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D. R. OLANDER

*University of California*
*Berkeley, California*

*Received February 25, 1963*

## Effect of Temperature Variation on "Intermediate-Resonance" Formulas

The "intermediate-resonance" formulas derived by Goldstein and Cohen (*1*) for effective resonance integrals in homogeneous systems have found wide acceptance as a means of interpolating between the extreme "narrow-resonance" and "infinite-mass" approximations at absolute zero temperature. However, there appears to be no reference in the literature to the validity of applying these formulas to the determination of effective resonance integrals at working temperatures. The effect of temperature variation is considered in this note.

*Theoretical Background*

Neglecting interference scattering and the variation in the reciprocal of the energy over a resonance, we may write the first and second order approximations to the effective resonance integral at working temperatures in the form

$$I_\lambda^{(1)} = \frac{\Gamma_\gamma \sigma_0 a_\lambda}{2E_0} \int_{-\infty}^{\infty} \frac{\psi(\theta, x)}{a_\lambda + \psi(\theta, x)}\, dx \tag{1}$$

and

$$I_\lambda^{(2)} = I_1^{(1)} \left[\frac{1 + \sigma_{pa}(1-\alpha)}{\alpha\sigma_p}\right] + \frac{\Gamma_\gamma \sigma_{pa}(a_\lambda - a_\infty)}{2E_0 x_0 a_\infty} \cdot \int_{-\infty}^{\infty} \frac{\psi(\theta, x)}{a_1 + \psi(\theta, x)} \int_x^{\frac{x+x_0}{\alpha}} \frac{\psi(\theta, x')}{a_\lambda + \psi(\theta, x')}\, dx'\, dx, \tag{2}$$

where the notation is the same as that used by Dresner (*2*), except that

$$a_\lambda = \Gamma(\sigma_m + \lambda\sigma_{pa})/\sigma_0(\Gamma_\gamma + \lambda\Gamma_n),$$

$$a_1 = \sigma_p/\sigma_0 = \text{Dresner's } \beta,$$

$$a_\infty = \Gamma\sigma_{pa}/\Gamma_n\sigma_0$$

and

$$x_0 = 2E_0(1-\alpha)/\Gamma.$$

Equations (1) and (2) give, to first and second order respectively, the "infinite-mass" approximation if $\lambda$ is put equal to zero and the "narrow-resonance" approximation if $\lambda$ is taken as unity. These extreme approximations may be combined linearly, following Goldstein and Cohen (*1*), to give

$$I_\mu^{(1)} = (I_0^{(1)} + \mu I_1^{(1)})/(1+\mu) \tag{3}$$

and

$$I_\mu^{(2)} = (I_0^{(2)} + \mu I_1^{(2)})/(1+\mu), \tag{4}$$

where the "best" value of $I$ results from the choice of $\mu$ in such a way that $I_\mu^{(1)} = I_\mu^{(2)}$. Hence

$$\mu = (I_0^{(1)} - I_0^{(2)})/(I_1^{(2)} - I_1^{(1)}) = \frac{a_0 J(\theta, a_0) - a_1 J(\theta, a_1)\left[\frac{1+\sigma_{pa}(1-\alpha)}{\alpha\sigma_p}\right] - \frac{a_1\sigma_{pa}(a_0 - a_\infty)}{2a_\infty \sigma_p x_0} L(\theta, a_1, a_0, x_0)}{a_1 J(\theta, a_1)\sigma_{pa}\frac{(1-\alpha)}{\alpha\sigma_p} + \frac{a_1\sigma_{pa}(a_1 - a_\infty)}{2a_\infty\sigma_p x_0} L(\theta, a_1, a_1, x_0)}, \tag{5}$$

where

$$L(\theta, a_1, a_\lambda, x_0) = \int_{-\infty}^{\infty} \frac{\psi(\theta, x)}{a_1 + \psi(\theta, x)} \cdot \int_x^{(x+x_0)/\alpha} \frac{\psi(\theta, x')}{a_\lambda + \psi(\theta, x')}\, dx'\, dx$$

and $J(\theta, a_\lambda)$ is the well-known function tabulated by Dresner (*2*) and others.

Equation (5) may be used to give an interpolation parameter, $\mu$, appropriate for use in (3) or (4) at any given temperature.

*Numerical Procedure*

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

The line shape function was obtained by solving the differential equation

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

where the primes denote differentiation with respect to the variable $x$. The infinite range required for the integrals was truncated to the range $x = -d$ to $x = d$, and the range subdivided into $2j$ equal steps in $x$ of width $h$. It was necessary to choose $d$ so that $x_0/h$ was exactly an even integer $n$.

Using the notation

$$x_i = -d + (i-1)h$$

and

$$\psi_i = \psi(\theta, x_i),$$

the line shape function was obtained from the following algorithm.

$i = j + 1$ (center of resonance): (7)

$$\psi_i = \tfrac{1}{2}\sqrt{\pi}\,\theta e^{\theta^2/4}\,\operatorname{erfc}\tfrac{1}{2}\theta,$$

$$\psi_i' = 0.$$

$2j + 1 + n \geqq i > j + 1$ and $x_i < 12/\theta$:

$$\psi_i = \psi_{i-1} + h\psi_{i-1}' + \tfrac{1}{2}h^2\psi_{i-1}'' + \tfrac{1}{6}h^3\psi_{i-1}''',$$

$$\psi_i' = \psi_{i-1}' + h\psi_{i-1}'' + \tfrac{1}{2}h^2\psi_{i-1}'''$$

$$\psi_i'' = \tfrac{1}{4}\theta^4 - \theta^2 x_i\psi_i' - \tfrac{1}{4}\theta^2(2 + \theta^2 + \theta^2 x_i^2)\psi_i,$$

$$\psi_i''' = -\theta^2 x_i\psi_i'' - \tfrac{1}{4}\theta^2(6 + \theta^2 + \theta^2 x_i^2)\psi_i' - \tfrac{1}{2}\theta^4 x_i\psi_i.$$

$2j + 1 + n \geqq i > j + 1$ and $x_i \geqq 12/\theta$:

$$\psi_i = \frac{1}{1 + x_i^2}\left\{1 + \frac{2(3x_i^2 - 1)}{\theta^2(1 + x_i^2)^2}\right\}.$$

$1 \leqq i < j + 1$:

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

(ii) Evaluation of $J(\theta, a_\lambda)$

The Doppler broadening function was evaluated using Simpson's rule, with a correction for the truncated range based on the assumption that $\psi = (1 + x^2)^{-1}$ in the wings of the resonance.

$$J(\theta, a) = h \sum_{i=1}^{i+1} S_i r_i^{(\lambda)} + \frac{1}{a_\lambda c_\lambda}\left(\frac{\pi}{2} - \tan^{-1}\frac{d}{c_\lambda}\right), \qquad (8)$$

where

$$(S_i) = \tfrac{1}{3}(1, 4, 2, 4, \cdots, 2, 4, 1),$$

$$c_\lambda = \left(1 + \frac{1}{a_\lambda}\right)^{1/2}$$

and

$$r_i^{(\lambda)} = \frac{\psi_i}{a_\lambda + \psi_i}.$$

(iii) Evaluation of $L(\theta, a_1, a_\lambda, x_0)$

To facilitate the calculation of the $L$-function, $\alpha$ was set equal to unity in the limit of integration. The effect of this simplification is negligible. Simpson's rule was again used and an end correction was added assuming $\psi = (1 + x^2)^{-1}$.

$$L(\theta, a_1, a_\lambda, x_0) = h^2 \sum_{i=1}^{2j+1} S_i r_i^{(1)} q_i^{(\lambda)} + \frac{1}{a_1 a_\lambda (x_0^2 + c_\lambda^2)}\left[\ln\left(\frac{d + x_0}{d - x_0}\right) - \frac{2x_0}{c_\lambda}\left(\frac{\pi}{2} - \tan^{-1}\frac{d}{c_\lambda}\right)\right], \qquad (9)$$

where

$$q_i^{(\lambda)} = \sum_{k=i}^{i+n} S_k r_k^{(\lambda)} = q_{i-1}^{(\lambda)} + \tfrac{1}{24}\{9(r_{i+n}^{(\lambda)} - r_{i-1}^{(\lambda)}) + 19(r_{i+n-1}^{(\lambda)} - r_i^{(\lambda)}) - 5(r_{i+n-2}^{(\lambda)} - r_{i+1}^{(\lambda)}) + (r_{i+n-3}^{(\lambda)} - r_{i+2}^{(\lambda)})\}. \qquad (10)$$

Equation (10) was used for all except the first step and is based on fitting cubics through the points that lie near $k = i$ and $k = i + n$.

(iv) Order of Accuracy

The values found to be suitable for the numerical parameters were $h = 0.25$ and $d = 120$. Using these parameters, $\psi$ was checked against the tabulation of Rose *et al.* (*3*) and found to differ on spot checks by at most 2%. The $J$-function was similarly checked against the accurate table values of Bell *et al.* (*4*) and the greatest error found was 0.1%. The $L$-function was checked in the limits

$$\theta \to \infty \quad \text{and} \quad x_0 \to \infty$$

and was found in each case to differ from the analytic result by less than ½%. (See Eq. (11).)

The numerical procedure was coded in FORTRAN for an IBM 1620 computer and each run took approximately 25 min.

*Discussion of Results*

Values of $\mu$ and $I_\mu$ have been determined from Eqs. (5) and (3) for several resonances of $U^{238}$ in a homogeneous 1:1 mixture with hydrogen at temperatures ranging from 0°K to 900°K. These values are recorded in Table I together with corresponding values of $I_{\mu(0)}$, which result from interpolation between the "infinite-mass" and "narrow-resonance" approximations at the specified temperatures using the appropriate 0°K value of $\mu$.

TABLE I

COMPARISON OF RESONANCE INTEGRALS FOR $U^{238}$:H = 1:1

| $E_0$ (ev) | Temp. (°K) | $\mu$ | $I_\mu$ (barns) | $I_{\mu(0)}$ (barns) |
|---|---|---|---|---|
| 6.68 | 0 | 0.0510 | 4.06 | 4.06 |
| | 300 | 0.0496 | 4.10 | 4.10 |
| | 600 | 0.0485 | 4.15 | 4.15 |
| | 900 | 0.0476 | 4.20 | 4.20 |
| 21 | 0 | 0.262 | 1.80 | 1.80 |
| | 300 | 0.252 | 1.83 | 1.83 |
| | 600 | 0.244 | 1.87 | 1.87 |
| | 900 | 0.237 | 1.90 | 1.90 |
| 36.8 | 0 | 0.0189 | 1.46 | 1.46 |
| | 300 | 0.0204 | 1.49 | 1.49 |
| | 600 | 0.0220 | 1.51 | 1.51 |
| | 900 | 0.0234 | 1.53 | 1.53 |
| 66.3 | 0 | 0.337 | 0.492 | 0.492 |
| | 300 | 0.359 | 0.522 | 0.523 |
| | 600 | 0.348 | 0.553 | 0.553 |
| | 900 | 0.325 | 0.581 | 0.581 |
| 103 | 0 | 0.554 | 0.402 | 0.402 |
| | 300 | 0.583 | 0.415 | 0.418 |
| | 600 | 0.593 | 0.430 | 0.433 |
| | 900 | 0.588 | 0.445 | 0.448 |
| 117 | 0 | 1.28 | 0.182 | 0.182 |
| | 300 | 1.38 | 0.221 | 0.222 |
| | 600 | 1.23 | 0.252 | 0.252 |
| | 900 | 1.06 | 0.278 | 0.277 |
| 192 | 0 | 1.57 | 0.172 | 0.172 |
| | 300 | 1.68 | 0.178 | 0.180 |
| | 600 | 1.74 | 0.184 | 0.188 |
| | 900 | 1.74 | 0.191 | 0.195 |
| 209 | 0 | 3.01 | 0.107 | 0.107 |
| | 300 | 3.32 | 0.121 | 0.122 |
| | 600 | 3.16 | 0.134 | 0.135 |
| | 900 | 2.93 | 0.146 | 0.146 |

The results show that, for a 1:1 mixture of $U^{238}$ and hydrogen, there is virtually no difference between $I_{\mu(0)}$ and $I_\mu$ for most of the resonances considered, the maximum variation being about 2% for the 192 ev resonance.

In the case of the 192 ev resonance, the calculations were carried out for mixtures of $U^{238}$ with hydrogen of various dilutions ranging up to 1:100, and the results are recorded in Table II. It appears that the difference between $I_{\mu(0)}$ and $I_\mu$ does not become significant except in very dilute mixtures, when the resonance escape probability is not very sensitive to changes in the effective resonance integral.

TABLE II

COMPARISON OF RESONANCE INTEGRALS FOR THE 192 ev RESONANCE OF $U^{238}$

| $U^{238}$:H | Temp. (°K) | $\mu$ | $I_\mu$ (barns) | $I_{\mu(0)}$ (barns) |
|---|---|---|---|---|
| 1:1 | 0 | 1.57 | 0.172 | 0.172 |
| | 300 | 1.68 | 0.178 | 0.180 |
| | 600 | 1.74 | 0.184 | 0.188 |
| | 900 | 1.74 | 0.191 | 0.195 |
| 1:5 | 0 | 3.50 | 0.302 | 0.302 |
| | 300 | 3.82 | 0.329 | 0.335 |
| | 600 | 3.73 | 0.355 | 0.360 |
| | 900 | 3.53 | 0.380 | 0.381 |
| 1:10 | 0 | 4.92 | 0.393 | 0.393 |
| | 300 | 5.11 | 0.443 | 0.446 |
| | 600 | 4.70 | 0.488 | 0.484 |
| | 900 | 4.25 | 0.529 | 0.514 |
| 1:20 | 0 | 6.71 | 0.516 | 0.516 |
| | 300 | 6.25 | 0.608 | 0.602 |
| | 600 | 5.34 | 0.681 | 0.657 |
| | 900 | 4.62 | 0.742 | 0.700 |
| 1:100 | 0 | 11.0 | 0.983 | 0.983 |
| | 300 | 6.74 | 1.23 | 1.20 |
| | 600 | 5.07 | 1.37 | 1.30 |
| | 900 | 4.12 | 1.46 | 1.37 |

As expected, the trend in the interpolation parameter with increasing dilution is towards the "narrow-resonance" limit. Another trend which becomes apparent from a consideration of dilute mixtures is that $\mu$ moves back towards the "infinite-mass" value as the temperature increases.

The results as a whole show that, although the interpolation parameter $\mu$ may exhibit quite marked changes with temperature in some cases, the variation has a comparatively small effect on the effective resonance integral. Thus it appears that, in applying the formulas of Goldstein and Cohen, no significant error should result from the use of the 0°K value of $\mu$ in the calculation of the total effective resonance integral, except, perhaps, when determining the Doppler coefficient, for which a more thorough investigation may be needed.

It is interesting to note that, for the values of the parameters relevant to the resonances of $Th^{232}$ and $U^{238}$ under practical conditions, the function $L(\theta, a_1, a_\lambda, x_0)$ has been found to be given within a few percent by the formula

$$L(\theta, a_1, a_\lambda, x_0) \simeq \frac{4}{\pi} J(\theta, a_1) J(\theta, a_\lambda) \tan^{-1} \frac{x_0}{c_1 + c_\lambda}, \quad (11)$$

which is exact in the limit as $\theta \to \infty$ and also in the limit as $x_0 \to \infty$.

The work reported here was undertaken by one of the authors (M. H. M.) as part of project sponsored by the Australian Institute of Nuclear Science and Engineering.

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M. H. MCKAY
*The University of New South Wales*
*Kensington, N.S.W.*
*Australia*

J. P. POLLARD
*Australian Atomic Energy Commission*
*Private Mail Bag*
*Sutherland, N.S.W.*
*Australia*

*Received November 12, 1962*
*Revised February 11, 1963*

## The Average Capture/Fission Ratio of $U^{233}$ for Epithermal Neutrons

In thermal reactors using $U^{233}$ as fuel somewhere around 10% of all absorption in the fuel may be expected to involve epithermal neutrons. While the capture/fission ratio $\alpha$ for thermal neutrons is known to be close to 0.10 (*1*) and while the fission, scattering, and total (i.e., fission plus capture plus scattering) cross sections have been studied as a function of energy (*1*), nevertheless there remains significant uncertainty as to the average capture cross section and capture/fission ratio for epithermal neutrons. If the latter ratio were sufficiently high the consequent effect on the neutron economy of a $U^{233}$ thermal breeder could be serious. The purpose of the work described here was to to compare the epithermal capture and fission values to the thermal values by the use of Cd ratios, radiochemical analyses of fission products, and mass-spectrographic ratios of $U^{234}/U^{233}$. Thereby an experimental $\alpha_{epi}$ for epithermal neutrons was evaluated, as were infinitely dilute resonance integrals for capture and fission, $I_c$ and $I_f$, for $U^{233}$.

Microgram quantities of $U^{233}$ (prepared to be especially free of $U^{234}$ by milking $U^{233}$ from $Pa^{233}$) were irradiated in both the LITR (ORNL Low Intensity Test Reactor) and ORR (Oak Ridge Research Reactor), both with and without 40 mil Cd filters surrounding them. The thermal fluxes were about $2 \times 10^{13}$ and $1 \times 10^{14}$ $n/cm^2$-sec respectively. Both thermal and epithermal fluxes were monitored at the sample positions with cobalt in a dilute Co–Al alloy (containing 0.151% Co).

After irradiation, the uranium was separated from fission products and other impurities and analyzed mass-spectrographically for $U^{234}$ produced. Analyses were made on the four fission products, 12.8-day $Ba^{140}$, 67-hr $Mo^{99}$, 54-day $Sr^{89}$ and 65-day $Zr^{95}$, by using standard procedures (*2*) with few modifications, in order to determine the number of fissions which occurred during irradiation.[1]

[1] The yield of $I^{131}$ was also measured and found to give a resonance integral some 36% higher than that computed from $Sr^{89}$, $Mo^{99}$, and $Ba^{140}$. Since $I^{131}$ is on the slope of the