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1TABLES FOR COMPUTING EFFECTIVE RESONANCE INTEGRALS, INCLUDING THE
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It has been long recognized that in calculating the absorption of neutrons in the resonance energy region, careful account must be taken of the thermal motion of the absorbing atoms.¹ Indeed, the relevant absorption cross section is just $\sigma_{a \text{ eff}}(E)$, where

$$\sigma_{a \text{ eff}}(E) \equiv \int \sigma_a(E_{\text{eff}}) P(E_{\text{eff}}) dE_{\text{eff}} \quad (1)$$

where E is the relative energy in the center of mass system, assuming the target nucleus to be at rest; E_{eff} is the actual relative energy including thermal motion of the absorber; where $P(E_{\text{eff}})$ is the probability that the relative energy will have the value E_{eff} . The integral represents an average over the thermal velocity distribution of the absorber. E_{eff} is given by

$$E_{\text{eff}} = \frac{1}{2} \mu (\vec{v} - \vec{V})^2 \quad (2)$$

where μ is the reduced mass of the neutron, and equals $\frac{A}{A+1}$ times the ordinary neutron mass, $\vec{v}$ is the neutron velocity, and $\vec{V}$ the velocity of the moderating nucleus. If we expand the right side of Eq. (2) we can neglect the square of V against the other terms since $\frac{V}{v} \sim \left(\frac{kT}{AE}\right)^{\frac{1}{2}} \ll 1$. Here kT is the absorber temperature expressed in energy units. We can furthermore, choose as our reference

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direction for $\vec{V}$ the direction of $\vec{v}$, i.e., we can choose as our z - axis the direction of $\vec{v}$. Then

$$E_{\text{eff}} = \frac{1}{2} \mu v^2 - \mu v V_z = E - (2\mu E)^{\frac{1}{2}} V_z \quad (3)$$

The V_z are distributed according to a normalized Maxwellian distribution, viz.,

$$P(V_z) dV_z = \left(\frac{M}{2\pi kT} \right)^{\frac{1}{2}} \exp \left(- \frac{M V_z^2}{2kT} \right) dV_z \quad (4)$$

where M is the mass of the absorbing nucleus. By combining Eq. (4) and (3) we can find the probability distribution of E_{eff} .

$$P(E_{\text{eff}}) dE_{\text{eff}} = \pi^{-\frac{1}{2}} \left(\frac{M}{4\mu E kT} \right)^{\frac{1}{2}} \exp \left(- \frac{M}{4\mu E kT} (E - E_{\text{eff}})^2 \right) dE_{\text{eff}} \quad (5)$$

$\sigma_a(E)$ is given by the Breit-Wigner formula, i.e.,

$$\sigma_a(E) = \sigma_0 \frac{\Gamma_\gamma}{\Gamma} \left(1 + \left[\frac{E - E_0}{\Gamma/2} \right]^2 \right)^{-1} \quad (6)$$

where $\sigma_0 = 4\pi \lambda^2 \frac{\Gamma_n}{\Gamma}$, Γ_γ is the radiative capture width, Γ_n is the neutron width, Γ is the total width, and E_0 the resonance energy, and λ the reduced wavelength. Combining Eq. (5) and (6) we have

$$\sigma_{a \text{ eff}}(E) = \int \sigma_0 \frac{\Gamma_\gamma}{\Gamma} \left(1 + \left[\frac{E_{\text{eff}} - E_0}{\Gamma/2} \right]^2 \right)^{-1} \pi^{-\frac{1}{2}} \left(\frac{M}{4\mu E kT} \right)^{\frac{1}{2}} \exp \left(- \frac{M}{4\mu E kT} (E - E_{\text{eff}})^2 \right) dE_{\text{eff}} \quad (7)$$

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Generally speaking, it is the case that the width Γ of absorption resonances is considerably less than the resonance energy. Only when E is near E_0 is there any appreciable contribution to the absorption cross section, for only then can both the exponential and the dispersion denominator be near unity. On the strength of this consideration we shall set σ_0 equal to its value at resonance under the integral sign, and also ignore the energy dependence of the total width, Γ . If we define

$$\Delta = \left(\frac{\ln E k T}{M} \right)^{\frac{1}{2}}, \quad \frac{\Gamma}{\Delta} = \xi, \quad \frac{E - E_0}{\Gamma/2} = x, \quad \frac{E_{\text{eff}} - E_0}{\Gamma/2} = y \quad (8)$$

then Eq. (7) becomes

$$\frac{\sigma_{a \text{ eff}}(x)}{\frac{\sigma_0 \Gamma}{\Gamma}} = \frac{\xi}{2\sqrt{\pi}} \int_{-\infty}^{+\infty} dy \frac{\exp\left(-\frac{\xi^2}{4} [x - y]^2\right)}{1 + y^2} \equiv \psi(\xi, x) \quad (9)$$

ξ depends still on E through Δ ; we shall in the remainder of this work make the assumption that this dependence is unimportant by virtue of the narrowness of the resonances, and replace E in Δ by E_0 .

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II. Properties of $\psi(\xi, x)$

1. Normalization: $\int_{-\infty}^{+\infty} dx \psi(\xi, x) = \pi$
2. Symmetry: $\psi(\xi, x) = \psi(\xi, -x)$
3. Monotonicity: $\psi(\xi, x)$ decreases as x increases.
4. Boundedness: $\psi(\xi, x) \leq \psi(\xi, 0) = \xi \exp(\xi^2/4) \cdot x$
 $\int_{\xi/2}^{\infty} \exp(-\zeta^2) d\zeta \leq 1$
5. Asymptotic Expansion:

$$\psi(\xi, x) \sim (1+x^2)^{-1} \left(1 - \frac{2}{\xi^2} \frac{1-3x^2}{(1+x^2)^2} + \frac{12}{\xi^4} \frac{1-10x^2+5x^4}{(1+x^2)^4} + \dots \right)$$

The first four properties are easy to prove directly from the definition of $\psi(\xi, x)$; the fifth has been proven by Born, as well as others.²

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III. The Effective Resonance Integral

The effective resonance integral, I , of a single absorption resonance is defined by

$$I = \int \frac{\sigma_a(E)}{1 + \frac{\sigma_a(E) + \sigma_s(E)}{\sigma_p}} \frac{dE}{E} \quad (10)$$

where

$$\sigma_a(E) = \sigma_{a \text{ eff}}(x) = \sigma_0 \frac{\Gamma_\gamma}{\Gamma} \phi(\xi, x)$$

$$\sigma_s(E) = \sigma_{s \text{ eff}}(x) = \sigma_0 \frac{\Gamma_n}{\Gamma} \phi(\xi, x)$$

and where Γ_n is the neutron width, and σ_p is the non-resonance scattering cross section per absorbing atom. By rearranging the terms in Eq. (10) it can be written as

$$I = \frac{\pi}{2} \frac{\sigma_0 \Gamma_\gamma}{E_0} \cdot \frac{2\beta}{\pi} \int_0^\infty \frac{\phi(\xi, x)}{\beta + \phi(\xi, x)} dx \quad (11)$$

where $\beta = \frac{\sigma_p}{\sigma_0}$. In the derivation of Eq. (11) use again has been made of the narrowness of absorption resonances, and E has again been replaced by E_0 . In form Eq. (11) consists of the infinitely dilute integral, $\frac{\pi \sigma_0 \Gamma_\gamma}{2 E_0}$, multiplied by a correcting factor which accounts for finite dilution and Doppler broadening. The integral in Eq. (11) will henceforth be denoted $J(\xi, \beta)$.

1. Approximate behavior of $J(\xi, \beta)$ for large β and small ξ

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IV. Properties of $J(\xi, \beta)$

1. Asymptotic behavior for large β . We can write

$$\frac{\psi}{\psi + \beta} = \frac{\psi}{\beta} \left(1 - \frac{\psi}{\beta} + \left(\frac{\psi}{\beta}\right)^2 - \dots \right) \quad (12)$$

when $\beta > 1$, the series expansion on the right converges uniformly, and can be integrated term-by-term. Since the terms alternate in sign, it is clear that

$$\int_0^{\infty} \frac{\psi(\xi, x)}{\beta} dx > J(\xi, \beta) > \int_0^{\infty} \frac{\psi(\xi, x)}{\beta} dx - \int_0^{\infty} \left[\frac{\psi(\xi, x)}{\beta} \right]^2 dx \quad (13)$$

Since $\psi^2(\xi, x) \leq \psi(\xi, x)$ and $\int_0^{\infty} \psi(\xi, x) dx = \pi/2$, we can write

$$\frac{\pi/2}{\beta} > J(\xi, \beta) > \frac{\pi/2}{\beta} \left(1 - \frac{1}{\beta} \right) \quad (14)$$

2. Asymptotic behavior for small β . When β is small the integrand $\psi(\xi, x) / \psi(\xi, x) + \beta$ is virtually unity until $\psi(\xi, x) \cong \beta$. If the value of x at which this approximate equality is fulfilled is sufficiently large so that $\psi(\xi, x)$ is essentially given by $(1 + x^2)^{-1}$, then we may replace $\psi(\xi, x)$ by $(1 + x^2)^{-1}$ not only for large x , but for small x as well. For the integrand is virtually unity for small x , whether we use $\psi(\xi, x)$ or $(1 + x^2)^{-1}$ in place of it. In this event

$$J(\xi, \beta) \cong \int_0^{\infty} \frac{(1 + x^2)^{-1}}{\beta + (1 + x^2)^{-1}} dx = \frac{\pi/2}{(\beta [1 + \beta])^{1/2}} \quad (15)$$

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If when $\varphi(\xi, x) \cong \beta$, $\varphi(\xi, x) \cong (1 + x^2)^{-1}$ then the value of x determined by the first equality is $x \cong \beta^{-1/2}$. The approximation of replacing $\varphi(\xi, x)$ by $(1 + x^2)^{-1}$ will then be a good one if $6\beta/\xi^2 < 1$, as we can easily see from property 5 of $\varphi(\xi, x)$.

3. Asymptotic behavior for large ξ . $\varphi(\xi, x) \cong (1 + x^2)^{-1}$ for large ξ . Then $J(\xi, \beta) \cong \frac{\pi/2}{(\beta[1 + \beta])^{1/2}}$ for large ξ . This corresponds to no Doppler broadening.

4. For the purposes of computation of $J(\xi, \beta)$ it is also useful to know that

$$\int_{-\infty}^{\infty} \frac{\varphi(\xi, x)}{\varphi(\xi, x) + \beta} dx \cong \frac{\frac{\pi}{2} - \tan^{-1} \left(C \sqrt{\frac{\beta}{1 + \beta}} \right)}{\sqrt{\beta(1 + \beta)}} \quad (16)$$

for fairly large C . This expression is derived by replacing $\varphi(\xi, x)$ by $(1 + x^2)^{-1}$. For sufficiently large C it can be shown that the percentage error in this expression is bounded by

$$\frac{6}{\xi^2 (C^2 + \frac{1}{\beta})}$$

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V. Description of the Numerical Procedure Error Analysis

$J(\xi, \beta)$ has been calculated on the ORACLE in the form

$$J(\xi, \beta) = \sum_{k=1}^N \int_{(k-1)\Delta}^{k\Delta} \frac{\phi(\xi, x)}{\phi(\xi, x) + \beta} dx + \frac{\frac{\pi}{2} - \tan^{-1} \left(N\Delta \sqrt{\frac{\beta}{1-\beta}} \right)}{\sqrt{\beta(1+\beta)}} \quad (17)$$

and with

$$\phi(\xi, x) = \int_{x - \frac{a}{\xi/2}}^{x + \frac{a}{\xi/2}} \frac{\xi}{2\sqrt{\pi}} \frac{\exp\left(-\frac{\xi^2}{4} [x - y]^2\right)}{1 + y^2} dy \quad (18)$$

The integrals have all evaluated with Gauss' integration rule. The integrals in the sum in Eq. (17) have been evaluated using 64 points of integration per interval width Δ . The accuracy of the calculation depends on the parameters N, Δ, a , the number of points of integration used in evaluating $\phi(\xi, x)$ ($= 16 \cdot 2^n$), and the number of points of integration used in determining the arc tangent ($= 16 \cdot 2^m$).

Let us first consider the parameter a . It can be shown without difficulty that the difference between the right hand sides of Eq. (18) and Eq. (9) is less than

$$\frac{2}{\xi\sqrt{\pi}} \frac{\exp(-a^2)}{a} \left(\frac{1}{1 + (x - \frac{2a}{\xi})^2} + \frac{1}{1 + (x + \frac{2a}{\xi})^2} \right). \quad (19)$$

Expression (19) has maxima near $x = \pm \frac{2a}{\xi}$. At these points, since a is at least several times unity, $\phi \cong (1 + x^2)^{-1}$. The maximum relative error in $\phi(\xi, x)$ will then be, very roughly, equal to

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$$\frac{8}{\sqrt{\pi}} \xi^{-3} \exp(-a^2) a^{-1} \quad (20)$$

In this work the smallest ξ considered will be $\xi=0.1$. For this value, $a = 4$ causes Expression (20) to be $\sim 0.2\%$. We shall use this value of a . The effect of this error in ϕ will not be felt to its full extent in the J integral since the relative error in ϕ is only as large as Expression (20) in at most two places. The analysis leading to Expression (20) was intentionally carried out in a simple and unprecise fashion so as to easily achieve a rough estimate of the relative error in ϕ . As a final word on this point, it deserves to be pointed out that as ξ increases, the error in ϕ decreases.

The value of n (which gives the number of ϕ - integration points) is determined as follows: Arbitrarily we selected $N = 1$, $\Delta = 150$, $a = 4$, $\xi = 0.1$, and $m = 5$ (the number which gives the number of points of integration employed in evaluating the arctangent). $J(\xi, \phi)$ was calculated for $n = 2, 3$, and 4 , and for $\phi = 2^k \times 10^{-5}$; $k = 0, 1, \dots, 31$. The cases for $n = 3$ and $n = 4$ agreed within a maximum relative error of 0.7% for all values of ϕ . This close agreement indicates that for $n \geq 3$ the value $J(\xi, \phi)$ is essentially independent of the choice of n . The choice of n of course depends heavily on a and ξ , but not very much on N or Δ . The error will be greatest for the smallest ξ and will decrease rapidly as ξ increases. To the choices $a = 4$, $\xi \geq 0.1$, we add the choice $n = 3$.

The only choices which remain are now N and Δ and m . The product $N\Delta$ will introduce error only through the use of property (4) of $J(\xi, \phi)$ (Eq. (16)). For $N\Delta = 256$, the error in $J(\xi, \phi)$ due to using Eq. (16) is about 1% for $\xi = 0.1$, and less for larger ξ . The dependence of $J(\xi, \phi)$ on the values of N and Δ was

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was analyzed as follows: $J(\xi, \beta)$ was calculated for $\beta = 2^k 10^{-5}$, $k = 0, 1, \dots, 31$, and $\xi = 0.1$. Also $a = 7$, $m = 5$, $N\Delta = 128$. For $N = 2$, $\Delta = 64$ and $N = 4$, $\Delta = 32$ the relative difference for all β of the two values of $J(\xi, \beta)$ was about 0.5% at most. The first choice corresponds to 1 point of integration per unit interval of the x-axis; the second choice corresponds to 2 points per unit interval of the x-axis. If we make the first choice, then N and Δ are determined as $N = 4$, $\Delta = 64$.

The determination of m is done by similar techniques. With $C = 15$, the expression on the right hand side of Eq. (15) was determined for $m = 2, 3$, and 4. For $m = 3$ and $m = 4$ the RHS of Eq. (16) varied by at most 2%. However, in the neighborhood of β where its variation was near 2%, it contributed only about 0.5% to $J(\xi, \beta)$. On the other hand, in regions of β where its contribution is large, the two values of the RHS of Eq. (16) agreed to 5 or 6 significant figures. Choosing $m = 5$ will therefore annihilate any dependence of $J(\xi, \beta)$ on m .

We expect, therefore that the choices

$$\begin{array}{lll} N = 4 & n = 3 & \xi \geq 0.1 \\ \Delta = 64 & m = 5 & \\ N\Delta = 256 & a = 4 & \end{array} \quad (21)$$

will produce $J(\xi, \beta)$ for $\beta = 2^k 10^{-5}$, $k = 0, 1, \dots, 31$ to an accuracy of about 1%. With the program used the computing time for one value of ξ and all β is approximately $N2^n + 1$ minutes, or about one hour for the choice (21). The choice (21) was made in order to achieve reasonable accuracy ($\cong 1\%$) and still have the computing time remain within reasonable bounds.

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VI. Results and Discussion

In Table I are presented the values of β at which $J(\xi, \beta)$ was evaluated in this calculation, i.e., $\beta = 2^k 10^{-5}$, $k = 0, 1, \dots, 31$. The numbers are to be interpreted as follows: In the first digit is 0 the number is positive, if it is F the number is negative. The second to seventh digits are the decimal parts of the number; the decimal point is between the first and second digits. The ninth and tenth digits are the exponent of 10, this power of which multiplies the decimal part. Finally the seventh digit is the sign digit of the exponent. For example:

$$0123467F02 = .123467 \times 10^{-2} \text{ and}$$

$$F315296003 = -315.296, \text{ etc.}$$

In Table II is presented $J(\xi, \beta)$ for the β in Table I and for $\xi = 0.1$ (0.1) 1.0. The β corresponding to a given entry in Table II can be found in the corresponding position in Table I.

In Fig. 1 $J(\xi, \beta)$ is plotted vs. β for various ξ for a restricted range of β . It appears from the figure that as ξ increases, $J(\xi, \beta)$ decreases, and indeed it can be shown that this is a general property of the $J(\xi, \beta)$. In Fig. 2 $J(\xi, \beta)$ is plotted for $\xi = 0.1$ and $\xi = 1.0$ for the full range of β . In the first place, for $\beta \leq 1.6 \times 10^{-4}$ or $\beta \geq 2.6$ all the curves for $\xi = 0.1$ (0.1) 1.0 have essentially the same value. What is more important, is that the curve for $\xi = 1.0$ is virtually indistinguishable from the curve $\pi/2 [\beta(\beta+1)]^{-1/2}$, which is correct in the limit $\xi \rightarrow \infty$. Hence, the Doppler effect is only important in computing effective resonance integrals if $2.6 \geq \beta \geq 1.6 \times 10^{-4}$, and $\xi \leq 1$. It is also clear from this result that $J(\xi, \beta)$ has the predicted asymptotic form in the limit of both large and small β .

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Fig. 2. $J(\xi, \beta)$ vs. β for $\xi = 0.1, 1.0$.

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VII. Acknowledgements

I wish to gratefully acknowledge the help of S. G. Campbell and C. L. Gerberich of the ORNL Mathematics Panel for advice and assistance in coding this problem for ORACLE. In particular, I should like to thank the latter for the use of his Gaussian integration subroutine.

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Table I. $\beta = 2^k \times 10^{-5}$ ($k = 0, 1, \dots, 31$)

0100000F04	0199999F04	0399999F04	0799999F04
0159999F03	0319999F03	0639999F03	0127999F02
0255999F02	0511999F02	0102399F01	0204799F01
0409599F01	0819199F01	0163839000	0327679000
0655359000	0131071001	0262143001	0524287001
0104857002	0209715002	0419430002	0838860002
0167772003	0335544003	0671088003	0134217004
0268435004	0536870004	0107374005	0214748005

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Table II. $J(\xi, \beta)$ for all β in Table I and $\xi = 0.1$ (0.1) 1.0

$\xi = 0.1$

0497919003	0353201003	0251413003	0180149003
0130657003	0966738002	0735538002	0577298002
0464737002	0378127002	0304473002	0236654002
0172986002	0116449002	0717193002	0408780001
0220375001	0114768001	0586163000	0296280000
0148955000	0746837F01	0373935F01	0187097F01
0935811F02	0467986F02	0234013F02	0117011F02
0585072F03	0292539F03	0146270F03	0731354F04

$\xi = 0.2$

0497008003	0351698003	0249070003	0176663003
0125684003	0899298002	0650095002	0477726002
0358904002	0275900002	0215296002	0167556002
0126829002	0908070001	0601364001	0365817001
0206746001	0110878001	0575749000	0293594000
0140279000	0745169F01	0373536F01	0187007F01
0935636F02	0467967F02	0234021F02	0117020F02
0585124F03	0292567F03	0146285F03	0731430F04

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Table II. (Continued)

Σ 0.3

0496850003	0351438003	0248669003	0176068003
0124825003	0887177002	0633517002	0456153002
0332795002	0247076002	0186656002	0142255002
0107353002	0781475001	0534166001	0337070001
0196604001	0107779001	0567110000	0291314000
0147696000	0743709F01	0373179F01	0186922F01
0935450F02	0467934F02	0234019F02	0117022F02
0585147F03	0292581F03	0146292F03	0731470F04

Σ = 0.4

0496796003	0351349003	0248532003	0175866003
0124535003	0883071002	0627820002	0448487002
0322982002	0235414002	0174070002	0130149002
0971750001	0708707001	0491400001	0316885001
0188884001	0105282001	0559896000	0289363000
0147186000	0742402F01	0372844F01	0186836F01
0935223F02	0467872F02	0234001F02	0117016F02
0585125F03	0292572F03	0146288F03	0731451F04

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Table II. (Continued)

$\xi = 0.5$

0496771003	0351309003	0248469003	0175774003
0124402003	0881206002	0625225002	0444955002
0318348002	0229678002	0167541002	0123476002
0911911001	0662886001	0462422001	0302170001
0182890001	0103253001	0553865000	0287708000
0146752000	0741290F01	0372563F01	0186765F01
0935046F02	0467828F02	0233990F02	0117014F02
0585119F03	0292571F03	0146288F03	0731451F04

$\xi = 0.6$

0496757003	0351286003	0248435003	0175725003
0124331003	0880204002	0623831002	0443049002
0315816002	0226471002	0163762002	0119440002
0873900001	0632190001	0441873001	0291116001
0178149001	0101584001	0548776000	0286291000
0146377000	0740325F01	0372318F01	0186704F01
0934892F02	0467789F02	0233980F02	0117011F02
0585113F03	0292570F03	0146288F03	0731450F04

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Table II. (Continued)

$\epsilon = 0.7$

0496749003	0351273003	0248415003	0175695003
0124289003	0879604002	0622997002	0441906002
0314287002	0224508002	0161394002	0116831002
0848358001	0610667001	0426790001	0282611001
0174341001	0100197001	0544453000	0285071000
0146052000	0739484F01	0372104F01	0186650F01
0934755F02	0467755F02	0233971F02	0117009F02
0585107F03	0292568F03	0146287F03	0731448F04

$\epsilon = 0.8$

0496744003	0351265003	0248402003	0175675003
0124261003	0879217002	0622458002	0441167002
0313295002	0223223002	0159819002	0115053002
0830434001	0595031001	0415409001	0275937001
0171241001	0990360000	0540759000	0284016000
0145769000	0738752F01	0371918F01	0186603F01
0934638F02	0467726F02	0233964F02	0117007F02
0585103F03	0292567F03	0146287F03	0731449F04

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Table II. (Continued)

$\xi = 0.9$

0496740003	0351259003	0248393003	0175662003
0124242003	0878952002	0622090002	0440661002
0312615002	0222337002	0158722002	0113792002
0817409001	0583340001	0406625001	0270612001
0168689001	0980545000	0537582000	0283099000
0145522000	0738108F01	0371754F01	0186562F01
0934534F02	0467699F02	0233958F02	0117006F02
0585099F03	0292566F03	0146287F03	0731448F04

$\xi = 1.0$

0496737003	0351255003	0248387003	0175653003
0124229003	0878763002	0621827002	0440301002
031213002	0221701002	0157927002	0112867002
0807667001	0574387001	0399716001	0266302001
0166566001	9072193000	0534836000	0282298000
0145305000	0737542F01	0371609F01	0186525F01
0934442F02	0467676F02	0233952F02	0117004F02
0585095F03	0292565F03	0146287F03	0731447F04

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Footnotes

- 1 H. A. Bethe and G. Placzek, Physical Review 51 450 (1937)
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