,x_k,a_\lambda) \quad (37)$$

and $$K(\theta,a_1,a_\lambda,x_0^*;d) = h\sum_{i=1}^{2j+1} S_i\, w(\theta,x_i,a_1)\, s(\theta,x_i,a_\lambda,x_0^*) . \quad (38)$$

We may greatly speed up the calculation if we use Equation 37 only for $i = 1$, as we may obtain a simple algorithm for $i > 1$ which uses the fact that the function $s$ is always integrated over a range of constant width $x_0^*$ ($x \leqslant x' \leqslant x + x_0^*$), with an integrand which is not dependent on the other outer variable of integration, $x$.

Provided $i>1$ we may obtain from Equation 28 the result:

$$s(\theta,x_i,a_\lambda,x_0^*) - s(\theta,x_{i-1},a_\lambda,x_0^*) = \left( \int_{x_{i-1}+x_0^*}^{x_i+x_0^*} - \int_{x_{i-1}}^{x_i} \right) w(\theta,x',a_\lambda)\, dx' \quad .$$

To achieve the same order of accuracy as Simpson's rule we calculate this integral by a method based on fitting cubic polynomials to the integrand at each end of the range which passes through the points $i+n-3$, $i+n-2$, $i+n-1$, $i+n$, and $i-1$, $i$, $i+1$, $i+2$. We obtain the result:

$$s(\theta,x_i,a_\lambda,x_0) = s(\theta,x_{i-1},a_\lambda,x_0) + h \sum_{k=1}^{4} C_k [w(\theta,x_{i+n+1-k},a_\lambda) - w(\theta,x_{i-2+k},a_\lambda)] \quad , \qquad (39)$$

where $(C_k) = \frac{1}{24}(9,19,-5,1)$ .

### 3.2.3 Resultant integrals

Using the results obtained from numerical integration (Equations 36 and 38), and the end corrections (Equation 34 and 35), the infinite range integrals (Equation 31 and 32) are obtained. The ratio function, r, is then calculated using the defining Equation 22. It is possible to test the validity of the end corrections and the integration rule, as the resultant integrals should be reasonably insensitive to change in d and h provided d is reasonably large, say $\simeq 250$, and h is reasonably small, say $\simeq 0.25$.

### 3.2.4 Actual calculation

The calculation procedure was coded in FORTRAN for an IBM 1620 computer and took about 10 minutes for each calculation. The line shape function and J–function were compared with selected values obtained from the subroutines by Bell et al. (1963). Both functions had less than 0.1 per cent. error when compared in this fashion. The K–function was checked in the limits $\theta \to \infty$ and $x_0^* \to \infty$ and was found to differ by less than $\frac{1}{2}$ per cent. from the analytic result, Equation 21.

The table of the function $r(\theta,a_1,a_\lambda,x_0^*)$, Table 1, was prepared, taking advantage of the symmetry in $a_1$ and $a_\lambda$ to save computational time. Regeneration of the line shape function was also avoided by carrying out a series of runs at constant $\theta$.

## 4. CONCLUDING REMARKS

Inspection of Table 1 shows the accuracy of the approximation (21a) for a wide range of values of the parameters, the error involved being only a few per cent. for the values of the parameters appropriate to most resonances under practical conditions. In general this error may be reduced by using approximation (24) in Equation 23 provided $x_0^*\theta \geqslant 4$. This criterion is satisfied for virtually all the entries in Table 1 between the bold lines, which are relevant for the resonances of the fertile nuclei $Th^{232}$, $U^{238}$, and $Pu^{240}$. In fact, for most resonances under practical conditions the product $x_0^*\theta$ is considerably greater than 4. Thus, since the accuracy of approximation (24) improves as $x_0^*\theta$ increases, Equation 23 used with this approximation generally gives $K(\theta,a_1,a_\lambda,x_0^*)$ very accurately. For greater accuracy, values of r for use in Equation 23 may be obtained from Table 1 by interpolation.

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## TABLE 1

THE FUNCTION $r(\theta, a_1, a_\lambda, x_0^*) = K(\theta, a_1, a_\lambda, x_0^*) / L(\theta, a_1, a_\lambda, x_0^*)$

Entries for fertile resonance data predominantly fall between bold lines

| $x_0^*$ | $a_\lambda$ \ $a_1$ | $\theta$ = 0.05 | | | $\theta$ = 0.1 | | | $\theta$ = 0.2 | | | $\theta$ = 0.5 | | | $\theta$ = 1.0 | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 0.001 | 0.01 | 0.1 | 0.001 | 0.01 | 0.1 | 0.001 | 0.01 | 0.1 | 0.001 | 0.01 | 0.1 | 0.001 | 0.01 | 0.1 |
| 5 | 0.001 | | | | | | | 1.05 | 1.04 | 0.98 | 1.01 | 1.02 | 1.01 | 1.00 | 1.00 | 1.01 |
| | 0.01 | | | | | | | 1.04 | 0.96 | 0.82 | 1.02 | 1.03 | 1.00 | 1.00 | 1.01 | 1.01 |
| | 0.1 | | | | | | | 0.98 | 0.82 | 0.64 | 1.01 | 1.00 | 0.94 | 1.01 | 1.01 | 1.01 |
| 20 | 0.001 | | | | 1.05 | 0.97 | 0.90 | 1.05 | 1.05 | 1.02 | 1.01 | 1.02 | 1.02 | 1.00 | 1.00 | 1.01 |
| | 0.01 | | | | 0.97 | 0.83 | 0.76 | 1.05 | 1.04 | 1.01 | 1.02 | 1.04 | 1.04 | 1.00 | 1.01 | 1.01 |
| | 0.1 | | | | 0.90 | 0.76 | 0.72 | 1.02 | 1.01 | 0.99 | 1.02 | 1.04 | 1.04 | 1.01 | 1.01 | 1.02 |
| 50 | 0.001 | 0.93 | 0.85 | 0.82 | 1.08 | 1.06 | 1.04 | 1.05 | 1.06 | 1.04 | 1.01 | 1.01 | 1.01 | 1.00 | 1.00 | 1.00 |
| | 0.01 | 0.85 | 0.79 | 0.79 | 1.06 | 1.05 | 1.04 | 1.06 | 1.07 | 1.05 | 1.01 | 1.02 | 1.02 | 1.00 | 1.00 | 1.01 |
| | 0.1 | 0.82 | 0.79 | 0.80 | 1.04 | 1.04 | 1.02 | 1.04 | 1.05 | 1.04 | 1.01 | 1.02 | 1.02 | 1.00 | 1.01 | 1.01 |
| 100 | 0.001 | 1.06 | 1.04 | 1.04 | 1.09 | 1.08 | 1.06 | 1.03 | 1.04 | 1.02 | 1.01 | 1.01 | 1.01 | 1.00 | 1.00 | 1.00 |
| | 0.01 | 1.04 | 1.03 | 1.02 | 1.08 | 1.07 | 1.04 | 1.04 | 1.04 | 1.03 | 1.01 | 1.01 | 1.01 | 1.00 | 1.00 | 1.00 |
| | 0.1 | 1.04 | 1.02 | 1.00 | 1.06 | 1.04 | 1.02 | 1.02 | 1.03 | 1.02 | 1.01 | 1.01 | 1.01 | 1.00 | 1.00 | 1.00 |
| 150 | 0.001 | 1.11 | 1.08 | 1.07 | 1.06 | 1.05 | 1.04 | 1.02 | 1.02 | 1.02 | 1.00 | 1.01 | 1.01 | 1.00 | 1.00 | 1.00 |
| | 0.01 | 1.08 | 1.06 | 1.04 | 1.05 | 1.04 | 1.03 | 1.02 | 1.03 | 1.02 | 1.01 | 1.01 | 1.01 | 1.00 | 1.00 | 1.00 |
| | 0.1 | 1.07 | 1.04 | 1.02 | 1.04 | 1.03 | 1.02 | 1.02 | 1.02 | 1.01 | 1.01 | 1.01 | 1.01 | 1.00 | 1.00 | 1.00 |
| 200 | 0.001 | 1.10 | 1.07 | 1.05 | 1.05 | 1.04 | 1.03 | 1.02 | 1.02 | 1.01 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| | 0.01 | 1.07 | 1.04 | 1.03 | 1.04 | 1.03 | 1.02 | 1.02 | 1.02 | 1.01 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| | 0.1 | 1.05 | 1.03 | 1.01 | 1.03 | 1.02 | 1.01 | 1.01 | 1.01 | 1.01 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |