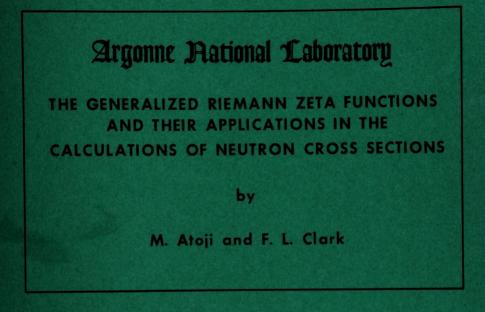
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THE GENERALIZED RIEMANN ZETA FUNCTIONS AND THEIR APPLICATIONS IN THE CALCULATIONS OF NEUTRON CROSS SECTIONS

by

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Chemistry Division

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I. INTRODUCTION

The Riemann Zeta function has been of fundamental importance in the theory of prime numbers and also for allied functions such as the Gamma function. The literature and numerical tables for the Riemann Zeta function are hence relatively abundant. This is, however, not the case for the generalized Riemann Zeta function.

This report introduces the Riemann Zeta function of incomplete mode, a further generalization. The values of the generalized Riemann function and those of the incomplete mode are given for a specific range of the variables. The present calculation was initiated in order to fulfill a need in the neutron cross-section study as described in Section IV below. Other physical applications of the tables in a wider scope are also suggested.

II. DEFINITIONS

The generalized Riemann Zeta function of incomplete mode is defined by the equation

$$\zeta_{N}(s,a) = \sum_{n=0}^{N} \frac{1}{(a+n)^{s}},$$
 (1)

where n and N are nonnegative integers, and we suppose that the constant "a" is a real number. The function $\zeta_N(s,a)$ is also defined in terms of infinite integrals as follows:

$$\Gamma(s)\zeta_{N}(s,a) = \sum_{n=0}^{N} \int_{0}^{\infty} x^{s-1} e^{-(n+a)x} dx$$

$$= \int_{0}^{\infty} \frac{x^{s-1}e^{-ax}}{1-e^{-x}} dx - \int_{0}^{\infty} \frac{x^{s-1}}{1-e^{-x}} e^{-(N+1+a)x} dx, \qquad (2)$$

where

$$\int_{0}^{\infty} \frac{x^{s-1}e^{-ax}}{1 - e^{-x}} dx = \Gamma(s)\zeta(s,a).$$
(3)

Here $\zeta(s,a)$ is the generalized Riemann Zeta function (of complete mode) (see Ref. 16, p. 265), and

$$\lim_{N \to \infty} \zeta_N(s,a) = \zeta(s,a). \tag{4}$$

It is evident that

$$\zeta_{N}(s,a+m) = \zeta_{N}(s,a) - \zeta_{m-1}(s,a),$$
(5)

where m is a positive integer and m \leq N. The Riemann Zeta function of incomplete mode, $\zeta_N(s),$ is defined by the equation

$$\zeta_{N}(s) = \zeta_{N-1}(s,1) = \sum_{n=1}^{N} \frac{1}{n^{s}}.$$
 (6)

Titchmarsh⁽¹⁵⁾ and Chandrasekharan⁽²⁾ have reviewed the literature on $\zeta(s)$ and $\zeta(s,a)$.

III. NUMERICAL CALCULATIONS

We confine ourselves to the case for which a > 0. Numerical tables for $\zeta(s,a)$ have been available for some specific cases:

- a = 0(0.1)2, s = -10(0.1)0 and (s-1) ζ (s,a) for a = 0(0.1)2, s = 0(0.1)1 (Ref. 8);
- a = 0.1(0.1)10 for s = -7, -6(0.5)0, 1.5(0.5)7.5 and for s = σ + it with σ = 1(1)5 and t = 0(1)5 (Ref. 13);
- a = 3(1/12)4 and a = 3(0.05)4, each for s = 2(2)8 (Ref. 3).

Pearson and Pearson⁽¹²⁾ have given tables for $\zeta_N(s)$ with s = 1(1)4and N = 1 to 100. Jones⁽¹¹⁾ has computed $\zeta_N(s)$ for s = 2 and N = 100, 200(200)1000. Several useful equations for evaluating $\zeta(s)$ and $\zeta_N(s)$ are given by Jolley.⁽¹⁰⁾ For other related tables, one may refer to Fletcher et al.⁽⁶⁾

For our numerical calculations, the following formulae were derived and found to be the most practical. We utilize the equation

$$\frac{\mathbf{x}}{\mathbf{e}^{\mathbf{x}}-1} = \sum_{n=0}^{\infty} \frac{\mathbf{B}_n}{n!} \mathbf{x}^n, \tag{7}$$

where B_n is Bernoulli's number. Equation (2) is then expressed as

$$\Gamma(s)\zeta_{N}(s,a) = \Gamma(s)\zeta(s,a) - \sum_{n=0}^{\infty} \frac{B_{n}(n+s-2)!}{n!(N+a)^{n+s-1}},$$
(8)

where $s \ge 2$. The series in (8) converges very rapidly for large N. We also obtain

$$\Gamma(s)\zeta(s,a) = \sum_{n=0}^{\infty} \frac{B_n(n+s-2)!}{n!(a-1)^{n+s-1}}$$
(9)

where $s \ge 2$ and $a \ne 1$. For a < 1, the series in (9) should be replaced by two terms:

$$\Gamma(s) \zeta(s,a) = \sum_{n=0}^{m} \frac{1}{(a+n)^s} + \sum_{n=0}^{\infty} \frac{B_n(n+s-2)!}{n!(a+m)^{n+s-1}},$$
(10)

where m is an arbitrary positive integer and the second series converges more rapidly for larger m.

The formulae for special cases are as follows. Taking s = 1 and a = 1, we have

$$\zeta_{N-1}(1,1) = \zeta_{N}(1) = \sum_{n=1}^{N} \frac{1}{n}$$

= Euler's constant + log_e N - $\sum_{n=1}^{\infty} \frac{B_{n}}{nN^{n}}$
= 0.57721566 + 2.30258509 log₁₀ N

$$+ \frac{1}{2N} - \frac{1}{12N^2} + \frac{1}{120N^4} - \frac{1}{252N^6} + \dots$$
(11)

The rate of divergence in $\zeta_N(1)$ is slow as demonstrated below:

When $s \ge 2$ and a = 1, we have

$$\zeta_{N-1}(s,1) = \zeta_N(s) = \zeta(s) - \sum_{n=0}^{\infty} \frac{1}{(N+1+n)^s}$$

$$= \zeta(s) - \frac{1}{\Gamma(s)} \sum_{n=0}^{\infty} \frac{B_n(n+s-2)!}{n! N^{n+s-1}},$$
(12)

where

$$\zeta(s) = \frac{(2\pi)^{s} |B_{s}|}{2(s!)}$$
(13)

for an even integer of s and the $\zeta(s)$ values for odd integers of s are given by Jolley.(10) When s = 2, we have

$$\zeta_{N-1}(2,1) = \zeta_{N}(2) = \sum_{n=1}^{N} \frac{1}{n^{2}} = \frac{\pi^{2}}{6} - \sum_{n=0}^{\infty} \frac{B_{n}}{N^{n+1}}$$
$$= 1.64493407 - \frac{1}{N} + \frac{1}{2N^{2}} - \frac{1}{6N^{3}} + \frac{1}{30N^{5}} - \frac{1}{42N^{7}} + \dots \quad (14)$$

In particular, if a = 0.5, since

$$\zeta(s, 0.5) = (2^{s} - 1)\zeta(s)$$
(15)

(see Ref. 16, p. 267), we have, as an example,

$$\zeta(2,0.5) = 3\zeta(2) = 4.93480220. \tag{16}$$

Table 1 lists 4 places-after-decimal values of the following:

$$\zeta_{N}^{1}(1,a) = \sum_{n=1}^{N} \frac{1}{a+n} = \zeta_{N}(1,a) - \frac{1}{a}, \qquad (17)$$

where a = 0.01(0.01)0.5; 0.5(0.02)1, and N = 1(1)100;

$$\zeta_{\rm N}^1(2,{\rm a}) = \sum_{\rm n=1}^{\rm N} \frac{1}{({\rm a}+{\rm n})^2} = \zeta_{\rm N}(2,{\rm a}) - \frac{1}{{\rm a}^2},$$
 (18)

where a = 0.01(0.01)0.5; 0.5(0.02)1, and N = 1(1)50. For a > 1, one may utilize the Equation (5).

In Table 2, 4 places-after-decimal values of $\zeta(2,a)$ are given for a = 0.01(0.0005)0.5; 0.5(0.001)1. The calculation was carried out by use of the relation,

$$\zeta(2,a) = \sum_{n=0}^{m} \frac{1}{(a+n)^2} + \sum_{n=0}^{\infty} \frac{B_n}{(a+m)^n}.$$
 (19)

For 6 places-after-decimal accuracy, if m = 10, only five terms are needed in the second summation.

The computer programs were coded in the FORTRAN language and are also given in Tables 1 and 2. The calculation was carried out with the Control Data 3600 computation. Table 1

COMPUTER PROGRAM AND NUMERICAL VALUES FOR $\zeta^1_N(1,A)$ and $\zeta^1_N(2,A)$

```
FTN4.10
                                                                                                                              01/05/65
           PROGRAM C114
        PROGRAM C114
DIMENSION ZETA(2,1001),AA(100)
FORMAT(6X,1HA,F5.2,3X,7(F5.2,3X))
FORMAT(2X,II3,8F8.4)
FORMAT(12X,8HCASE S =I2)
FORMAT(14X,1HN)
FORMAT(1H)
FORMAT(1H)
P2 = 01
1000
2000
4000
   p_2 = .01
p_2 = .01
p_0 = 1, 2
p_0 = 1, 2
p_0 = 1, 2
p_0 = 1, 1001
r_1 = 1, 2
r_2 = 1, 1001
r_1 = 0, 1001
r_2 = 1
r_3 = 1
8000
9000
  120 INI =
           INF
        INF

I1 = 1

I2 = 50

III = III + 1

WRITE OUTPUT TAPE 61,

WRITE OUTPUT TAPE 62,

WRITE OUTPUT TAPE 61,

DO 40 IN = I1, I2

INF - 1)*P2

- 1)*P2
                  = 8
    90
    60
                                                             8000
3000,
9000
                                                                           IS
           A = (INI - 1)*P2
IF (INI - 49)4196,4197,4197
4197 A = A - .5
4196 DO 1 IA =
          A = A - 5
D0 1 IA = INI, INF
IF (IA - 49) 4293, 4291, 4292
IF (IA - 51) 4293, 4294, 4293
A = A + 5
G0 T0 4293
P2 = .02
A = A + P2
2FTA(IS, IA) = 2FTA(IS, IA)
4292
4291
4294 4293
           ZETA(IS,IA) = ZETA(IS,IA) + 1./(A+IN)**IS
   100C, (AA(IA), IA = INI, INF)
400C
                                                            200C, IN, (ZETA(IS,IA),IA = INI,INF)
          IF (INI
P2 = .01
CONTINUE
    41
40
               (IS - 2)88,70,70
(II - 51)50,70,70
          IF
    88
    50
         I1 = I2 =
               = 51
= 100
          GO TO 60
    70 INI = INI
INF = INF
                                + 8
               F = INF + 8
(INI - 50)90,91,91
           IF
    91 P2
               = .02
    IF (INI -
54 INF = 75
                                73)90,54,110
          GC TO 90
```

01/05/65

```
FTN4.10

110 IF (IS - 1)112,112,119

112 IS = 2

P2 = .01

III = 0

GO TO 120

119 WRITE OUTPUT TAPE 61, 8000

END
```

N

0.02 0.

0.03

(1,A)

0.06 0

0.07

80.0

A 0.01

0.02

0.03

0.04

 $\zeta_{N}^{1}(1,A)$

0.05 4.4404 4.4596

0.06 4.4254

0.07 4.4106 4.4298 4.4486

0.08 4.3959 4.4152 4.452 5 6

123456789 11123456789012345678901234567890 50

N

A 0.09 9174

0.10 $\begin{array}{c} 0.11 \\ 0.12 \\ 0.$

0.12

 $\zeta_{N}^{1}(1,A)$

0.13 0.8850 544 739

0.14

0.15

0.16

Δ

0.09 4.3815 4.4007 •9983 •0087 •0190 •0292 039 190 292 392 492 5 0 .

0.10 4.3673 4.3865 4.4053

0.11

0.12 4.9867 4.9968 5.0068

 $\zeta_{\rm N}^{1}(1,A)$

0.13 4.9930

0.14 4.3122 4.3314 4.3502 4.3686 4.3868 $\begin{smallmatrix} & 0.6\\ & 0.6\\ & 0.4$ 4.9492 4.9593 4.9694 4.9794

0.15 9660 4.

0.16 $\begin{array}{c} 786 \\ 612057 \\ 62675 \\ 1548 \\ 2324 \\ 679 \\ 129 \\ 6267 \\ 636 \\ 801 \\ 2332 \\ 647 \\ 912 \\ 129 \\ 626 \\ 129 \\ 626 \\ 129 \\ 12$ 4.8699 4.8806 4.8912 4.9018 4.9122 4.9224 4.9326 4.9427 4.9527

0.18 0.8 475

0.19 0.8403 1.2970

0.20 0.8333 1.2879

 $\zeta_{\rm N}^{1}(1,A)$

0.21 0.8 264

0.22

0.23 0+0+6(250)

0.24

16

Δ N

Δ

0.17

0.18

0.19

0.20

 $\zeta_{N}^{1}(1,A)$

0.21 $\begin{array}{c} 1315\\ 24131\\ 564491\\ 06290\\ 864491\\ 06290\\ 864491\\ 06290\\ 864491\\ 06290\\ 864491\\ 06290\\ 864491\\ 06290\\ 864491\\ 06290\\ 864491\\ 06290\\ 864491\\ 06290\\ 86490\\ 86790\\ 1245679\\ 1357790\\ 12777777\\ 8567890\\ 12345680\\ 8800\\ 8800\\$

0.22

0.23 4.8339 4.8441 4.8541 4.8641

0.24

0.7937

0.26

0.27

0.28

 $\zeta_{N}^{1}(1,A)$

0.29

0.30

0.31

0.32

Δ

0.26 $\begin{array}{c} 231\\ 6449\\ 611\\ 86449\\ 995289\\ 72667\\ 8974$ \\ 8974\\ 8974\\ 8974\\ 8974\\ 8974\\ 8974\\ 8974\\ 8974\\ 8974\\ 8974\\ 8974\\

0.27 8066 4.

0.28

 $\xi_{N}^{1}(1,A)$

0.29 4.7936

0.30

0.31 4. 7711

N

Α 0 in n n 3.9807 3.9822 4.0034 4.0241 4.0443 4.0642

0.33 .7519 .1811 .9607

0.7463

0.34

0.35 0.7407

0.36

 $\zeta_{\rm N}^{1}(1,A)$

0.37 C.7299 1.1519 1.4486

0.38

0.39

0.40

0.33

0.34

0.35

0.36

 $\zeta_{\rm N}^{1}(1,A)$

0.37

0.38

0.39

0.40

A 0.41 .7092 C

0.42

0.43

0.45

0.46

0.47

0.48

22

N

 $\zeta_{N}^{1}(1,A)$

0.44

A

0.41 4.0007

0.42 4.6354 4.6454 4.6554

0.43

4.6455

0.44 3.9712 3.9903 4.0090

(1,A)

0.45

0.46

0.47 3. 9426 9617 ž . 3 ģ 804 .

0.48

Δ

0.49

3

8 9

0.50 54

0.54 3. 8 5 94

 $\xi_{N}^{1}(1,A)$

0.56

0.58

0.62 3. 7 911

Δ

0.49

0.50

0.52

0.54 3.8788 3.8978 3.9165

0.56 .8613

0.58

0.60 3.8271

0.62

0.64 0

.6098

0.66

0.68

0.70

0.72

0.74

0.76

0.78

26

Δ N

 $\zeta^1_N(1,A)$

A

0.64 .7941 ろうちょうちょうちょうちょう

0.66

0.68

0.70 $\begin{array}{c} 5551\\ 46551\\ 46551\\ 46551\\ 46551\\ 46551\\ 46551\\ 46551\\ 46551\\ 46551\\ 46551\\ 46551\\ 882858\\ 89251\\ 8558\\ 89251\\ 8558\\ 892951\\ 8558\\ 892955\\ 892951\\ 8929\\ 892951\\ 892857\\ 892270\\ 8911\\ 80223457\\ 89257\\ 89265757\\ 89265757\\ 89265757\\ 892657\\ 89265757\\ 89265757\\ 89265757\\ 892$

0.72

0.74

0.76

0.78

 $\zeta_{N}^{1}(1,A)$

0.80

0.82

0.84

0.86

 $\zeta_{N}^{1}(1,A)$

0.88 с.

0.90

0.92

0.94

2.8

٨ N

A

0.80

0.82

0.84 3.6437 3.6626 3.6812

0.86 3.6299 3.6488 .6674 ž

 $\xi_{N}^{1}(1,A)$

0.88 2 .6162 .6351

0.92 3.5895

0.94 3.5763 3.5952 3.6138

123456789012345678901234567890123456789012345678901234567890

N

0.96 Α

0.98 1697972582016622954077749412667407902109774494126779725801468295102394374040043951029774949412667407907369265050497444041549253502505048826037703952146913925350254077111114

1.00

N A 0.96

0.98

1.00 $\begin{array}{l} 0.94\, (4.50) \\$

 $\zeta_{N}^{1}(1,A)$

N

A 0.01 C.9803

0.02

0.03

0.04 C.9246 1.1648 1.2731 1.3343 1.3737 1.4011 1.4213 1.4267 1.44589

0.05

0.06

0.07

0.08

0.8573

 $\zeta_{N}^{1}(2,A)$

Δ

1.

0.10 1.4093 1.4098 1.4104 1.4109 1.4114 1.4118 1.4123 1.4123 1.4127 1.4131 4135

0.11

0.12 0.7972 27435291129866082305559622333555596223433527774555667482

CN(2,A)

C

0.13 7831 .

0.14 $\begin{array}{c} 585 \\ 5878364 \\ 6977773884 \\ 6978333364 \\ 6978364 \\ 6978364 \\ 6978364 \\ 6978364 \\ 6978364 \\ 6978364 \\ 697844 \\$

0.15

0.7432

0.16

A

N

0.17

0.18 0.

0.19

0.20 0.6944

0.21 C.6830 C.8878 C.9848 .

0.22

0.23

0.24 0.65C4 0.8497 0.9449

 $\zeta_{\rm N}^{1}(2,A)$

A 0.25 .6400 000 .837 5

Č.

0.26 C.6299 C.8257 C.9198 C.9749

0.27

0.28 0.6104 0.8027 0.8957 0.9503 $\begin{array}{c} 0.51\\ 0.51\\ 0.51\\ 0.51\\ 0.52\\$

 $\zeta_{\rm N}^{1}(2,A)$

С $^{\circ}_{\circ}$ (603) $^{\circ}_{\circ}$ (603) $^{\circ}_{\circ}$ (203) $^{\circ}_{\circ}$

0.29 .6009 .7916

0.30 $\begin{array}{c} $9808 \\ $9086 \\ $9780 \\ $9800 \\ $9780 \\ $9800 \\$

0.31 0.5827 0.8614

35

0.32

C.5739 C.7597 O.85C4 O.9040

.9394

1.

.8

36

Δ 0.33 •565 •749 •839 000 . 8 000 $\begin{array}{c} & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & & & \\ & & & &$

357

0.34

0.35

0.36 0468 1.

 $\zeta_{\rm N}^1(2,A)$

0.37

0.38

 $\begin{array}{c} \textbf{5} \textbf{1623} \textbf{84} \textbf{80} \textbf{474} \textbf{495} \textbf{536} \textbf{636} \textbf{6626} \textbf{688} \textbf{6639} \textbf{690} \textbf{111} \textbf{6678} \textbf{495} \textbf{1662} \textbf{1662$

0.39 0.40

Α

0.41 $\begin{array}{c} 0.567612681\\ 0.567612681\\ 0.567612681\\ 0.567612681\\ 0.567612681\\ 0.567612681\\ 0.567612681\\ 0.56761268\\ 0.56761268\\ 0.56761268\\ 0.56761268\\ 0.56761268\\ 0.56761268\\ 0.56761268\\ 0.56761268\\ 0.56761268\\ 0.56761268\\ 0.56761268\\ 0.56761268\\ 0.567628\\ 0.56$

.6.7 0000

0.42 0.4959 667 522 034

0.43 0.4890

0.44 $\begin{array}{c} 3227\\ 820$

 $\xi_{N}^{1}(2,A)$

0.45 C.4756 C.6422 C.7262

0.46 č 9495 .

0.47 0.4628

0.48 $\begin{array}{c} 456917\\ 67017518486\\ 6501775158486\\ 6507778086674\\ 780866747\\ 7808865072\\ 677808885607\\ 67780888991\\ 60000000000\\ 8889916000\\ 8889916000\\ 889911622\\ 8899117884\\ 69912012\\ 99120122\\ 99223450\\ 9922250\\ 9922250\\ 992250\\ 99250\\ 99250\\ 99250\\ 99250\\ 99250\\ 99250\\ 99250\\ 99250\\ 99250\\$ •9308 •9312 •9317 •9320

0.49 A .4504 0 .611 0.6938 0.7434 0.7766 0.80 0.80

0.50

0.52

0.54

0.56 0: . •

0.58

0.60

0.62

38

 $\zeta_{N}^{1}(2,A)$

Δ

0.64 $\begin{array}{c} 0.3718\\ 0.55153\\ 0.55153\\ 0.55153\\ 0.55153\\ 0.55153\\ 0.55153\\ 0.55153\\ 0.55153\\ 0.55153\\ 0.5512\\ 0.57212\\ 0.77222\\ 0.77212\\ 0.772222\\ 0.77222\\ 0.77222\\ 0.77222\\ 0.77222\\ 0.77222\\ 0.77222\\ 0.77222\\ 0.77222\\ 0.77222\\ 0.77222\\ 0.77222\\ 0.77222\\ 0.77222\\ 0.77222\\ 0.7722$ 0.8074 0.8080 0.8085 0.8090 0.8095 0.8099 0.8104 0.8108 0.8112 C.8116

0.66 $\begin{array}{c} 3624\\ 929\\ 0.552261\\ 712869\\ 0.5522661\\ 712869\\ 0.5522661\\ 712869\\ 0.57266\\ 712869\\ 0.7725699\\ 1.28599\\ 0.775599\\ 1.28599\\ 0.77778\\ 0.00\\ 0.77778\\ 0.00\\ 0.77778\\ 0.00\\ 0.77778\\ 0.00\\ 0.77778\\ 0.00\\ 0.7788\\ 0.00\\ 0.7788\\ 0.00\\ 0.7799\\ 0.779\\ 0.779\\ 0.779\\ 0.779\\ 0$

0.68

0.3543 0.4935 0.5674 $\begin{array}{c} & & + 0 \\ & + 0$

0.70

0.3460 0.4832 0.5562 $\begin{array}{c} 0.025\\ 0.025\\ 0.0223\\ 0$

0.72 C.3380 C.4732 C.5454 C.5903 247618 C.

0.74 0.3303 0.4635 0.5350 535 •

0.76 $\begin{array}{c} 3228\\ 0.45448\\ 0.5569910\\ 0.5629910\\ 0.663766\\ 0.665766\\ 0.666780\\ 0.668840\\ 0.668840\\ 0.669700\\ 0.668880\\ 0.668830\\ 0.669700\\ 0.770915\\ 0.7711894\\ 0.69970\\ 0.7711364\\ 0.772218\\ 0.7722655\\ 0.7722893\\ 0.773324\\ 1.73373\\ 0.773324\\ 0.773324\\ 0.773324\\ 0.773373494\\ 0.773373880\\ 0.7733880\\ 0.7733880\\ 0.7733880\\ 0.7733880\\ 0.7733880\\ 0.7733880\\ 0.7733880\\ 0.7733880\\ 0.7733880\\ 0.7733880\\ 0.7733880\\ 0.7733880\\ 0.7733880\\ 0.7733880\\ 0.7733880\\ 0.773880\\ 0.7733880\\ 0.778880\\ 0.778880\\ 0.778880\\ 0.778880\\ 0.778880\\ 0.778880$

 $\begin{array}{c} 31556\\ 0.556\\ 0.5578\\ 0.5772\\ 0$

0.78

0.80 .3086 0 7175 Õ .

0.82 0.3019 0.3019 0.4276 0.4962 0.53922 0.55687 0.5902 0.6066 0.6194 0.6298 0.6455 0.6384 0.6455 0.6516 0.6568 0.6614 0.6654 0.6689 0.6721 0.6724 0. .

7068

0.84 .2954 ŏ 0.6950 0.6955 0.6959 0.6963 0.6967 0.6971

0.86 0.2891 0.6852 0.6857 0.6861 0.6865 0.6865 0.6873

 $\zeta_{N}^{1}(2,A)$

0.88 C.6762 C.6766 C.6770 C.6774 C.6778

0.90 C.6669 C.6673 C.6677 C.6681 C.6685

0.92

0.2713 0.3886 0.4536 0.4949

0.94 0.2657 0.3814 0.4458

40

Δ

N123456789012345678901234567890123456789012345678901234567890

A

0.96 344290749033248827316908627146787765318890504931211000

0.98

1.00

Table 2

COMPUTER PROGRAM AND NUMERICAL VALUES FOR $\zeta(2, A)$

```
01/05/65
FTN4.10
         PROGRAM C114
         DIMENSION ZETA(1961), A(1981), B(7)
         B(1) = 1.
B(2) = -.5
B(3) = 1./6.
         B(4)
                  = 0.0
         B(5)
B(6)
B(7)
                  = -1./30.
= 0.0
                      1./42.
                  =
          110 = 11
        99
4111
4112
4113
         SUM = 0.0
DC 2 II = 1,II0
III = II - 1
SUM = SUM + 1./(A(I) + II1)**2
      2
         SUM = SUM + 1./(A(1) + 111)**2

SUM1 = 0.0

DC 3 I4 = 1,7

SUM1 = SUM1 + B(I4)/(A(I) + I10 - 1)**I4

ZETA(I) = SUM + SUM1
      3
          IDOWN = 1
          IUP = 58
          DO 25
WRITE
         DČ 25 J = 1,8
WRITE DUTPUT TAPE 61,
WRITE DUTPUT TAPE 61,
                                                   1000
    35
         FORMAT(1H1)
FORMAT(1OX,18HTABLE OF ZETA(2,A))
WRITE_OUTPUT TAPE 61, 3COC
 1000
 2000
    38
3000 FORMAT(1H
3000 FCRMAT(1H)

WRITE OUTPUT TAPE 61, 3001

3001 FORMAT(6X,3(1HA,9X,4HZETA,11X))

D0 225 J1 = IDOWN,IUP

225 WRITE OUTPUT TAPE 61, 400C, A(J1),ZETA(J1),A(J1+58),ZETA(J1+58),

XA(J1+116),ZETA(J1+116)

4000 FCRMAT(2X,3(F7.4,F12.4,6X))

IDOWN = IDOWN + 174

25 IUP = IDOWN + 57

IUP = 1421

J = 9
                9
          J
            =
         WRITE
                                  TAPE
                                                   1000
2000
3000
                     OUTPUT
                                            61,
    52
                     OUTPUT TAPE
OUTPUT TAPE
         WRITE
                                            61,
          WRITE
                     OUTPUT TAPE
                                                    3001
                                            61,
IUP
          DO
              60
                     J1 = IDOWN,
OUTPUT TAPE
    60 WRITE
                                            61, 4000, A(J1), ZETA(J1), A(J1+29),
    XZETA(J1+29),A(J1+58),ZETA(J1+58)
WRITE OUTPUT TAPE 61, 4000, A(1480),ZETA(1480),A(1481),ZETA(1481)
80 WRITE OUTPUT TAPE 61, 1000
          END
```

Δ $\begin{array}{c} 0.5 \\$ ŏ Õ

 $\begin{array}{c} {\tt ZETA}\\ {\tt 2ETA}\\ {\tt 10} {\tt col} {\tt 1.6} {\tt 212}\\ {\tt 9071} {\tt col} {\tt 1.6} {\tt 214}\\ {\tt 9071} {\tt 69466} {\tt .05417}\\ {\tt 755663} {\tt .054147}\\ {\tt 69461} {\tt .778127}\\ {\tt 59466} {\tt .655330}\\ {\tt 4163} {\tt 95731}\\ {\tt 47564} {\tt .655330}\\ {\tt 4163} {\tt 935737}\\ {\tt 4163} {\tt 935737}\\ {\tt 33674} {\tt .855340}\\ {\tt 4163} {\tt 935737}\\ {\tt 33674} {\tt .85026}\\ {\tt 300823} {\tt .6686} {\tt 022235}\\ {\tt 292731} {\tt .454880}\\ {\tt 292731} {\tt .48880}\\ {\tt 29266} {\tt .622435}\\ {\tt 29266} {\tt .626233}\\ {\tt 29263} {\tt .66868}\\ {\tt 1533052}\\ {\tt 21667} {\tt .7766023}\\ {\tt 1976} {\tt .99011}\\ {\tt 18812} {\tt .366022}\\ {\tt 16671} {\tt .756668}\\ {\tt 15380} {\tt .87775}\\ {\tt 14253} {\tt .899523}\\ {\tt 1277} {\tt .022755}\\ {\tt 11500} {\tt .66867167}\\ {\tt 10762} {\tt .5556618}\\ {\tt 10762} {\tt .5556618}\\ {\tt 10773} {\tt .6673}\\ {\tt 7732} {\tt .6780}\\ {\tt 676} {\tt .20702}\\ {\tt 8667} {\tt .20702}\\ {\tt 8667} {\tt .20702}\\ {\tt 8667} {\tt .20702}\\ {\tt 8676} {\tt .20702}\\ {\tt 8667} {\tt .20702}\\ {\tt 8676} {\tt .20702}\\ {\tt$

TABLE OF ZETA(2,A)

0

Δ 0680 0 . $\begin{array}{c} 0.000 \\$

0 Õ 0000 ŏ

000 0000

A $\begin{array}{c} \mathsf{A} \\ \mathsf{335} \\ \mathsf{000} \\ \mathsf{221445} \\ \mathsf{500} \\ \mathsf{000} \\ \mathsf{221455} \\ \mathsf{000} \\$

 $\begin{array}{c} \mathsf{X} \\ \mathsf{Z} \\ \mathsf{$

ZETA •786 •735 44 •

0 •

•

	•
A550506061120233445056667702777777777777777777777777777777	

7574
8.8711
8.8266
8.7825
8.7387
8.6953
8.6523
8.6096
8.5462
8.5043
8.4628
8.4216 8.4012
8.3808
8.3402
8.2801
8.2403 8.2206
8.2009
8.1618
8.1230
8.0653
8.0273
7.9895
7.9520 7.9334
7.9148
7.8779
7.8231
7.7869
$\begin{array}{c} \textbf{Z} \cdot \textbf{B} \\ \textbf{Z} \cdot \textbf{B} \\ \textbf{B} $

TABLE OF ZETA(2.A)

0. Õ

 $\begin{array}{c} \mathsf{A} \\ \mathsf{05} \\$

 $\begin{array}{c} \mathsf{A} & \mathsf{A} & \mathsf{B} & \mathsf{P} \\ \mathsf{A} & \mathsf{B} & \mathsf{P} & \mathsf{A} \\ \mathsf{B} & \mathsf{B} & \mathsf{P} & \mathsf{A} \\ \mathsf{B} & \mathsf{A} & \mathsf{B} & \mathsf{P} & \mathsf{A} \\ \mathsf{B} & \mathsf{A} & \mathsf{B} & \mathsf{P} & \mathsf{A} \\ \mathsf{B} & \mathsf{A} & \mathsf{B} & \mathsf{P} & \mathsf{A} \\ \mathsf{B} & \mathsf{A} & \mathsf{B} & \mathsf{P} & \mathsf{A} \\ \mathsf{B} & \mathsf{A} & \mathsf{B} & \mathsf{P} & \mathsf{A} \\ \mathsf{B} & \mathsf{A} & \mathsf{B} & \mathsf{P} & \mathsf{A} \\ \mathsf{B} & \mathsf{A} & \mathsf{P} & \mathsf{A} & \mathsf{A} \\ \mathsf{B} & \mathsf{A} & \mathsf{P} & \mathsf{A} & \mathsf{A} \\ \mathsf{B} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} \\ \mathsf{B} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} \\ \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} \\ \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} \\ \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} \\ \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} \\ \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} \\ \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} \\ \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} & \mathsf{A} \\ \mathsf{A} & \mathsf{A} \\ \mathsf{A} & \mathsf{A} \\ \mathsf{A} & \mathsf{A} \\ \mathsf{A} & \mathsf{A} \\ \mathsf{A} & \mathsf{$

	TABLE OF ZETA(2,A)	
$\begin{array}{c} 05050505050505050505050505050505050505$	ZE TAA $6 \cdot 0.2207$ 0.4746 $6 \cdot 0.2207$ 0.4745 $6 \cdot 0.2207$ 0.4755 $5 \cdot 9.656$ 0.4765 $5 \cdot 9.6566$ 0.4765 $5 \cdot 9.65739$ 0.47765 $5 \cdot 9.65088$ 0.47765 $5 \cdot 9.65088$ 0.47765 $5 \cdot 9.65088$ 0.47765 $5 \cdot 9.65088$ 0.47785 $5 \cdot 9.65088$ 0.47785 $5 \cdot 9.65088$ 0.47866 $5 \cdot 9.898760$ 0.48802 $5 \cdot 9.898760$ 0.48802 $5 \cdot 8.8876977$ 0.488265 $5 \cdot 8.8876977$ 0.4488775 $6 \cdot 8.8876977$ 0.4488775 $6 \cdot 8.8876977$ 0.4488775 $6 \cdot 8.88778929$ 0.4488775 $6 \cdot 8.8778929$ 0.4488775 $6 \cdot 8.8778929$ 0.4488775 $5 \cdot 8.8878822$ 0.49926 $5 \cdot 8.8778929$ 0.4488775 $5 \cdot 8.6588951$ 0.49926 $5 \cdot 8.6588951$ 0.49926 $5 \cdot 8.658789951$ 0.49926 $5 \cdot 8.658789951$ 0.49926 $5 \cdot 8.65877868822$ 0.49926 $5 \cdot 8.65877868822$ 0.49926 $5 \cdot 8.65877786$ 0.59773 $6 \cdot 8$	

	INDEE	J. 2
$ \begin{array}{c} A \\ 6450 \\ 5566670 \\ 0 \\ 5566670 \\ 0 \\ 0 \\ 5566670 \\ 0 \\ 0 \\ 557720 \\ 0 \\ 0 \\ 5577720 \\ 0 \\ 0 \\ 5577777780 \\ 0 \\ 0 \\ 0 \\ 557777780 \\ 0 \\ 0 \\ 0 \\ 557777780 \\ 0 \\ 0 \\ 0 \\ 557777780 \\ 0 \\ 0 \\ 0 \\ 55777780 \\ 0 \\ 0 \\ 0 \\ 5577780 \\ 0 \\ 0 \\ 0 \\ 5577780 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 5577880 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 $		4864219745320098745432110985437776664666666666666666666666666666666

23581594062976444454321298373885196646666666666677788889000112345670

TABLE OF ZETA(2,A)

 $\begin{array}{c} A \\ 0.6220 \\ 0.6230 \\ 0.6230 \\ 0.6230 \\ 0.6240 \\ 0.66240 \\ 0.66240 \\ 0.66240 \\ 0.66320 \\ 0.66320 \\ 0.66320 \\ 0.66330 \\ 0.66330 \\ 0.66330 \\ 0.66330 \\ 0.66330 \\ 0.66330 \\ 0.66330 \\ 0.66330 \\ 0.66440 \\ 0.66440 \\ 0.66440 \\ 0.66440 \\ 0.664510 \\ 0.665510 \\ 0.665560 \\ 0.665560 \\ 0.665560 \\ 0.665560 \\ 0.665560 \\ 0.665560 \\ 0.66550 \\ 0.66550 \\ 0.66550 \\ 0.66550 \\ 0.66550 \\ 0.66550 \\ 0.66570 \\ 0.66570 \\ 0.66570 \\ 0.66570 \\ 0.66570 \\ 0.66770 \\ 0.66770 \\ 0.66770 \\ 0.66770 \\ 0.6779 \\ 0.679 \\$

 $\begin{array}{c} \mathsf{A} = \mathsf{$

 $\begin{array}{c} A\\ 0.680\\ 0.6810\\ 0.6810\\ 0.6820\\ 0.6830\\ 0.6880\\ 0.6880\\ 0.6880\\ 0.6910\\ 0.6920\\ 0.69910\\ 0.69910\\ 0.69910\\ 0.69910\\ 0.69910\\ 0.6990\\ 0.6990\\ 0.6990\\ 0.6990\\ 0.6990\\ 0.6990\\ 0.6990\\ 0.6990\\ 0.6990\\ 0.7000\\ 0.7100\\ 0.71100\\ 0.71100\\ 0.71200\\ 0.71200\\ 0.71200\\ 0.72200\\ 0.72200\\ 0.73200\\ 0.73300\\ 0.73300\\ 0.73300\\ 0.73300\\ 0.73370\\ 0.73300\\ 0.73300\\ 0.73300\\ 0.73370\\ 0.73300\\ 0.73370\\ 0.73300\\ 0.73300\\ 0.73300\\ 0.73370\\ 0.73300\\ 0.73300\\ 0.73370\\ 0.73300\\ 0.73300\\ 0.73300\\ 0.73300\\ 0.73370\\ 0.73300\\ 0.7300\\ 0.7300\\ 0.7300\\ 0.7300\\ 0.7300\\ 0.7300\\ 0.7300\\ 0.7300\\ 0.7300\\ 0.7300\\ 0.7300\\ 0.7300\\ 0.7300\\ 0.7300\\ 0.7300\\ 0.7300\\ 0.7300\\$

	TABLE	OF	ZET	Α (2,	4)
$ \begin{array}{c} A\\ 73800\\ 0\\ 0\\ 7734200\\ 0\\ 0\\ 7744120\\ 0\\ 0\\ 0\\ 0\\ 7744120\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0\\ 0$			0494951629529631864219876655555667891246803581470482604938			

Z E TA 1.8848 1.8848 1.887565 1.887565 1.886634 1.885544 1.8855444 1.8855444 1.8855444 1.8855444 1.885333666 1.88239666 1.88239666 1.8821962 1.8821962 1.88107574 1.8800473 1.880047478 1.880047478 1.8800473 1.880047478 1.88004778 1.88004778 1.88004778 1.88004778 1.88004778 1.88004778 1.88004778 1.880047778 1.88004778 1.880047778 1.8800478 1.88004778 1.88004778 1.88004788 1.88004788 1.8800478 1.8800478 1.880 $\begin{array}{c} A\\ 0.9410\\ 0.9420\\ 0.9430\\ 0.9440\\ 0.9440\\ 0.9440\\ 0.9440\\ 0.9440\\ 0.9450\\ 0.9550\\ 0.9550\\ 0.9550\\ 0.9550\\ 0.9550\\ 0.9550\\ 0.9550\\ 0.9550\\ 0.9550\\ 0.9550\\ 0.9550\\ 0.9550\\ 0.9550\\ 0.9550\\ 0.9550\\ 0.9550\\ 0.9550\\ 0.9560\\ 0.96620\\ 0.96620\\ 0.96620\\ 0.96650\\ 0.$

ZE79902 L.79902 L.79902 L.79907 L.79335 L.78849 L.78849 L.77768 L.77768 L.77768 L.77768 L.77768 L.77768 L.77768 L.775203 L.773080 L.773080 L.773080 L.772257 L.72280 L.7280

TABLE OF ZETA(2,A)

IV. APPLICATIONS

The numerical results given in Tables 1 and 2 have been employed to evaluate the unmeasured resonance-level contribution in calculations of the neutron cross section and amplitude.⁽¹⁾ If the total resonance width is much smaller than the level spacing, the radiative neutron capture cross section is expressed in terms of the single-level Breit-Wigner formula:⁽⁹⁾

$$\sigma_{\rm c} = \frac{6.509 \times 10^{-19}}{\sqrt{\rm E}} \sum_{\rm level} \frac{{\rm g} \, \Gamma_{\rm p}^{\rm n} \, \Gamma_{\nu}}{({\rm E} - {\rm E}_{\lambda})^2 + (\Gamma^2/4)} \, ({\rm in \ cm}^2), \tag{20}$$

where g is the statistical weighing factor; Γ_n^0 the reduced neutron width, equal to $\sqrt{1 \text{ eV}/|E_\lambda|} \Gamma_n$, with Γ_n being the neutron width at the exact resonance; E and E_λ are the neutron energy and the resonance energy, respectively; Γ is the total width, expressed as $\Gamma = \Gamma_\nu + \sqrt{E/1 \text{ eV}} \Gamma_n^0$ with the radiation width Γ_ν . The energy parameters are all in eV. The summation should be taken for all positive and negative levels. In the region where $|E_\lambda| \gg E$, the $\Gamma^2/4$ term can be ignored. Therefore, for E = 0.0253 eV, we have

$$\sigma_{\rm c}({\rm distant}) = 4.0911 \times 10^{-18} \sum_{\rm level}' \frac{{\rm g} \Gamma_{\rm n}^0 \Gamma_{\nu}}{{\rm E}_{\lambda}^2}.$$
 (21)

The contribution of the unmeasured distant positive levels $\boldsymbol{\sigma}^u_c$ is calculated as follows:

$$\sigma_{\rm c}^{\rm u}({\rm distant}) = 4.0911 \ge 10^{-18} \frac{\langle g \Gamma_{\rm n}^0 \rangle \langle \Gamma_{\nu} \rangle}{\langle D \rangle^2} \sum_{\rm n=1}^{\infty} \frac{1}{(a_1 + n)^2}, \tag{22}$$

where

$$a_1 = E_{\lambda}^{(1)} / \langle D \rangle.$$
(23)

Here, the average resonance parameters obtained from the measured positive-level resonances are used; $\langle D \rangle$ is the mean level spacing; $E^{(1)}_{\lambda}$ is the highest measured positive level. The negative-level contribution $\Delta \sigma_c$ is then obtained from

$$\Delta \sigma_{\rm c} = \sigma_{\rm c} (\text{observed}) - \sigma_{\rm c} (\text{all positive levels}). \tag{24}$$

Statistical equivalence in the positive and negative level distributions near the binding energy is an established fact.(4,7) Therefore, we may use the approximation

$$\Delta \sigma_{\rm c} = 4.0911 \times 10^{-18} \frac{\langle {\rm g} \Gamma_{\rm n}^0 \rangle \langle \Gamma_{\nu} \rangle}{\langle {\rm D} \rangle^2} \sum_{\rm n=0}^{\infty} \frac{1}{({\rm a_2} + {\rm n})^2}, \tag{25}$$

where

$$a_2 = |E_{\lambda}^{(2)}|/\langle D \rangle,$$

and $E_{\lambda}^{(2)}$ is the highest negative level.

If the resultant $E_{\lambda}^{(2)}$ value does not satisfy the condition 0.0253 + $|E_{\lambda}^{(2)}| \gg \langle \Gamma \rangle / 2$, the first several terms may be computed by means of Equation (20); a few iterative refinements then lead to the final $E_{\lambda}^{(2)}$ value. In most cases, Equations (22) to (25) give a satisfactory result, unless $\sigma_{c}(obs)$ is abnormally large. The value of a_{1} is usually larger than unity, and hence the summation in Equation (22) is evaluated by use of Equation (5) and Tables 1 and 2. The negative-level parameter thus obtained is far from unique, but is meaningful from a statistical view of point. The most orthodox method for obtaining the negative-level parameters is a least-square analysis using all of available cross-section data; including the resonance-integral values.

The thermal-neutron coherent scattering amplitude b of an isotope is expressed as

$$b = a' + f' + if'',$$
 (26)

where a' is the potential scattering amplitude. For the resonance amplitudes f' and f'', we have

$$f' = 227.6 \sum_{\text{level}} \frac{g\Gamma_n^0(E - E_{\lambda})}{(E - E_{\lambda})^2 + (\Gamma^2/4)},$$
(27)

and

f'' = -113.8
$$\sum_{\text{level}} \frac{g\Gamma_n^0\Gamma}{(E - E_{\chi})^2 + (\Gamma^2/4)}$$
 (in 10⁻¹² cm). (28)

The imaginary component of the amplitude is usually negligibly small, except when the neutron energy is in the vicinity of a resonance level. In other words, the distant-level contribution to f" is in general too small to be significant. However, when high accuracy is required, one may evaluate the distant-level contribution by formulae similar to those previously derived for the capture cross section and $E_{\lambda}^{(2)}$.

The thermal-neutron value of f' for the unmeasured distant levels is obtained from the equation

$$f'_{\rm u}({\rm distant}) = -227.6 \times 10^{12} < g \Gamma_{\rm n}^{0} > \sum_{\rm level}^{\prime} \frac{1}{E_{\lambda}},$$
 (29)

where

$$\sum_{\text{evel}}^{\prime} \frac{1}{E_{\lambda}} = \frac{1}{\langle D \rangle} \left\{ \sum_{n=1}^{m_{1}} \frac{1}{a_{1}+n} - \sum_{n=0}^{m_{2}} \frac{1}{a_{2}+n} \right\}.$$
 (30)

The values of m_1 and m_2 should be chosen so that $a_1 + m_1 \approx a_2 + m_2$ and $m_2 \gg a_2$. The sum values for Equation (30) are obtained from Table 1.

$$\sum_{\text{level}}^{\prime} \frac{1}{E_{\lambda}^2} \approx \frac{1}{\langle D \rangle} \int_{E_1}^{\infty} \frac{1}{E^2} dE = \frac{1}{\langle D \rangle E_1}.$$
(31)

Equation (22) then becomes

$$\sigma_{\rm c}^{\rm u}({\rm distant}) = 4.0911 \times 10^{-18} \frac{\langle {\rm g} \Gamma_{\rm n}^{\rm o} \rangle \langle \Gamma_{\rm v} \rangle}{\langle {\rm D} \rangle {\rm E}_{\rm 1}}.$$
 (32)

A similar equation can be derived for f" as expressed in (28).

The distant-level contribution in the reduced R function^(5,14) is calculated similarly, using Table 1. The analytical form of the neutron resonance is analogous to the formula for anomalous optical dispersion. Hence, our tables are also useful in the interpretation of anomalous scattering and dispersion of X rays, mechanical resonance, resonating electric circuit, etc.

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