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# STUDIES OF THE SPHERICAL HARMONICS METHOD IN NEUTRON TRANSPORT THEORY

## IV. Completion of the Analysis of the Limit-Process $L \to \infty$ for the Milne Problem with Anisotropic Scattering and Absorption. Planning of the Numerical Calculations.

Walter Kofink

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ORNL-2901

Contract No. W-7405-eng-26

Director's Department

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DATE ISSUED

[illegible] 1960

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for the Milne Problem

with Anisotropic Scattering and Absorption.

Planning of the Numerical Calculations.

Walter Kofink*

## Introduction

In two earlier reports(1) it was shown that:

(1) the spherical harmonics solution in $P_L$-approximation for the angular distribution of neutrons at any point of the space in plane geometry is the exact solution of an equation, which one obtains by adding an "error-source" term to the original Boltzmann equation. This error-source is a multipole of the order $2^{L+1}$;

(2) the sum over $\ell = 0$ through L, which occurs in the $P_L$-approximation of the angular distribution, can be performed explicitly in the case of plane geometry by application of two Christoffel formulae. This summation enables one to show

(3) that the spherical harmonics solution for the angular distribution can be split in two expressions at every degree L of approximation. One of these two expressions is the corresponding solution which follows by application of the Gauss-quadrature method in the same degree L of approximation to the Boltzmann equation. This expression is in $\frac{L+1}{2}$ positive directions ($\mu_j = \cos \vartheta_j > 0$; $j = 1, 2, \ldots, \frac{L+1}{2}$) identical with the corresponding expression of the spherical harmonics method, namely, in those directions in which the second member of the split expression vanishes.

*On leave of absence from the Institute of Technology, Karlsruhe, Germany. This work is supported by the Bundesminister fuer Atomkernenergie und Wasserwirtschaft, Bad Godesberg, Germany.

(1) W. Kofink, "Studies of the Spherical Harmonics Method in Neutron Transport Theory", ORNL-2334 and ORNL-2358. Published partially in Nuovo Cimento, Sup. 2 to Vol. IX, p. 497-541 (1958). The equations of these reports are quoted here by the numerals I and II before their numbers.

In all other directions the angular distributions according to the spherical harmonics and the Gauss-quadrature method are different.

(4) This difference is removed by integration over all directions, and the average of the "error-source" over all directions vanishes, of course. Therefore the density, the flux, the characteristic equation and the coefficients in the Milne problem are identical in both methods at every degree L of approximation.

(5) These coefficients of the partial solutions entering the solution of the Milne problem were calculated for anisotropic scattering with absorption.

(6) It was shown that the second part of the spherical harmonics solution, which arose by the splitting, does not contribute at all to the exact solution in the limit-process $L \to \infty$. It is the Gauss-quadrature part of the angular distribution which converges straight forwardly to the exact solution of the Boltzmann equation for positive directions $\mu = \cos \vartheta$ (pointing to the vacuum). Using once more the Boltzmann equation to avoid the poles of the Gauss-quadrature solution in some negative directions (pointing to the deeper interior of the medium), an expression of the angular distribution for negative directions was obtained which should converge to the exact solution for $L \to \infty$.

(7) By application of Euler's sum formula the limit process was performed for the distance $\Lambda$ of the extrapolated endpoint, for the emerging angular distribution of the neutrons at the boundary of the medium into the vacuum and for the current-density.

In a third report,[2] the properties of the exact characteristic equation were investigated more closely. Furthermore, the degree $L_1$ of approximation by the spherical harmonics or the Gauss-quadrature method was calculated, at which

(2) W. Kofink, "Studies of the Spherical Harmonics Method in Neutron Transport Theory, Part III", ORNL-2850, (1959).

the largest root $\lambda_0$ of the approximate characteristic equation leaves the interval $0 \leq \lambda \leq 1$ converging to the corresponding root of the exact characteristic equation, which lies always on the outside of this interval for $c > 0$.

The purpose of this report is to complete the limit-process for the distance $\Delta$ of the extrapolated endpoint (see Equations 18a and 18b), for the linear extrapolation distance $\delta$ (see Equation 29), for some constants of normalizations N, $\rho(0)$ and $j(0)$ (see Equations 27, 28; 33a and 33b; 35a and 35b), for the angular distribution of the emerging neutrons at the boundary of the medium (see Equations 36a and 36b), for the current-density $j(\zeta)$ and for the density $\rho(\zeta)$ of the neutrons at an arbitrary point $\zeta$ in the interior of the medium (see Equations 38, 39, 43, 44, 46). All these expressions are calculated for anisotropic scattering with, respectively, a positive or a negative constant of anisotropy $a = 3\gamma_a(1-\gamma_t)$; that is, respectively, for preferred forward or preferred backward scattering, and for prevailing absorption, $\gamma_a > 0$ $(c < 1)$. The case of prevailing multiplication $\gamma_a < 0$, $c > 1$ is left for the future. Incidentally, the case of no absorption $c = 1$, $\gamma_a = 0$ is treated as an extraordinary case in section 3. In the sections 1 through 6 it will be shown that all quantities, mentioned above, can be represented with the aid of eight different integrals, denoted by $\Theta_0$, $\Theta^+$, $\Theta^-$, $\phi_a$, $\phi_0$, $\chi(\mu)$, $\chi_1$ and $\chi_2$ (see Equations 2 to 7 and 52, 53). All these integrals contain in their integrands a common weight function W(u) as a factor. W(u) is singular at the upper end $u = 1$ of the integration as $\sim(1-u)^{-1}\left[\log(1-u)\right]^{-2}$. This fact is inconvenient for the numerical calculation with the electronic computer. But the integrals are convergent in the area of the c,a-plane $\left[c < 1,\ -c(1-c) \leq a \leq c(1-c)\right]$, for which we want to produce tables this time. There are of course different ways to remove the singularity from the process of integration by the computer. Two methods are given in sections 7e and 7f. In the first method the integrals are integrated in their original form from $u = 0$ to $u = p$ $(p < 1)$ and the remainder of the integral

from $u = p$ to $u = 1$ is transformed into an integral without a singularity on a new finite path of integration. In the second method the whole integral is transformed into the new form.

Incidentally, the transformation of the integrals has some heuristic value also. The weight function $W(u)$ (see Equation 1, 1a, 1b and 56) mentioned above is connected with the continuous spectrum of the Boltzmann operator, which is a "non-normal" operator. By the transformation of the integrals a connection of the function $W(u)$ related to the continuous spectrum with the characteristic function (i.e., the secular determinant for $L \to \infty$) $Ch(\lambda)$ is uncovered. The roots of $Ch(\lambda) = 0$ form the discrete spectrum of the Boltzmann operator. $W(u)$ is replaced in the transformed integrands by the logarithmic derivative of $Ch(\lambda)/\lambda$ in a complex w-plane and the path of integration $u = 0$ to $u = 1$ is replaced by a finite complex path in the w-plane ($\lambda = \text{cotanh } w$ and see Equation 74). The procedure, starting with the spherical harmonics or Gauss quadrature approximations, going to the limit $L \to \infty$ and transforming the occurring integrals, will yield always the logarithmic derivative of $Ch(\lambda)/\lambda$. This function could be derived easily for any more complicated scattering law than that assumed here.

1. Some Notations.

Some results of the sections 3 to 7 of part II[1] will be rewritten here in a more concise form. To do that the following notations are introduced: A weight function

$$W(u) = \frac{hg}{1 - u^2} \equiv \frac{h(c,a;u)\ g(c,a,u)}{1 - u^2} \quad ; \tag{1}$$

$h(c,a;u)$ and $g(c,a;u)$ were defined in the equations (II 52 and 53)

$$h(c,a;u) = c + \left[c^2 - c + a(3-c)\right] u^2 + a\left[a + 3(c-1)\right] u^4 \tag{1a}$$

$$g(c,a;u) = 1\Big/\left\{\left[1 + au^2 - u(c+au^2)\ \tanh^{-1} u\right]^2 + \left[\frac{\pi}{2}\ u(c+au^2)\right]^2\right\} ; \tag{1b}$$

the function $W(u)$ occurs in the following integrals:

$$\Theta_0 = \frac{1}{2}\int_0^1 \left(\tanh^{-1} \frac{u}{\lambda_{0\infty}}\right) W(u)\ du \tag{2}$$

$$\Theta^+ = \frac{1}{2}\int_0^1 \left(\tan^{-1} \sqrt{\frac{a}{c}}\ u\right) W(u)\ du \qquad \left(\begin{array}{l}\text{for } a > 0 \\ \text{and } \frac{a}{c} < 1\end{array}\right) \tag{3}$$

$$\Theta^- = \frac{1}{2}\int_0^1 \left(\tanh^{-1} \sqrt{\frac{|a|}{c}}\ u\right) W(u)\ du \qquad \left(\begin{array}{l}\text{for } a < 0 \\ \text{and } \frac{|a|}{c} < 1\end{array}\right) \tag{4}$$

$$\phi_0 = \frac{1}{4}\int_0^1 \left[\log\left(1 - \frac{u^2}{\lambda_{0\infty}^2}\right)\right] W(u)\ du \tag{5}$$

$$\phi_a = \frac{1}{4}\int_0^1 \left[\log\left(1 + \frac{a}{c}\ u^2\right)\right] W(u)\ du \qquad (\text{for } a > -c) \tag{6}$$

$$\chi(\mu) = \frac{1}{2}\int_0^1 \left[\log(\mu + u)\right] W(u)\ du \qquad (\text{for } \mu \ \underline{\text{not}} \text{ in } -1 \leq \mu < 0)\ . \tag{7}$$

The functions (2) to (7) depend all on c and a by $\lambda_{0\infty}$ and W(u) in their integrands; but c and a are omitted mostly in the writing below. In part II (between the equations II 54 and II 55) it was shown that

$$\frac{1}{2}\int_0^1 W(u)\,du = 1 . \tag{8}$$

This integral is convergent; no doubt its integrand has a singularity at u = 1, but only of the kind

$$1\Big/\left\{(1-u)\left[\log(1-u)\right]^2\right\} = \frac{d}{du}\left[\log(1-u)\right]^{-1} .$$

This point, however, makes numerical calculations rather difficult and will be avoided by a transformation of the integrals, which contain W(u) in their integrands, in section 7.

By the integrals (2) to (7) defined above we shall express a sequence of constants and functions which appear in the neutron transport theory of the Milne problem. They were found in part II from their expressions in the spherical harmonics and Gauss-quadrature method in L-th approximation by going to the limit $L \to \infty$.

From the Equations I 33 and II 53 one recognizes that the function (7) is the limit

$$\lim_{L\to\infty} \log\left[-\frac{p(-\lambda)}{r(-\lambda)}\right] = \lim_{L\to\infty} \log \frac{\prod_{j=1}^{(L+1)/2}(\lambda+\mu_j)}{\prod_{s=1}^{(L-1)/2}(\lambda+\lambda_s)} = \chi(\lambda) . \tag{9}$$

$\lambda$ has to be chosen on the outside of the interval $-1 \le \lambda < 0$ in (9). The equation remains valid for $\lambda = 0$, for which Equations II 54 and 63 show that

$$\lim_{L\to\infty} \log\left[-\frac{p(0)}{r(0)}\right] = \chi(0) = \log\left(\sqrt{\gamma_a\gamma_t}\,\lambda_{0\infty}\right) \equiv \log\left(\sqrt{1-c-\frac{a}{3}}\,\lambda_{0\infty}\right) . \tag{9a}$$

2. The Distance of the Extrapolated Endpoint.

Equation (8) enables one to extract a factor $\mu$ from the integral $\chi(\mu)$. This yields Equation (II 55) which is valid under exclusion of the interval $-1 \leq \lambda \leq 0$:

$$\lim_{L \to \infty} \log \left( \frac{p(-\lambda)}{-\lambda\, r(-\lambda)} \right) = \frac{1}{2} \int_0^1 \log \left(1 + \frac{u}{\lambda}\right) W(u)\, du \,. \tag{10}$$

The reversal of the sign of $\lambda$ is then easy and leads to Equation (II 56). The difference of both is (with exclusion of the interval $-1 \leq \lambda \leq 1$)

$$\lim_{L \to \infty} \log \left[ - \frac{p(-\lambda)}{r(-\lambda)} \Big/ \left( \frac{p(\lambda)}{r(\lambda)} \right) \right] = \int_0^1 \left(\tanh^{-1} \frac{u}{\lambda}\right) W(u)\, du \,. \tag{11}$$

This function occurs in the distance of the extrapolated endpoint and in some normalization constants. For the characteristic root $\lambda = \lambda_{0\infty}$ it is the quantity named $\Theta_0$ in (2) and for $\lambda = \sqrt{\frac{c}{|a|}}$ it is the quantity named $\Theta^-$ in (4). The distance $\Delta$ of the extrapolated endpoint contains a function $\delta(\lambda)$, which is related to the expression on the left side of (11).

$$\tanh^{-1} \frac{\delta(\lambda)}{\lambda} = \frac{1}{2} \log \left[ - \frac{p(-\lambda)}{r(-\lambda)} \Big/ \left( \frac{p(\lambda)}{r(\lambda)} \right) \right]. \tag{12}$$

By comparison with (11) one recognizes that $\delta(\lambda)$ converges in the limit $L \to \infty$ to

$$\delta(\lambda) = \lambda \tanh \left[ \frac{1}{2} \int_0^1 \left(\tanh^{-1} \frac{u}{\lambda}\right) W(u)\, du \right] \tag{13}$$

for real $\lambda$ without writing the sign $\lim_{L \to \infty}$ before $\delta(\lambda)$ from now on. For pure imaginary $\lambda = ix$ one obtains

$$\delta(ix) = x \tan \left[ \frac{1}{2} \int_0^1 \left(\tan^{-1} \frac{u}{x}\right) W(u)\, du \right]. \tag{13a}$$

We consider in this report only the case $0 < c < 1$, in which the two roots $\pm \lambda_{0\infty}$ of the exact characteristic equation (II 58)

$$Ch(\lambda_{0\infty}) \equiv 1 + a\lambda_{0\infty}^2 - \lambda_{0\infty}(c+a\lambda_{0\infty}^2)\ \mathrm{cotanh}^{-1}\lambda_{0\infty} = 0 \tag{14}$$

are <u>real</u>. The constant of anisotropy a can be positive or negative. In anisotropic scattering the quantity (I 35)

$$\lambda_a = i\sqrt{\frac{c}{a}} = \begin{cases} i\sqrt{\frac{c}{a}} & \underline{\text{pure imaginary for positive a}} \quad (15a) \\ \sqrt{\frac{c}{|a|}} & \underline{\text{real for negative a}} \quad (15b) \end{cases}$$

plays a role. $\lambda_{0\infty}$ and $\lambda_a$ enter $\delta(\lambda)$ as a possible $\lambda$ and we shall meet later the following different versions

$$\delta(\lambda_a) = \begin{cases} \sqrt{\frac{c}{a}}\tan\left[\frac{1}{2}\int_0^1 (\tan^{-1}\sqrt{\frac{a}{c}}\,u)\,W(u)\,du = \sqrt{\frac{c}{a}}\tan\theta^+\right. & \text{for } a > 0 \quad (16a) \\ \sqrt{\frac{c}{|a|}}\tanh\left[\frac{1}{2}\int_0^1 (\tanh^{-1}\sqrt{\frac{|a|}{c}}\,u)\,W(u)\,du = \sqrt{\frac{c}{|a|}}\tanh\theta^-\right. & \text{for } a < 0 \quad (16b) \end{cases}$$

and

$$\delta(\lambda_{0\infty}) = \lambda_{0\infty}\tanh\left[\frac{1}{2}\int_0^1 \left(\tanh^{-1}\frac{u}{\lambda_{0\infty}}\right) W(u)\,du = \lambda_{0\infty}\tanh\theta_0\right. \quad \text{for } 0 < c < 1. \tag{17}$$

Then <u>the distance $\Delta$ of the extrapolated endpoint</u> is in the limit $L \to \infty$ [according to Equation (II 70), omitting the times sign before $\Delta$]

$$\Delta = \lambda_{0\infty}\begin{cases} \left[\theta_0 + \tanh^{-1}\left(\sqrt{\frac{a}{c}}\,\lambda_{0\infty}\tan\theta^+\right)\right] & a > 0 \quad (18a) \\ \left[\theta_0 - \tanh^{-1}\left(\sqrt{\frac{|a|}{c}}\,\lambda_{0\infty}\tanh\theta^-\right)\right] & a = -|a| < 0. \quad (18b) \end{cases}$$

3. The Case of No Absorption ($c = 1$).

Incidentally, we should remember the well-known special case of no absorption $c = 1$, $a = 0$. In this case $a = 3\gamma_a(1-\gamma_t) = 3(1-c)(1-\gamma_t)$ becomes 0 because of $c = 1$ for every arbitrary $\gamma_t$. But

$$\lim_{a\to 0,\ c\to 1,\ L\to\infty} \frac{a}{c}\lambda_{0\infty}^2 = \frac{1-\gamma_t}{\gamma_t}$$

is a finite constant, different from 0 for $\gamma_t \neq 1$, because the characteristic root $\lambda_{0\infty}$ (mean diffusion length in units of mean free path) goes to infinity for $c \to 1$ [see section I 9(a)]. Therefore this special case needs a more careful performance of the limit-process $a \to 0$. From (18b) one obtains for instance

$$\Delta = \frac{1}{\gamma_t}\cdot\frac{1}{2}\int_0^1 u\,W(u)\,du \quad \text{for } c = 1 \text{ and arbitrary } \gamma_t. \tag{19}$$

($\gamma_t \neq 1$ for anistropic scattering, $\gamma_t = 1$ for isotropic scattering.)

This simple limit will be assumed, because the arguments of all the $\tanh^{-1}$ and tanh involved in $\Delta$, $\Theta_0$ and $\Theta^-$ converge to 0. Hence the first and the second terms on the right side of equation (18b) converge to the following limits:

$$\lim_{(a\to 0,\, c\to 1)} \lambda_{0\infty}\,\Theta_0 = \frac{1}{2}\int_0^1 u\,W(u)\,du$$

$$\lim_{(a\to 0,\, c\to 1)} \lambda_{0\infty}\tanh^{-1}\left(\sqrt{\frac{|a|}{c}}\,\lambda_{0\infty}\tanh\Theta^-\right) = \lim_{(a\to 0,\, c\to 1)} \frac{|a|}{c}\lambda_{0\infty}^2\cdot\frac{1}{2}\int_0^1 u\,W(u)\,du$$

$$= \frac{\gamma_t - 1}{\gamma_t}\cdot\frac{1}{2}\int_0^1 u\,W(u)\,du\,.$$

From the last equation we see that the second term gives a contribution to $\Delta$ for no absorption ($c = 1$) but anisotropic scattering $\gamma_t \neq 1$, although the constant a vanishes. This was well known long ago.

One may add a further interesting remark to this special case. The <u>limit of the difference</u> $M_1 - \Lambda_1$ between the sum $M_1$ of the positive roots $\mu_j$ of the characteristic equation (I 14) for $\sigma = 0$

$$P_{L+1}(\mu_j) = 0 \quad (j = 1, 2, \ldots, \frac{L+1}{2})$$

and the sum $\Lambda_1$ of the positive roots of the characteristic equation (I 65) for $c = 1$ (leaving out $\lambda_0$ however), both in L-th approximations,

$$P_{L+1}(\lambda_s) - \lambda_s W_L(\lambda_s) = 0 \quad (s = 1, 2, \ldots, \frac{L-1}{2})$$

is connected with $\bar{u}$, the mean value of u over $\frac{1}{2} W(u)$,

$$\lim_{L\to\infty} (M_1 - \Lambda_1) \equiv \lim_{L\to\infty} \left\{ \sum_{j=1}^{(L+1)/2} \mu_j - \sum_{s=1}^{(L-1)/2} \lambda_s \right\} = \frac{1}{2} \int_0^1 u\, W(u)\, du \equiv \bar{u} = 0.7104 \tag{20}$$

for arbitrary $\gamma_t$ and $c = 1$. In this case the distance $\Delta$ of the extrapolated end-point and the linear extrapolation distance $\delta$ become equal, namely

$$\Delta = \delta = \frac{\bar{u}}{\gamma_t} . \tag{19a}$$

A last remark to this special case of no absorption results from the comparison of $\lim_{a=0,\, c\to 1} \gamma_a \gamma_t \lambda_0^2 = \frac{1}{3}$ (equation I 59) and equation (9a), which gives the mean value of log u over $\frac{1}{2} W(u)$

$$\overline{\log u} \equiv \frac{1}{2} \int_0^1 (\log u)\, W(u)\, du \equiv \chi(0) \Big/_{\substack{c=1 \\ a=0}} = \lim_{\substack{a\to 0,\, c\to 1 \\ L\to\infty}} \log\left(\sqrt{\gamma_a \gamma_t}\, \lambda_0\right) = -\frac{1}{2} \log 3 \tag{21}$$

for arbitrary $\gamma_t$ and $c = 1$.

W(u) has of course in this section its form for c = 1, a = 0, namely,

$$W(u) = \frac{1}{(1-u^2)\left[(1-u\tanh^{-1}u)^2 + (\frac{\pi}{2}u)^2\right]} \quad . \tag{1a}$$

4. Different Ways of Normalization.

(a) For normalization to unit density at the boundary $\zeta = 0$ one has to calculate [see equation (I 53)]

$$\rho(0) = 2\pi \int_{-1}^{+1} f(0,\mu)\, d\mu = \lim_{L\to\infty} 4\pi \sum_{k=\bar{0},0,1\ldots}^{(L-1)/2} \alpha_k = \lim_{L\to\infty} 8\pi\, N(1+\frac{a}{c}\lambda_0^2)\frac{p(0)}{r(0)}$$

$$= 8\pi(1+\frac{a}{c}\lambda_{0\infty}^2)\lim_{L\to\infty} N\frac{p(0)}{r(0)} \tag{22}$$

$$= -8\pi\sqrt{1-c-\frac{a}{3}}\,\lambda_{0\infty}\,(1+\frac{a}{c}\lambda_{0\infty}^2)\lim_{L\to\infty} N$$

after the application of equation (II 63). It remains to calculate $\lim_{L\to\infty} N$. N was defined by equation (I 36). We consider

$$\lim_{L\to\infty}\frac{1}{N} = \lim_{L\to\infty}\frac{\delta(\lambda_0)+\frac{a}{c}\lambda_0^2\delta(\lambda_a)}{\delta(\lambda_0)}\left[\frac{p(-\lambda_0)}{r(-\lambda_0)}+\frac{p(\lambda_0)}{r(\lambda_0)}\right] . \tag{23}$$

The first factor results immediately from the equations (16a, b, 17)

$$\frac{\delta(\lambda_0)+\frac{a}{c}\lambda_{0\infty}^2\delta(\lambda_a)}{\delta(\lambda_0)} = \begin{cases} 1+\sqrt{\frac{a}{c}}\,\lambda_{0\infty}\tan\theta^+\operatorname{cotanh}\theta_0 & \text{for } a>0 \quad (24a)\\ 1-\sqrt{\frac{|a|}{c}}\,\lambda_{0\infty}\tanh\theta^-\operatorname{cotanh}\theta_0 & \text{for } a<0 \quad . \quad (24b)\end{cases}$$

The second factor of the equation (23) follows from the equation (10)

$$\lim_{L\to\infty}\left\{\frac{p(-\lambda_0)}{r(-\lambda_0)}+\frac{p(\lambda_0)}{r(\lambda_0)}\right\} = -\lambda_{0\infty}\left[e^{\frac{1}{2}\int_0^1\log(1+\frac{u}{\lambda_{0\infty}})W(u)\,du} - e^{\frac{1}{2}\int_0^1\log(1-\frac{u}{\lambda_{0\infty}})W(u)\,du}\right] \tag{25}$$

$$= -2\lambda_{0\infty}e^{\phi_0}\sinh\theta_0$$

with $\phi_0$ from equation (5) and $\theta_0$ from equation (2) and the formula

$$e^{x_1} - e^{x_2} = 2\, e^{\frac{1}{2}(x_1+x_2)} \sinh \tfrac{1}{2}(x_1-x_2) \; .$$

Hence one obtains

$$\lim_{L\to\infty} \frac{1}{N} = -2\lambda_{0\infty}\, e^{\phi_0} \cdot \begin{cases} \left[\sinh\theta_0 + \sqrt{\frac{a}{c}}\,\lambda_{0\infty} \tan\theta^+ \cosh\theta_0\right] & \text{for } a > 0 \quad (26a) \\ \left[\sinh\theta_0 - \sqrt{\frac{|a|}{c}}\,\lambda_{0\infty} \tanh\theta^- \cosh\theta_0\right] & \text{for } a < 0 \,. \quad (26b) \end{cases}$$

Both of these versions for $a > 0$ and $a < 0$, respectively, can be rewritten as <u>one</u> formula by the introduction of the distance $\Delta$ of the extrapolated endpoint from equations (17a, b), which gives

$$\left.\begin{array}{ll} \text{for } a > 0: & \sqrt{\frac{a}{c}}\,\lambda_{0\infty} \tan\theta^+ \\ \text{for } a < 0: & -\sqrt{\frac{|a|}{c}}\,\lambda_{0\infty} \tanh\theta^- \end{array}\right\} = \tanh\left(\frac{\Delta}{\lambda_{0\infty}} - \theta_0\right) . \qquad (18)$$

Therefore one gets finally

$$\lim_{L\to\infty} N = \frac{e^{-\phi_0}}{2\,\lambda_{0\infty}} \left[\sinh\theta_0 - \cosh\theta_0 \operatorname{cotanh}\frac{\Delta}{\lambda_{0\infty}}\right] \qquad (27)$$

and

$$\rho(0) = 4\pi\sqrt{1 - c - \frac{a}{3}}\left(1 + \frac{a}{c}\lambda_{0\infty}^2\right) e^{-\phi_0}\left[\cosh\theta_0 \operatorname{cotanh}\frac{\Delta}{\lambda_{0\infty}} - \sinh\theta_0\right] . \qquad (28)$$

One remembers from equation (I 20) that the <u>linear extrapolation distance</u> $\delta$ is just

$$\frac{\delta}{\lambda_{0\infty}} = \tanh\frac{\Delta}{\lambda_{0\infty}} \; . \qquad (29)$$

Hence one may introduce $\delta$ instead of $\Delta$ in equation (27)

$$\rho(0) = 4\pi\sqrt{1 - c - \frac{a}{3}}\left(1 + \frac{a}{c}\lambda_{0\infty}^2\right)\left[\frac{\lambda_{0\infty}}{\delta} \cosh\theta_0 - \sinh\theta_0\right] . \qquad (30)$$

(b) For normalization to unit current density at the boundary $\zeta = 0$ one has to calculate [see equation (I 55)]

$$j(0) = 2\pi \int_{-1}^{+1} \mu f(0,\mu)\, d\mu = \lim_{L\to\infty} \left( - 4\pi(1-c) \sum_{k=\bar{0},0,1\ldots}^{(L-1)/2} \alpha_k \lambda_k \right)$$

$$= 16\pi(1-c)\, \lambda_{0\infty}^2 \lim_{L\to\infty} N \frac{p(\lambda_a)\, p(-\lambda_a)}{\lambda_a \left[ r(-\lambda_a)\, p(\lambda_a) - r(\lambda_a)\, p(-\lambda_a) \right]} \quad . \tag{31}$$

For the reciprocal of the last factor follows again from equation (10)

$$\lim_{L\to\infty} \lambda_a \left\{ \frac{r(-\lambda_a)}{p(-\lambda_a)} - \frac{r(\lambda_a)}{p(\lambda_a)} \right\} = - 2 e^{-\phi_a} \begin{cases} \cos\theta^+ & \text{for } a > 0 \quad (32a) \\ \cosh\theta^- & \text{for } a < 0 \quad (32b) \end{cases}$$

and we obtain

$$j(0) = \frac{4\pi(1-c)\, \lambda_{0\infty}\, e^{(\phi_a - \phi_0)}}{\begin{Bmatrix} \cos\theta^+ \sinh\theta_0 + \sqrt{\frac{a}{c}}\, \lambda_{0\infty} \sin\theta^+ \cosh\theta_0 & (33a) \\ \cosh\theta^- \sinh\theta_0 - \sqrt{\frac{|a|}{c}}\, \lambda_{0\infty} \sinh\theta^- \cosh\theta_0 & (33b) \end{Bmatrix}}$$

with the upper expression in the denominator for $a > 0$ and the lower expression for $a < 0$. Using the distance $\Delta$ of the extrapolated endpoint for the representation of $j(0)$, we get

$$j(0) = \frac{4\pi(1-c)\, \lambda_{0\infty}\, e^{(\phi_a - \phi_0)}}{\begin{Bmatrix} \cos\theta^+ \\ \cosh\theta^- \end{Bmatrix}} \left[ \cosh\theta_0 \operatorname{cotanh} \frac{\Delta}{\lambda_{0\infty}} - \sinh\theta_0 \right] \quad . \qquad \begin{matrix} (34a) \\ (34b) \end{matrix}$$

The gradient of both normalization constants (28) and (34) is

$$\frac{\rho(0)}{j(0)} = \frac{\sqrt{1 - c - \frac{a}{3}}\, (1 + \frac{a}{c} \lambda_{0\infty}^2)\, e^{-\phi_a}}{(1-c)\, \lambda_{0\infty}} \cdot \begin{cases} \cos\theta^+ & \text{for } a > 0 \quad (35a) \\ \cosh\theta^- & \text{for } a < 0 \quad (35b) \end{cases} \quad .$$

## 5. The Angular Distribution of the Emerging Neutrons at the Boundary of the Medium.

In equation (II 75) the angular distribution $f(0,\mu)$ at $\zeta = 0$ in the direction $\mu = \cos\vartheta$ was normalized to unit current density $j(0) = 2\pi\int_0^1 \mu\, f(0,\mu)\, d\mu$ at $\zeta = 0$. The limit $L \to \infty$ was taken from the Gauss quadrature expression $f^I(0,\mu)$ in L-th approximation (I 41). Applying the equations (9; 16a, b; 32a, b) to equation (II 75) one gets for $0 \leq \mu \leq 1$

$$\frac{f(0,\mu)}{j(0)} = \lim_{L\to\infty} \frac{f^I(0,\mu)}{2\pi\int_{-1}^{+1} \mu\, f(0,\mu)\, d\mu}$$

$$= \frac{c + a\lambda_{0\infty}^2}{8\pi(1-c)} \; \frac{1 + \frac{a}{c}\,\delta(\lambda_a)\mu}{\lambda_{0\infty}^2 - \mu^2} \cdot \lim_{L\to\infty}\left\{\lambda_a\left[\frac{r(\lambda_a)}{p(\lambda_a)} - \frac{r(-\lambda_a)}{p(-\lambda_a)}\right] \cdot \left(-\frac{p(-\mu)}{r(-\mu)}\right)\right\}$$

$$= \frac{c + a\lambda_{0\infty}^2}{4\pi(1-c)(\lambda_{0\infty}^2 - \mu^2)}\, e^{[\chi(\mu) - \phi_a]} \cdot \begin{cases} \cos\theta^+ + \sqrt{\frac{a}{c}}\,\mu\,\sin\theta^+ & a > 0 \quad (36a) \\ \cosh\theta^- - \sqrt{\frac{|a|}{c}}\,\mu\,\sinh\theta^- & a < 0 \quad (36b) \end{cases}$$

$$= \frac{c + a\lambda_{0\infty}^2}{4\pi(1-c)} \; \frac{1 + \frac{\mu}{\lambda_{0\infty}}\tanh\left(\frac{\Delta}{\lambda_{0\infty}} - \theta_0\right)}{\lambda_{0\infty}^2 - \mu^2} \cdot e^{[\chi(\mu) - \phi_a]} \cdot \begin{cases} \cos\theta^+ & a > 0 \quad (36c) \\ \cosh\theta^- & a < 0 \quad (36d) \end{cases}$$

## 6. The Current-Density and the Density of the Neutrons.

It was shown in part II, section 7, that the limit-process $L \to \infty$ can be performed with higher mathematical precision for the current density $j(\zeta)$ than for the density $\rho(\zeta)$ itself. For $c \neq 1$ the relation

$$(c-1)\,\rho(\zeta) = \frac{\partial j(\zeta)}{\partial \zeta} \qquad (37)$$

may be used to derive $\rho(\zeta)$ later from $j(\zeta)$ . In L-th approximation the following expressions hold (I 21, 51)

$$\rho(\zeta) = 2\pi \int_{-1}^{+1} f(\zeta,\mu)\, d\mu = 4\pi\, f_{00}(\zeta) = 4\pi \sum_{k=\bar{0},0,1,\ldots}^{(L-1)/2} \alpha_k\, e^{\zeta/\lambda_k}$$

$$= 4\pi \left\{ \frac{\sinh\left[(\Delta-\zeta)/\lambda_0\right]}{\sinh \Delta/\lambda_0} + \sum_{s=1,2,\ldots}^{(L-1)/2} \alpha_s\, e^{\zeta/\lambda_s} \right\} \tag{38}$$

and by use of equation (37)

$$j(\zeta) = 4\pi(1-c) \left\{ \frac{\lambda_0 \cosh\,(\Delta-\zeta)/\lambda_0}{\sinh\,(\Delta/\lambda_0)} - \sum_{s=1,2,\ldots}^{(L-1)/2} \alpha_s\, \lambda_s\, e^{\zeta/\lambda_s} \right\} . \tag{39}$$

The first, so-called asymptotic parts of both expressions go immediately to the limit for $L \to \infty$

$$\rho_a(\zeta) = 4\pi \frac{\sinh\left[(\Delta-\zeta)/\lambda_{0\infty}\right]}{\sinh(\Delta/\lambda_{0\infty})} \qquad \zeta \leq 0 \tag{40}$$

and

$$j_a(\zeta) = 4\pi(1-c)\, \lambda_{0\infty} \frac{\cosh\left[(\Delta-\zeta)/\lambda_{0\infty}\right]}{\sinh(\Delta/\lambda_{0\infty})} \qquad \zeta \leq 0 \tag{41}$$

in which $\Delta$ now has the meaning of equations (18a, b) and $\lambda_{0\infty}$ is the root of the exact characteristic equation (14). The normalization of (38) and (39) is such that the two coefficients $\alpha_{\bar{0}}$ and $\alpha_0$ of the 2 asymptotic partial solutions have the sum $\alpha_{\bar{0}} + \alpha_0 = 1$. Consequently, the asymptotic part of the density $\rho_a(0)$ at the boundary is normalized to $4\pi$ and the asymptotic part of the current-density is normalized to

$$j_a(0) = 4\pi(1-c)\, \lambda_{0\infty} \operatorname{cotanh}\left(\frac{\Delta}{\lambda_{0\infty}}\right) \tag{42a}$$

$$= \frac{4\pi(1-c)\, \lambda_{0\infty}^2}{\delta} . \tag{42b}$$

In the last expression the linear extrapolation length is introduced by applying equation (29). Other normalizations may be introduced for instance by using equations (28) or (34).

Finally we have to perform the limit-process $L \to \infty$ for the transient parts

$$j_t(\zeta) = 4\pi(c-1) \lim_{L \to \infty} \sum_{s=1,2,\ldots}^{(L-1)/2} \alpha_s \lambda_s \, e^{\zeta/\lambda_s} \tag{43}$$

and

$$\rho_t(\zeta) = \frac{1}{c-1} \frac{\partial j_t(\zeta)}{\partial \zeta} \qquad (c \neq 1) \quad . \tag{44}$$

The last equation suggests to obtain $\rho_t(\zeta)$ by numerical differentiation from $j_t(\zeta)$. We perform the $\lim\limits_{L \to \infty}$ for $j_t(\zeta)$ according to part II, section 7:

$$j_t(\zeta) = 4\pi(c-1) \lim_{L \to \infty} \sum_{s=1,2\ldots}^{(L-1)/2} \alpha_s \lambda_s \, e^{\zeta/\lambda_s}$$

$$= \frac{4\pi(c-1)}{2\pi i} \lim_{L \to \infty} \oint_{C_j} \chi(\mu) \, e^{\zeta/\mu} \, d\mu \quad \left[\text{see equation (II 82)}\right]$$

$$= -\frac{4\pi(1-c)}{2\pi i} \, 2\lambda_{0\infty}^2 \, (c + a\lambda_{0\infty}^2) \lim_{L \to \infty} \left\{ N \oint_{C_j} \frac{\left[1 - \frac{a}{c}\mu\,\delta(\lambda_a)\right] e^{\zeta/\mu}}{(c + a\mu^2)(\mu^2 - \lambda_{0\infty}^2)} \frac{p(\mu)}{r(\mu)} \, d\mu \right\} \tag{45}$$

$$= \frac{4\pi(1-c)(c+a\lambda_{0\infty}^2) \; e^{-\phi_0}}{\cosh\theta_0 \, \mathrm{cotanh}\,\frac{\Delta}{\lambda_{0\infty}} - \sinh\theta_0} \; \frac{1}{2\pi i} \oint_{C_j} \frac{\lambda_{0\infty} - \mu \tanh\left(\frac{\Delta}{\lambda_{0\infty}} - \theta_0\right)}{(c+a\mu^2)(\lambda_{0\infty}^2 - \mu^2)} \, e^{\left[\chi(-\mu) + \frac{\zeta}{\mu}\right]} d\mu \; .$$

One finds the last equation by applying the equations (27; 16a, b; 18; 9) to the third. Finally we remember that the medium lies on negative $\zeta = -|\zeta|$ and we obtain

$$j_t(\zeta) = \frac{2(1-c)(c+a\lambda_{0\infty}^2)\, e^{-\phi_0}}{\cosh\theta_0 \operatorname{cotanh}\frac{\Delta}{\lambda_{0\infty}} - \sinh\theta_0} (-i) \oint_{C_j} \frac{\lambda_{0\infty} - \mu \tanh\left(\frac{\Delta}{\lambda_{0\infty}} - \theta_0\right)}{(c+a\mu^2)(\lambda_{0\infty}^2 - \mu^2)} e^{\left[\chi(-\mu) - \frac{|\zeta|}{\mu}\right]} d\mu \,. \tag{46}$$

The closed complex path $C_j$ of integration has to encircle the real interval $0 \leq \mu \leq 1$ counter-clockwise <u>excluding</u>, however, <u>the points</u> $\mu = \pm\lambda_a$ and $\mu = \pm\lambda_{0\infty}$.

For $a < 0$ it is easy to show that $\lambda_a = \sqrt{\frac{c}{|a|}}$ is larger than $\lambda_{0\infty}$. In part III it was shown that $\lambda_{0\infty}$ remains constant on a straight line in the c, a-plane. If we name $c_0$ the point in which this straight line cuts the c-axis, we can represent <u>the anistropy constant</u> a by c, $c_0$, $\lambda_{0\infty}$, using the characteristic equation (14) for $a \neq 0$ and $a = 0$:

$$a = \frac{c_0 - c}{\lambda_{0\infty}^2(1-c_0)} \quad \text{with} \quad c_0 = \frac{1}{\lambda_{0\infty} \operatorname{cotanh}^{-1} \lambda_{0\infty}} \,.$$

For $a < 0$ we have $c_0 < c$, because $1 - c_0$ is always $>0$, and we may express

$$\lambda_a = \sqrt{\frac{c}{|a|}} = \lambda_{0\infty}\sqrt{\frac{c(1-c_0)}{c - c_0}} \,.$$

The radicand

$$\frac{c(1-c_0)}{c - c_0} = 1 + \frac{c_0(1-c)}{c - c_0} > 1$$

is larger than 1, because the additional term to 1 is $> 0$ in consequence of $c_0 > 0$ and $c_0 < c < 1$ for $a < 0$ (compare for instance l.c.[2] Figure 2). Hence we have always

$$\lambda_a > \lambda_{0\infty} \quad \text{for} \quad a < 0 \quad \text{and} \quad 0 < c < 1 \ . \tag{47}$$

Furthermore we know that $\lambda_{0\infty} > 1$ for $0 < c < 1$. A convenient path $C_j$ of integration would be a circle with its center in $\mu = \frac{1}{2}$ and with its radius $\frac{1}{2}\lambda_{0\infty}$ for the case $a < 0$. This circle cuts the real axis in the point $\frac{1}{2}(1+\lambda_{0\infty}) < \lambda_{0\infty}$ on the right side between 1 and $\lambda_{0\infty}$ and in the point $\frac{1}{2}(1-\lambda_{0\infty}) < 0$ between 0 and $-\lambda_{0\infty}$ on the left side of its center. Therefore this path fulfills the conditions which were imposed on it.

The equation of the circle in the complex $\mu$-plane is

$$\mu \equiv \mu_1 + i\mu_2 = \frac{1}{2}(1+\lambda_{0\infty}e^{i\eta}) \ , \tag{48}$$

if $\eta$ is the angle between the real $\mu$-axis and the radius to the point $\mu$. Then we have

$$\mu_1 = \frac{1}{2}(1+\lambda_{0\infty}\cos\eta) \ , \qquad \mu_2 = \frac{1}{2}\lambda_{0\infty}\sin\eta \ ; \tag{48a}$$

furthermore, we use the abbreviations

$$m = \mu_1^2 + \mu_2^2 = \frac{1}{4}(\lambda_{0\infty}^2 + 1 + 2\lambda_{0\infty}\cos\eta), \quad m_1 = \mu_1/m \ , \quad m_2 = \mu_2/m \ ,$$

$$m_0 = \mu_1^2 - \mu_2^2 = \frac{1}{4}(1 + 2\lambda_{0\infty}\cos\eta + \lambda_{0\infty}^2\cos 2\eta) \ . \tag{48b}$$

The differential $d\mu$ becomes

$$d\mu = i\,\frac{\lambda_{0\infty}}{2}\,e^{i\eta}\,d\eta = \left[-\mu_2 + i(\mu_1 - \tfrac{1}{2})\right] d\eta\,. \tag{49}$$

The introduction of $\eta$ into the transient part $j_t(\zeta)$ of the current (equation 46) yields

$$j_t(\zeta) = \frac{2(1-c)(c+a\lambda_{0\infty}^2)\,e^{-\phi_0}}{\cosh\theta_0\,\mathrm{cotanh}\,\dfrac{\Delta}{\lambda_{0\infty}} - \sinh\theta_0}\,\cdot \tag{46a}$$

$$\cdot\int_0^{2\pi} d\eta\,\frac{e^{(\chi_1 - m_1|\zeta|)}}{V_1^2 + V_2^2}\left\{(V_1Y_2 - V_2Y_1)\cos(\chi_2 + m_2|\zeta|) - (V_1Y_1 + V_2Y_2)\sin(\chi_2 + m_2|\zeta|)\right\},$$

in which some new abbreviations have the following meaning:

$$\left.\begin{aligned}
V_1 &= c(\lambda_{0\infty}^2 - m_0) + a\left[m^2 + m_0(\lambda_{0\infty}^2 - 2m_0)\right]\\
V_2 &= 2\mu_1\mu_2\left[c - a(\lambda_{0\infty}^2 - 2m_0)\right]\\
Y_1 &= -\mu_2(\lambda_{0\infty} - \frac{t_o}{2} - 2t_o\,\mu_1)\\
Y_2 &= -\frac{1}{2}\lambda_{0\infty} - (\lambda_{0\infty} - \frac{t_o}{2})\,\mu_1 + t_0 m_0\;;
\end{aligned}\right\} \tag{50}$$

$$t_0 = \tanh\left(\frac{\Delta}{\lambda_{0\infty}} - \theta_0\right)\;; \tag{51}$$

$$\chi_1 \equiv \chi_1(\mu_1,\mu_2) = \frac{1}{4}\int_0^1 \log\left[m - 2\mu_1 u + u^2\right] W(u)\, du \tag{52}$$

$$\chi_2 \equiv \chi_2(\mu_1,\mu_2) = \frac{1}{2}\int_0^1 \left(\tan^{-1}\frac{\mu_2}{\mu_1 - u}\right) W(u)\, du \tag{53}$$

and in which $\mu_1$, $\mu_2$, m, $m_0$, $m_1$, $m_2$ are given as functions of $\eta$ by the equations (48a, b) and $\chi_1(\mu_1,\mu_2) + i\,\chi_2(\mu_1,\mu_2) = \chi(-\mu)$.

For $a > 0$, however, a similar simple estimate of the position of

$$\lambda_a = i\sqrt{\frac{c}{a}} = i\,\lambda_{0\infty}\sqrt{\frac{c(1-c_0)}{c_0 - c}} \tag{54}$$

gives only $0 < |\lambda_a| < \infty$; this inequality does not give any information in which case $\lambda_a$ lies on the outside of the circle $C_j$, which we chose as the path of integration for $a < 0$. If we want to use this circle also for $a > 0$, $\lambda_a$ has to fulfill the following inequation:

$$|\lambda_a|^2 \equiv \frac{c}{a} > \frac{1}{4}\left(\lambda_{0\infty}^2 - 1\right) . \tag{55}$$

The right side of this inequation is the square of the ordinate at which the circle $C_j$ cuts the imaginary axis in the complex $\mu$-plane.

On curve I in Figure 1 is $|\lambda_a|^2 \equiv \frac{c}{a} = \frac{1}{4}\lambda_{0\infty}^2 - 1$ and for all c, a-values below this curve the inequality (55) is fulfilled. In the area above curve I the inequality (55) is not satisfied; in fact, $\lambda_{0\infty}$ increases to the limit $\infty$, if a increases (at c = const.) until it reaches the straight line $a = 3(1 - c)$, whereas $|\lambda_a|^2$ decreases to the limit $c/\left[3(1 - c)\right]$ on that line. The straight

line $a = 3(1 - c)$ in Figure 1 is the border of all cases belonging to exponentially decreasing or increasing solutions of the Boltzmann equation. On the right side of this line we have oscillatory solutions, which we do not consider in this report.

The curve I, however, comprehends a much ampler area of c, a-values than curve III with the equation $a = c(1 - c)$. The points below curve III satisfy the condition that the probability of a single neutron scattering event (including fission and absorption) is non-negative in every direction, and it is assumed that scattering, absorption and fission obey the same linear anisotropic law. This condition is called sometimes the "geometrical condition". Under these assumptions the area of the c, a-values, for which stationary solutions exist is so much restricted that the use of the circle $C_j$ as the path of integration is also allowed for $a > 0$.

Curve II in Figure 1 finally satisfies the equation $|\lambda_a| = \lambda_{0\infty}$; $|\lambda_a|$ is larger than $\lambda_{0\infty}$ below resp. smaller than $\lambda_{0\infty}$ above curve II.

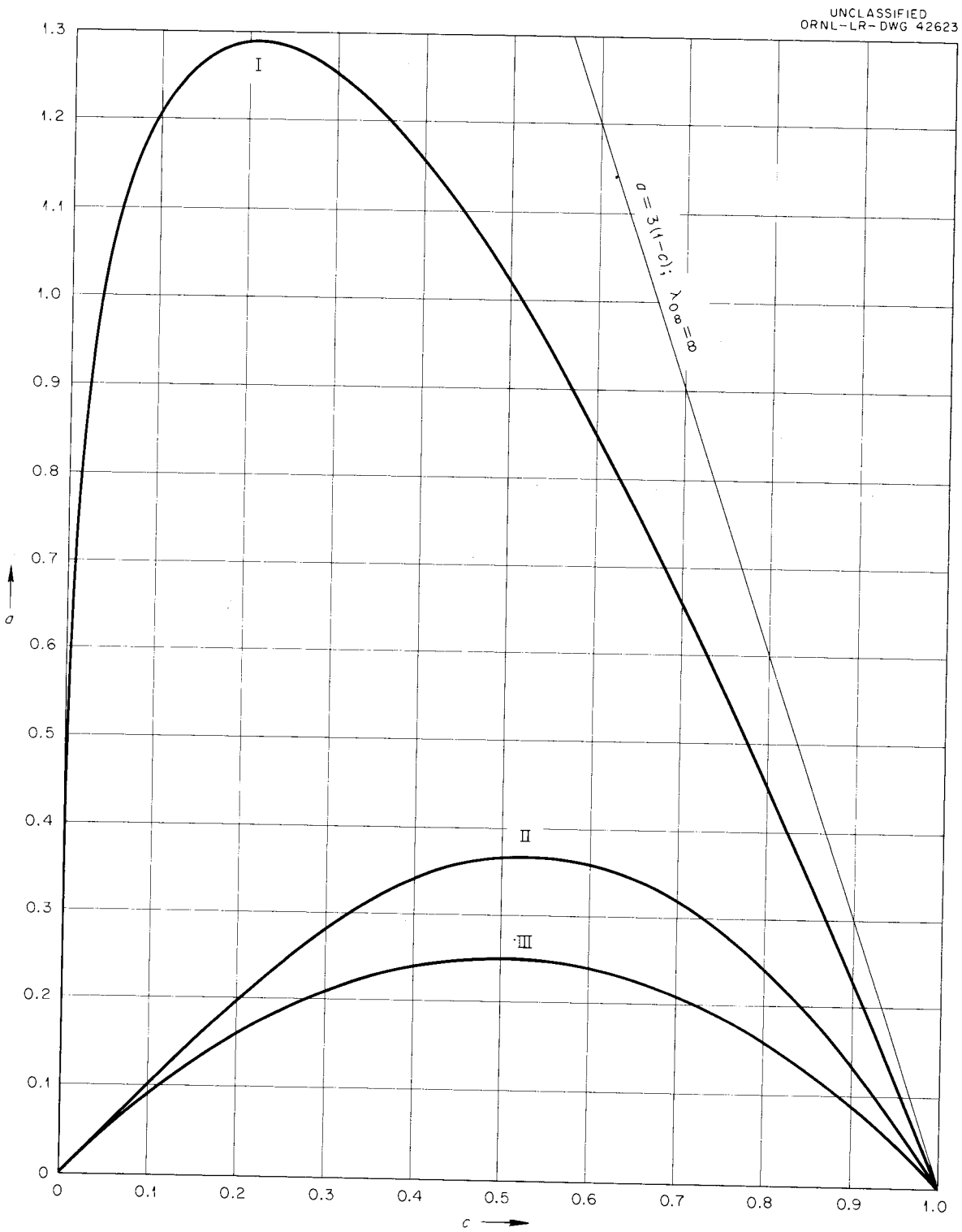


Fig. 1. Three Curves as Borders of Different Areas in the $c$, $a$-Plane, in which Interesting Inequations Hold.

The following tables give some information about the characteristic values $\lambda_{0\infty}$ as functions of c and a on the 3 curves.

1) For curve I with the equation $\frac{c}{a} = \frac{1}{4}(\lambda_{0\infty}^2 - 1)$:

TABLE I

| $\lambda_{0\infty}$ | c | a | $\lambda_{0\infty}$ | c | a |
|---|---|---|---|---|---|
| 1 | 0 | 0 | 1.5 | 0.370 | 1.186 |
| 1.0001 | $12{,}6 \cdot 10^{-6}$ | 0.253 | 1.6 | 0.433 | 1.110 |
| 1.001 | $177 \cdot 10^{-6}$ | 0.356 | 1.7 | 0.488 | 1.033 |
| 1.005 | $1{,}23 \cdot 10^{-3}$ | 0.490 | 1.8 | 0.536 | 0.957 |
| 1.01 | $2{,}91 \cdot 10^{-3}$ | 0.580 | 1.9 | 0.578 | 0.886 |
| 1.02 | $7{,}05 \cdot 10^{-3}$ | 0.698 | 2 | 0.616 | 0.821 |
| 1.05 | 0.0234 | 0.912 | 2.3 | 0.703 | 0.655 |
| 1.1 | 0.0581 | 1.106 | 2.6 | 0.764 | 0.531 |
| 1.15 | 0.0976 | 1.211 | 3 | 0.821 | 0.410 |
| 1.2 | 0.139 | 1.266 | 3.5 | 0.867 | 0.308 |
| 1.25 | 0.181 | 1.288 | 4 | 0.898 | 0.239 |
| 1.3 | 0.222 | 1.289 | 4.5 | 0.919 | 0.191 |
| 1.35 | 0.264 | 1.275 | 5 | 0.934 | 0.156 |
| 1.4 | 0.300 | 1.251 | 10 | 0.983 | 0.040 |
| 1.45 | 0.336 | 1.221 | $\infty$ | 1 | 0 |

2) For curve II with the equation $\frac{c}{a} = \lambda_{0\infty}^2$:

TABLE II

| $\lambda_{0\infty}$ | $c_o$ | c | a | $\lambda_{0\infty}$ | $c_o$ | c | a |
|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 0 | 1.2 | 0.695 | 0.532 | 0.370 |
| 1.0001 | 0.2019 | 0.11230 | 0.11228 | 1.5 | 0.828 | 0.707 | 0.314 |
| 1.001 | 0.2628 | 0.15131 | 0.15101 | 2 | 0.910 | 0.835 | 0.209 |
| 1.005 | 0.332 | 0.199 | 0.197 | 5 | 0.987 | 0.973 | 0.0389 |
| 1.01 | 0.373 | 0.230 | 0.225 | 10 | 0.9967 | 0.9933 | 0.0099 |
| 1.02 | 0.425 | 0.270 | 0.259 | 20 | 0.99916 | 0.99832 | 0.0025 |
| 1.05 | 0.513 | 0.345 | 0.313 | 80 | 0.99992 | 0.99984 | 0.00016 |
| 1.1 | 0.597 | 0.426 | 0.352 | $\infty$ | 1 | 1 | 0 |

3) For curve III with the equation $a = c(1 - c)$:

TABLE III[3]

| $c$ | $a$ | $\lambda_{0\infty}$ | $c/a$ | $\frac{1}{4}(\lambda_{0\infty}^2 - 1)$ |
|---|---|---|---|---|
| 0.99 | 0.0099 | 7.082 | 100 | 12.288 |
| 0.95 | 0.0475 | 3.187 | 20 | 2.289 |
| 0.9 | 0.09 | 2.272 | 10 | 1.041 |
| 0.85 | 0.1275 | 1.872 | 6.67 | 0.626 |
| 0.8 | 0.16 | 1.637 | 5 | 0.420 |
| 0.75 | 0.1875 | 1.480 | 4 | 0.297 |
| 0.7 | 0.21 | 1.366 | 3.33 | 0.216 |
| 0.65 | 0.2275 | 1.280 | 2.86 | 0.160 |
| 0.6 | 0.24 | 1.213 | 2.5 | 0.118 |
| 0.55 | 0.2475 | 1.160 | 2.22 | 0.086 |
| 0.5 | 0.25 | 1.118 | 2 | 0.062 |
| 0.45 | 0.2475 | 1.084 | 1.82 | 0.044 |
| 0.4 | 0.24 | 1.057 | 1.67 | 0.029 |
| 0.35 | 0.2275 | 1.036 | 1.54 | 0.018 |
| 0.3 | 0.21 | 1.020 | 1.43 | 0.010 |
| 0 | 0 | 1 | 1 | 0 |

The last two columns of this table may show how much larger $c/a$ is than $\frac{1}{4}(\lambda_{0\infty}^2 - 1)$. The inequality $c/a > 8 \cdot \frac{1}{4}(\lambda_{0\infty}^2 - 1)$ is satisfied always for $0 \leq c \leq 1$; for $c = 1$ both sides become equal and infinite.

[3] I owe the characteristic numbers $\lambda_{0\infty}$ of this table to Mr. H. S. Moran.

## 7. Transformation of the Occurring Integrals into a Form in which they Remain Finite Along a Finite Path of Integration.

### a. Properties of W(u).

The function W(u) defined by equation (1) is one factor in the integrand of the integrals $\Theta_0$, $\Theta^+$, $\Theta^-$, $\phi_0$, $\phi_a$, $\chi(\lambda)$ (equations 2 through 7) which are important in this report. W(u) is a representative of the continuous spectrum[4] of the Boltzmann-operator; this is easily recognized if one follows the limit-process $L \to \infty$ backward to its origin. Reviewing the equations (II 47, 45, 44, 41, 40) of the second report l.c.[1] one may find that W(u) is related to the quotient of the angular differences $\Delta\vartheta_s^{(1)} = \vartheta_s^{(1)} - \vartheta_{s+1}^{(1)}$ and $\Delta\vartheta_s^{(2)} = \vartheta_s^{(2)} - \vartheta_{s+1}^{(2)}$ by

$$\frac{1}{2} W(u)\, du = \lim_{L \to \infty} \left(1 - \frac{\Delta\vartheta_s^{(2)}}{\Delta\vartheta_s^{(1)}}\right) \Delta s \,. \tag{56}$$

$\vartheta_s^{(1)} = \cos^{-1} \mu_s$ and $\vartheta_s^{(2)} = \cos^{-1} \lambda_s$ are the angles which belong to the eigenvalues of two different characteristic equations in $P_L$-approximations; namely, $\mu_s = \cos \vartheta_s^{(1)}$ resp. $\lambda_s = \cos \vartheta_s^{(2)}$ are the roots of the characteristic equations in L-th degree of approximation

$$P_{L+1}(\mu_s) = 0 \qquad \text{(for } c = 0,\ a = 0\text{; perfect absorption)} \tag{57}$$

$$\text{resp.} \quad (1+a\lambda_s^2)\, P_{L+1}(\lambda_s) - \lambda_s(c+a\lambda_s^2)\, W_L(\lambda_s) = 0 \ (\text{for } c \neq 0,\ a \neq 0). \tag{58}$$

s takes only the values $s = 2, 3, \ldots \frac{L+1}{2}$ in the first equation and $s = 1, 2, \ldots \frac{L-1}{2}$ in the second equation. The largest roots $\mu_1$ and $\lambda_0$ are excluded. $\lambda_0$ converges to $\lambda_{0\infty}$ on the outside of the interval $0 \leq \lambda \leq 1$, whereas $\mu_1$ converges

(4) Wigner, E. P., Colloquium Publication of the Amer. Math. Soc. (Meeting on the Mathematical Aspects of Reactor Theory, New York, April 23-24, 1959.)

to 1, yielding a finite difference $\lambda_{0\infty} - 1$ in the limit $L \to \infty$. The differential quotient, involved in the right side of Equation (56), would therefore become infinite. So these two roots have in fact no place in a finite $W(u)$. In the course of the limit process they separate themselves from the other eigenvalues in a quite natural way. Hence $\frac{1}{2} W(u)\, du$ is the $\lim\limits_{L \to \infty}$ of a function of those roots of the characteristic equations (57) and (58) which lie <u>certainly in the interior</u> of the interval $0 \leq \lambda \leq 1$ for every degree L of approximation. In the limit $L \to \infty$, however, the roots in the interior of this interval create two continuous spectra: the set of $\lambda_s^{(1)}$ builds up the continuous spectrum of the perfect absorber and the set of $\lambda_s^{(2)}$ that of the problem with $c, a \neq 0$.

By partial integration of Equation (II 50) l.c.[1] one recognizes that

$$W(u) = \frac{hg}{1 - u^2} = \frac{2}{\pi} \frac{d}{du} \tan^{-1} \left\{ \frac{\pi}{2} \frac{u(c+au^2)}{P(u)} \right\} \tag{59}$$

with

$$P(u) = 1 + au^2 - u(c+au^2) \tanh^{-1} u \,. \tag{60}$$

(An additional remark is important for partial integrations, namely, that the branches of the inverse tangent involved in Equation (59) are those on which $\tan^{-1}$ is $-\pi$ for $u = 0$ and 0 for $u = 1$. $P(u)$ vanishes at $u = u_0$, where the $\tan^{-1}$ of the expression in curly brackets is therefore $-\frac{\pi}{2}$. This branch condition was found during the performance of the limit process $L \to \infty$ in section 3 of Part II l.c.[1] This peculiarity does not occur in the following.)

$P(u)$ is different from the characteristic function for the discrete spectrum, Equation (14), because it contains a $\tanh^{-1}$ instead of a $\text{cotanh}^{-1}$. $P(u)$ is also a representative of the continuous spectrum.

The functions h and g may be written with the aid of $P(u)$ and $P'(u)$:

$$h(c,a;u) = (1-u^2)\left[(c+3au^2)\ P(u) - u(c+au^2)\ P'(u)\right] \tag{61}$$

$$g(c,a;u) = 1\Big/\left\{P^2(u) + \left[\frac{\pi}{2}\ u(c+au^2)\right]^2\right\}. \tag{62}$$

b. Transformation of W(u) and of the path of integration.

We consider an integral of the form

$$I = \int_0^1 T(u)\ W(u)\ du \tag{63}$$

where T(u) stands for the different first factors in the integrals of the equations (2) through (7). By the transformation of the variable u of integration $u = \tanh \nu$, $\nu = \tanh^{-1} u$, $du = (1-u^2)\ d\nu$ we remove the pole $\frac{1}{1-u}$ in W(u) at the upper limit $u = 1$ of the path of integration:

$$I = \int_0^\infty T(\tanh \nu)\ h(\tanh \nu)\ g(\tanh \nu)\ d\nu\ . \tag{64}$$

The path of integration, however, now has infinite length. The denominator of g(u) can be written as the product of two complex conjugate factors

$$\begin{aligned} \frac{1}{g} &= \left[P(u) - \frac{\pi i}{2}\ u(c+au^2)\right]\cdot\left[P(u) + \frac{\pi i}{2}\ u(c+au^2)\right] \\ &= \left[1 + au^2 - (\nu + \frac{\pi i}{2})\ u(c+au^2)\right]\cdot\left[1 + au^2 - (\nu - \frac{\pi i}{2})\ u(c+au^2)\right]\ . \end{aligned} \tag{65}$$

Using this we can divide the integral I in many ways. A reasonable way is found by the additional request that no factor of the integrand should go to zero or infinity in the limit $c \to 1$, $a \to 0$. As a guide, the first factor of the integral $\lambda_{0\infty}\ \Theta_0$ (see equations 18a, b, and 2) which for $c = 1$, $a = 0$ goes over in the finite distance of the extrapolated endpoint. The first factor is $T(u) = \frac{\lambda_{0\infty}}{2}$ $\tanh^{-1} \frac{u}{\lambda_{0\infty}}$. If we divide T(u) by u, we have in T(u)/u a factor which goes to 1 in the case $c \to 1$, $a \to 0$, where $\lambda_{0\infty}$ goes to infinity. Hence it appears

reasonable to split

$$u\ h(u)\ g(u) \quad = \quad (1-u^2)\ u\ W(u) \tag{66}$$

in its partial fractions. The result is (with $u = \tanh \nu$ as an abbreviation)

$$u\ h(u)\ g(u) \quad = \quad \frac{1}{\pi i} \left\{ \frac{1 + (c-1+a)\ u^2 + 2a\left[(\nu + \frac{\pi i}{2})\ u - 1\right]\ u^2(1-u^2)}{1 + au^2 - (\nu + \frac{\pi i}{2})\ u(c+au^2)} \right.$$

$$\left. - \frac{1 + (c-1+a)\ u^2 + 2a\left[(\nu - \frac{\pi i}{2})\ u - 1\right]\ u^2(1-u^2)}{1 + au^2 - (\nu - \frac{\pi i}{2})\ u(c+au^2)} \right\} \quad . \tag{67}$$

Verification: we have to show that

$$\begin{aligned} u\ h(u) \quad = \quad \frac{1}{\pi i} \Bigg( & \left\{\left[1 + (c-1+a)\ u^2 + 2a(\nu u-1)\ u^2(1-u^2)\right] + \pi i a u^3(1-u^2)\right\} \\ & \cdot \left\{\left[1 + au^2 - \nu u(c+au^2)\right] + \frac{\pi i}{2}\ u(c+au^2)\right\} \\ & - \left\{\left[1 + (c-1+a)\ u^2 + 2a(\nu u-1)\ u^2(1-u^2)\right] - \pi i a u^3(1-u^2)\right\} \\ & \cdot \left\{\left[1 + au^2 - \nu u(c+au^2)\right] - \frac{\pi i}{2}\ u(c+au^2)\right\}\Bigg) \\ = \quad & u \left\{ 2\left[1 + au^2 - \nu u(c+au^2)\right]\ au^2(1-u^2) \right. \\ & \left. + \left[1 + (c-1+a)\ u^2 + 2a(\nu u-1)\ u^2(1-u^2)\right](c+au^2) \right\} \\ = \quad & u \left\{ c + \left[c^2 - c + a(3-c)\right]\ u^2 + a\left[a + 3(c-1)\right]\ u^4 \right\} \quad . \end{aligned}$$

Compare the last expression with equation (1a) to see that it is in fact $u\ h(u)$.

For real u the second expression in (67) is the complex conjugate of the first. If we apply now different transformations, namely

$$w = \nu + \frac{\pi i}{2} \qquad \text{to the first} \tag{68a}$$

and

$$w = \nu - \frac{\pi i}{2} \qquad \text{to the second} \tag{68b}$$

expression in (67), we obtain the same integrand in both cases because

$$u = \tanh \nu = \tanh\left(w \mp \frac{\pi i}{2}\right) = \operatorname{cotanh} w \tag{69}$$

yields the same function in w. The paths of integration, however, are different now for the two parts of the integrand. w runs from $\frac{\pi i}{2}$ to $\infty + \frac{\pi i}{2}$ for the first part and from $-\frac{\pi i}{2}$ to $\infty - \frac{\pi i}{2}$ for the second part. Hence we may write with $\lambda$ = cotanh w as an abbreviation

$$I = \frac{1}{\pi i}\left\{\left(\int_{\frac{\pi i}{2}}^{\infty+\frac{\pi i}{2}} - \int_{-\frac{\pi i}{2}}^{\infty-\frac{\pi i}{2}}\right)\frac{T(\lambda)}{\lambda}\;\frac{1 + (c-1+a)\,\lambda^2 + 2a(w\lambda-1)\,\lambda^2(1-\lambda^2)}{1 + a\lambda^2 - w\lambda(c+a\lambda^2)}\,dw\right\}$$

$$= -\frac{1}{\pi i}\left\{\left(\int_{-\frac{\pi i}{2}}^{\infty-\frac{\pi i}{2}} + \int_{\infty+\frac{\pi i}{2}}^{\frac{\pi i}{2}}\right)\frac{T(\lambda)}{\lambda}\;\frac{1 + (c-1+a)\,\lambda^2 + 2a(w\lambda-1)\,\lambda^2(1-\lambda^2)}{Ch(\lambda)}\,dw\right\} \tag{70}$$

$$= -\frac{1}{\pi i}\int_C T(\lambda)\cdot\frac{1 + (c-1+a)\,\lambda^2 + 2a(w\lambda-1)\,\lambda^2(1-\lambda^2)}{\lambda\, Ch(\lambda)}\,dw\ . \tag{71}$$

The two paths of integration in (70) could be joined at $w = \infty$; the integrand vanishes for large w and $c > 0$. The denominator behaves there like $-(c+a)\,w$ and the numerator like $2aw(1 - \operatorname{cotanh}^2 w) \sim 8aw\,e^{-2w}$. Hence the path C of integration obtains the form shown in Figure 2.

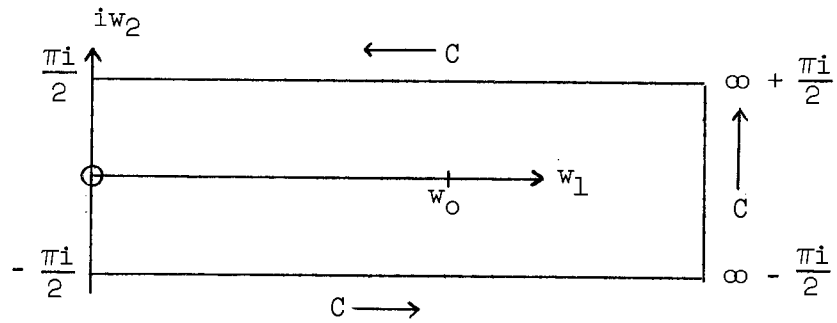


Figure 2. Path C of integration in the complex w-plane.

The denominator of the integrand is the characteristic function $Ch(\lambda)$ (see equation 14). It has, as we know, a zero at $\lambda = \lambda_{0\infty}$ or at $w = w_o = \text{cotanh}^{-1} \lambda_{0\infty}$ on the real $w_1$-axis in the complex $w = w_1 + iw_2$ plane. $w_o$ lies for $c = 1$, i.e., $\lambda_{0\infty} = \infty$, in the origin of the w-plane and joins there the second root $- w_o = \text{cotanh}^{-1} (- \lambda_{0\infty})$ of the characteristic equation. $w_o$ shifts to the right side, $- w_o$ to the left side on the real $w_1$-axis for decreasing c. It follows from the characteristic equation (14) that $w_o$ is connected simply with the point of intersection $c_o$, at which the straight line, labeled by a fixed characteristic number $\lambda_{0\infty}$, cuts the c-axis in the c,a plane (see l.c.[2] Equation 14). The straight line contains all c,a-values for which the characteristic equation has the same characteristic number $\lambda_{0\infty}$ and therefore also the same

$$w_o = \text{cotanh}^{-1} \lambda_{0\infty} = \frac{1 + a\lambda_{0\infty}^2}{\lambda_{0\infty}(c+a\lambda_{0\infty}^2)} = \frac{1}{\lambda_{0\infty} c_o} . \tag{72}$$

$c_o$ is the special c-value for $a = 0$. For $c_o \to 0$ (perfect absorption) $\lambda_{0\infty}$ goes to 1 and $w_o$ to infinity; this is a limit case which we have to exclude if we want to make the path of integration finite later.

The whole factor of $T(\lambda)$ in the integrand of (71) can be written

$$- \frac{1}{\lambda\, Ch(\lambda)} \left[1 + (c-1+a)\, \lambda^2 + 2a(w\lambda-1)\, \lambda^2(1-\lambda^2)\right] = \frac{d}{dw} \log \left(\frac{Ch(\lambda)}{\lambda}\right) . \tag{73}$$

This is easily verified remembering $\lambda = \text{cotanh}\, w$ and $d\lambda/dw = 1 - \lambda^2$. Hence the integral (63) takes the simple form

$$I = \frac{1}{\pi i} \int_C T(\lambda) \frac{d}{dw} \log \left(\frac{Ch(\lambda)}{\lambda}\right) \cdot dw . \tag{74}$$

It is to be expected that the procedure (which begins with the spherical harmonics $P_L$-approximation and ends with the limit process $L \to \infty$) to find the second factor $\frac{d}{dw} \log \left(\frac{Ch(\lambda)}{\lambda}\right)$ will be always the same, irrespective of the number of terms supposed in the scattering law for single neutrons. Therefore one will always have this second factor in plane geometry and the special scattering law will be represented in it by the corresponding characteristic function of the problem. The first factor $T(\lambda)$ and the combination of expressions occurring in the quantities to calculate, however, depend also on the boundary conditions. They cannot be predicted without further study.

c. Separation of the real and imaginary part in the integral I.

To prepare numerical calculations of the integral I we separate real and imaginary parts. We denote $w = w_1 + iw_2$, $\lambda = \lambda_1 + i\lambda_2$, $Ch(\lambda) = Ch_1 + iCh_2$, $T(\lambda) = T_1 + iT_2$, $\frac{d}{dw} \log \left(\frac{Ch(\lambda)}{\lambda}\right) = S_1 + iS_2$. These quantities are the following functions of $w_1$ and $w_2$:

$$\lambda_1 = \frac{\sinh 2w_1}{\cosh 2w_1 - \cos 2w_2} \tag{75}$$

$$\lambda_2 = \frac{-\sin 2w_2}{\cosh 2w_1 - \cos 2w_2} \tag{76}$$

$$\Lambda \equiv |\lambda|^2 \equiv \lambda_1^2 + \lambda_2^2 = \frac{\sinh^2 2w_1 + \sin^2 2w_2}{(\cosh 2w_1 - \cos 2w_2)^2} \tag{77}$$

$$M \equiv \lambda_1^2 - \lambda_2^2 = \frac{\sinh^2 2w_1 - \sin^2 2w_2}{(\cosh 2w_1 - \cos 2w_2)^2} \quad . \tag{78}$$

These quantities are abbreviations which are used in the following more complicated expressions:

$$\begin{aligned} |Ch(\lambda)|^2 \equiv Ch_1^2 + Ch_2^2 = {} & 1 + 2aM + a^2\Lambda^2 + (w_1^2+w_2^2)\,\Lambda(c^2+2acM+a^2\Lambda^2) \\ & - 2w_1\lambda_1\left[c + 2aM + a(c-1)\,\Lambda + a^2\Lambda^2\right] \\ & + 2w_2\lambda_2\left[c + 2aM - a(c-1)\,\Lambda + a^2\Lambda^2\right] \end{aligned} \tag{79}$$

and with $' = d/dw_1$

$$\begin{aligned} Ch_1\,Ch_1' + Ch_2\,Ch_2' = {} & \lambda_1\left[2a - c + a(3-c+2a)\,\Lambda - 3a^2\Lambda^2 - 6aM\right] \\ & + w_1\Big\{- c + c(c-2a)\,\Lambda + a(c-3-3a)\,\Lambda^2 + 3a^2\Lambda^3 \\ & \quad + M\left[(c-3a-ac) + 2a(2c-a)\,\Lambda + 3a^2\Lambda^2 + 6aM\right]\Big\} \\ & - 2w_2\lambda_1\lambda_2\left[(c-3a+ac) - 2a(c+a)\,\Lambda + 3a^2\Lambda^2 + 6aM\right] \\ & + (w_1^2+w_2^2)\,\lambda_1\left[c^2 + c(2a-c)\,\Lambda + a(2c+3a)\,\Lambda^2 - 3a^2\Lambda^3 + 2acM(1-3\Lambda)\right] \end{aligned} \tag{80}$$

$$
\begin{aligned}
Ch_1\, Ch_2' - Ch_2\, Ch_1' \;=\; & \lambda_2\Big[2a - c - a(3-c+2a)\,\Lambda - 3a^2\Lambda^2 - 6aM\Big] \\
& + w_2\Big\{- c - c(c-2a)\,\Lambda + a(c-3-3a)\,\Lambda^2 - 3a^2\Lambda^3 \\
& \qquad + M\Big[(c-3a-ac) - 2a(2c-a)\,\Lambda + 3a^2\Lambda^2 + 6aM\Big]\Big\} \qquad (81) \\
& + 2w_1\lambda_1\lambda_2\Big[(c-3a+ac) + 2a(c+a)\,\Lambda + 3a^2\Lambda^2 + 6aM\Big] \\
& + (w_1^2+w_2^2)\,\lambda_2\Big[- c^2 + c(2a-c)\,\Lambda - a(2c+3a)\,\Lambda^2 - 3a^2\Lambda^3 - 2acM(1+3\Lambda)\Big] .
\end{aligned}
$$

The last expressions occur in $S_1$ and $S_2$

$$
S_1 \;=\; \lambda_1\,\frac{\Lambda - 1}{\Lambda} + \frac{Ch_1\, Ch_1' + Ch_2\, Ch_2'}{|Ch(\lambda)|^2} \;=\; \frac{R(w_1,w_2)}{\Lambda|Ch(\lambda)|^2} \qquad (82)
$$

$$
S_2 \;=\; \lambda_2\,\frac{\Lambda + 1}{\Lambda} + \frac{Ch_1\, Ch_2' - Ch_2\, Ch_1'}{|Ch(\lambda)|^2} \;=\; \frac{Q(w_1,w_2)}{\Lambda|Ch(\lambda)|^2} . \qquad (83)
$$

With these denotations the integral (74) will become $\Big[R \equiv R(w_1,w_2)$, $Q \equiv Q(w_1,w_2)\Big]$

$$
\begin{aligned}
I \;=\; \frac{1}{\pi}\iint\limits_{\underbrace{w_1,w_2}_{C}} \frac{1}{\Lambda|Ch(\lambda)|^2}\Big\{ & T_1(Rdw_2 + Qdw_1) + T_2(Rdw_1 - Qdw_2) \\
& + i\Big[T_2(Rdw_2 + Qdw_1) + T_1(Qdw_2 - Rdw_1)\Big]\Big\} \quad . \qquad (84)
\end{aligned}
$$

The double-integral sign in (84) means that one has to integrate over the $w_1$ and $w_2$ ranges which occur on the curve C. Hence there is always a relation between $dw_1$ and $dw_2$. If one expresses $w_1$ and $w_2$ for instance by an angle $\varphi$ along the curve C (a circle or an ellipse), the integral (84) will become a single integral over the range of $\varphi$.

Finally we give the expressions R and Q for numerical calculations

$$R = \lambda_1(D-E) - w_2(F-G) - w_1(J-H) \tag{85a}$$

$$Q = \lambda_2(D+E) - w_1(F+G) - w_2(J+H) \tag{85b}$$

with

$$\left.\begin{aligned}
D &= \Lambda\left[(1-c+2a) - 4aM - 2a^2\Lambda^2 + 2a(w_1^2+w_2^2)\,\Lambda(c-2cM-a\Lambda^2)\right] \\
E &= 1 + 2aM + a(c-3-a)\,\Lambda^2 - 2a(c+a)(w_1^2+w_2^2)\,\Lambda^3 \\
F &= 2\lambda_1\lambda_2\left[c + 2aM - a(1+c+a)\,\Lambda^2\right] \\
G &= 4a\lambda_1\lambda_2(1-2M-a\Lambda^2) \\
H &= M(c+2aM) + \Lambda^2\left[(c^2-c-ac-a) + a(3c-a-1)\,M + 2a^2\Lambda^2\right] \\
J &= 2a\Lambda\left[(1+a)\,\Lambda^2 + M(1-a\Lambda^2) - 2M^2\right] .
\end{aligned}\right\} \tag{86}$$

d. Finite paths of integration.

As long as one does not move over a singularity by contracting the path of integration C of Figure 2, one may take any finite path in the complex w-plane which joins the points $w = -\frac{\pi i}{2}$ and $w = \frac{\pi i}{2}$. There is, however, a pole of the expression $\frac{d}{dw}\log Ch(\lambda)$ at $w = w_0$ (see equation 72). At this point lies the root of the characteristic equation $Ch(\lambda_{0\infty}) = 0$. The first factors $T(\lambda)$ are different functions. In the case of the integral $\Theta_0$ (see equation 2) the first factor $T(\lambda) = \tanh^{-1}\frac{\lambda}{\lambda_{0\infty}}$ has a branch point at $w_0 = \text{cotanh}^{-1}\lambda_{0\infty}$, because $\lambda/\lambda_{0\infty}$ is just 1 at this point. The same is true for the integral $\phi_0$ (see equation 5). In other cases, in which the first factor is regular at $w = w_0$, one could use the residue theorem at $w = w_0$ and contract the integration path for the remaining integral to the straight junction from $w = -\frac{\pi i}{2}$ to $w = \frac{\pi i}{2}$. But we shall use

always the same contour in the w-plane to have the same program for the numerical calculations of all integrals (2) to (7) and (52, 53). We prefer therefore to use always an integration path which passes the point $w = w_0$ on the right side. This method has the advantage also that it remains practicable for $c = 1$ where the pole of the second factor at $w = w_0 = 0$ joins another from the left side of the w-plane, namely $w = - w_0 = 0$, to a double pole at $w = 0$.

e. A half parallelogram as the path C of integration.

$W(u)$ becomes infinite at the upper end of the integration path $u = 0$ to $u = 1$. This is inconvenient for numerical integration. One has to detach the environment of $u = 1$ from the integral and to treat it separately. This can be performed by choosing the half parallelogram in Figure 3 as path C of integration.

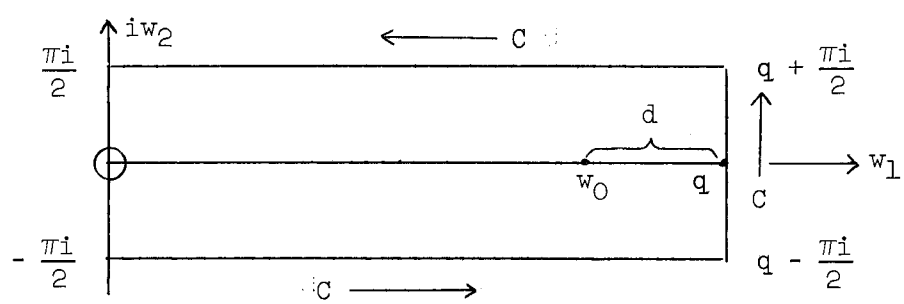


Figure 3. How to make the path of integration finite.

Then we may write

$$I = \int_0^1 T(u)\, W(u)\, du = \int_0^p T(u)\, W(u)\, du + \frac{1}{\pi i} \int_{q-\frac{\pi i}{2}}^{q+\frac{\pi i}{2}} T(\lambda) \frac{d}{dw} \log \left( \frac{Ch(\lambda)}{\lambda} \right) dw \qquad (87)$$

$$= I^{(1)} + I^{(2)}$$

with $p = \tanh q$. The point $q$ of intersection may lie at every finite distance $d > 0$ on the right side of $w_0$:

$$q = d + w_0 = d + \operatorname{cotanh}^{-1} \lambda_{0\infty} \equiv d + \frac{1}{2} \log \frac{\lambda_{0\infty} + 1}{\lambda_{0\infty} - 1} \tag{88}$$

$$p = \tanh q = \frac{1 + \lambda_{0\infty} \tanh d}{\lambda_{0\infty} + \tanh d} \equiv \frac{1}{\lambda_{0\infty}} \left[ 1 + \frac{(\lambda_{0\infty}^2 - 1) \tanh d}{\lambda_{0\infty} + \tanh d} \right] > \frac{1}{\lambda_{0\infty}} \quad . \tag{89}$$

The first integral on the right side of the equation (87) from $u = 0$ to $u = p$ is equal to the two parts on the path C in Figure 3 which are parallel to the real axis $w_1$

$$I^{(1)} = \int_0^p \frac{T(u)}{1 - u^2} \frac{c + \left[c^2 - c + a(3-c)\right] u^2 + a\left[a + 3(c-1)\right] u^4}{\left[1 + au^2 - u(c+au^2) \tanh^{-1} u\right]^2 + \left[\frac{\pi}{2} u(c+au^2)\right]^2} du \quad . \tag{90}$$

To write down $I^{(2)}$ we remember (84) and that $dw_1 = 0$ on its integration path. Hence from (84) remains

$$I^{(2)} = \frac{1}{\pi} \int_{-\pi/2}^{+\pi/2} \frac{dw_2}{\Lambda \left| Ch(\lambda) \right|^2} \left[ (T_1 R - T_2 Q) + i(T_2 R + T_1 Q) \right] \tag{91}$$

$T_1$ and $T_2$ in (91) are the real and the imaginary parts of $T(\lambda) = T_1 + iT_2$; and $\Lambda$, $\left|Ch(\lambda)\right|^2$, R and Q are given by (77), (79), (85a), (85b), together with (86).

$I^{(2)}$ is always real for the integrals $\Theta_0$, $\Theta^+$, $\Theta^-$, $\phi_0$, $\phi_a$ [see equations (2) through (6)], and it is real also for the integral $\chi(\lambda)$ [see (7)], if $\lambda$ is real, for instance if $\lambda$ has the meaning of $\mu = \cos \vartheta$ of the direction $\vartheta$ of neutrons in $f(0,\mu)/j(0)$ of the equations (36a and 36b). Then the imaginary part of (91) is zero and we obtain simply

$$I^{(2)}_{real} = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} \frac{dw_2}{\Lambda|Ch(\lambda)|^2} (T_1R - T_2Q) \quad . \tag{92}$$

Finally, one finds that the integrands are symmetric to $w_2 = 0$ and may be written as twice the integrals from $w_2 = 0$ to $\pi/2$:

$$I^{(2)}_{real} = \frac{2}{\pi} \int_{0}^{\pi/2} \frac{dw_2}{\Lambda|Ch(\lambda)|^2} (T_1R - T_2Q) \ . \tag{92a}$$

Because d is an arbitrary positive number, we get a check of our numerical calculations with the electronic computer by choosing different values for d. The form (90) of the integral $I^{(1)}$ is the original one, but without the diverging part of the integrand from $u = p$ to $u = 1$. One has to choose d, which is involved in p and q according to the equations (88) and (89), in such a manner that both integrals $I^{(1)}$ and $I^{(2)}$ can be calculated with good precision. If d is too small one comes too near to the singularity of the integrand of $I^{(2)}$ at $w = w_0$; if d is too large one comes too near to the singularity of the integrand of $I^{(1)}$ at $u = 1$. It is to suppose also that the best value of d could be a function of c and a. By taking 2 or 3 different positive values of d one obtains a check of the accuracy of the result.

Finally, we consider the double integral $j_t(\zeta)$; see equations (46) and (46a). We chose there a circle in the complex $\mu$-plane as one path of integration. We separated real and imaginary parts of $\chi(-\mu) = \chi_1(\mu_1,\mu_2) + i\chi_2(\mu_1,\mu_2)$. $\chi_1$ and $\chi_2$ depend on $\mu_1$, $\mu_2$, c, a and u. As long as we integrate over u each of these functions is a real function T(u), suitable to be put in $I^{(1)}$ of equation (90). By the transformation of the path of integration into the complex w-plane, however, $\chi_1 \equiv \chi_1(\mu_1,\mu_2;\lambda_1+i\lambda_2)$ and $\chi_2 = \chi_2(\mu_1,\mu_2;\lambda_1+i\lambda_2)$ become complex functions

again, now in the w-plane. In equations (52) and (53) the functions T(u) in the sense of (63) are given for $\chi_1$ and $\chi_2$. They shall be written down in the following, together with their separated real and imaginary parts $T(\lambda) = T_1 + iT_2$ in the complex variables $w = w_1 + iw_2$ and $\lambda = \lambda_1 + i\lambda_2$, respectively:

(a) for $\chi_1$

$$T(u) = \frac{1}{4} \log (m-2\mu_1 u+u^2) \tag{93a}$$

$$T_1 = \frac{1}{8} \log \left[ (m+M-2\mu_1\lambda_1)^2 + 4\lambda_2^2(\mu_1-\lambda_1)^2 \right] \tag{93b}$$

$$T_2 = -\frac{1}{4} \tan^{-1} \left( \frac{2\lambda_2(\mu_1-\lambda_1)}{m + M - 2\mu_1\lambda_1} \right) ; \tag{93c}$$

(b) for $\chi_2$

$$T(u) = \frac{1}{2} \tan^{-1} \frac{\mu_2}{\mu_1 - u} \tag{94a}$$

$$T_1 = \frac{1}{4} \left( \tan^{-1} \frac{\mu_2(\mu_1-\lambda_1)}{(\mu_1-\lambda_1)^2 + \lambda_2^2 + \mu_2\lambda_2} + \tan^{-1} \frac{\mu_2(\mu_1-\lambda_1)}{(\mu_1-\lambda_1)^2 + \lambda_2^2 - \mu_2\lambda_2} \right) \tag{94b}$$

$$T_2 = \frac{1}{8} \log \frac{(\mu_1-\lambda_1)^2 + (\mu_2+\lambda_2)^2}{(\mu_1-\lambda_1)^2 + (\mu_2-\lambda_2)^2} \equiv \frac{1}{4} \tanh^{-1} \frac{2\mu_2\lambda_2}{(\mu_1-\lambda_1)^2 + \mu_2^2 + \lambda_2^2} . \tag{94c}$$

The quantities $\mu_1$, $\mu_2$, m are related to the variable of integration $\eta$ by the equations (48a and 48b) and $\lambda_1$, $\lambda_2$, M to the variable $w_2$ ($w_1$ is a constant in section 7e) by the equations (75, 76, 78) or to the variable $\varphi$ on the elliptic path of integration in section 7f by the equations (97, 98). The integrands are symmetric to $w_2 = 0$ again and we may apply formula (92a) for the integral over $w_2$. Hence we obtain for the quantities $\chi_1$ and $\chi_2$ involved in the transient part of the current density $j_t(\zeta)$:

$$\chi_1 = \frac{1}{4}\int_0^p \log\,(m-2\mu_1 u+u^2)\; W(u)\; du$$

$$+ \frac{1}{4\pi}\int_0^{\pi/2} \frac{dw_2}{\Lambda\left|Ch(\lambda)\right|^2}\left\{R\cdot \log\left[(m+M-2\mu_1\lambda_1)^2 + 4\lambda_2^2\,(\mu_1-\lambda_1)^2\right] + 2Q\cdot\tan^{-1}\frac{2\lambda_2(\mu_1-\lambda_1)}{m+M-2\mu_1\lambda_1}\right\} \tag{95}$$

$$\chi_2 = \frac{1}{2}\int_0^p \left(\tan^{-1}\frac{\mu_2}{\mu_1-u}\right) W(u)\; du$$

$$+ \frac{1}{4\pi}\int_0^{\pi/2} \frac{dw_2}{\Lambda\left|Ch(\lambda)\right|^2}\left\{2R\cdot\left[\tan^{-1}\frac{\mu_2(\mu_1-\lambda_1)}{(\mu_1-\lambda_1)^2+\lambda_2^2+\mu_2\lambda_2} + \tan^{-1}\frac{\mu_2(\mu_1-\lambda_1)}{(\mu_1-\lambda_1)^2+\lambda_2^2-\mu_2\lambda_2}\right] - Q\cdot\log\frac{(\mu_1-\lambda_1)^2+(\mu_2+\lambda_2)^2}{(\mu_1-\lambda_1)^2+(\mu_2-\lambda_2)^2}\right\} . \tag{96}$$

The quantities $\Lambda$, $\left|Ch(\lambda)\right|^2$, R, Q have the meaning indicated by the equations (77, 79, 85a, 85b). Putting these expressions in (95) and (96) one gets the quantities $\chi_1$ and $\chi_2$ as functions of $\eta$, which is the variable of integration in the integral (46a) for the transient part of the current $j_t(\zeta)$.

f. <u>A half ellipse as path C of integration.</u>

We determine the ellipse by the request that $w_0$ and $-w_0$ should be the focuses of the ellipse and $\frac{\pi}{2}$ its minor half axis. This guarantees that the ellipse passes the point $w_0 = \text{cotanh}^{-1}\,\lambda_{0\infty}$ at the right side, its vertex being at $r_0 = \sqrt{w_0^2 + \frac{\pi^2}{4}}$ . A point P on the ellipse is defined by the angle $\varphi$ between the real $w_1$-axis and its distance between $w_1 = w_0$ and the point P (see Figure 4).

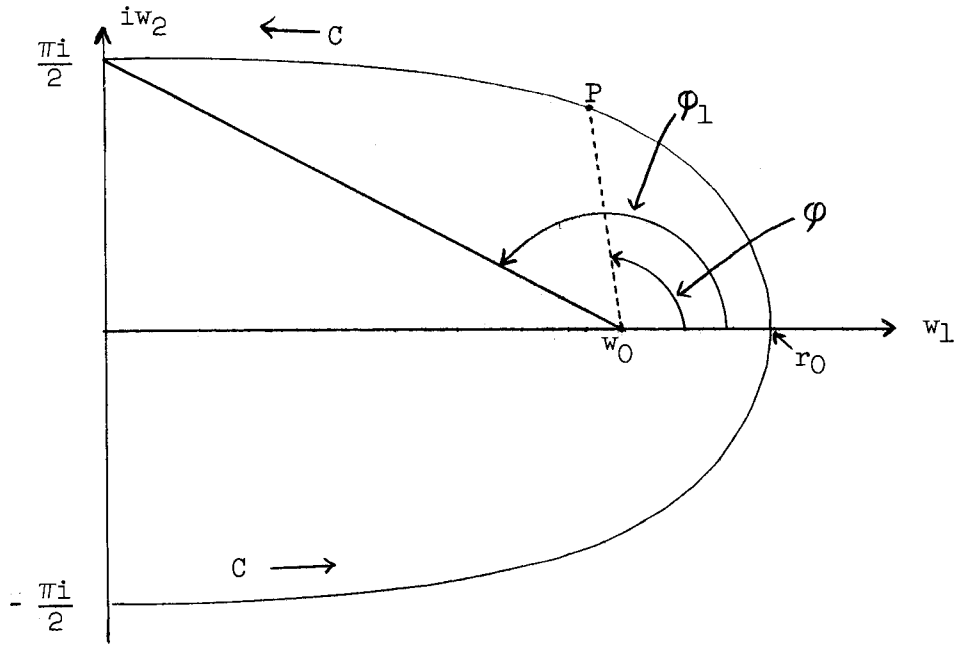


Figure 4. A schematical picture of the half ellipse as path C of integration in the complex w-plane.

The coordinates of the point P are $w = w_1 + iw_2$ with

$$w_1 = w_0 + \frac{\pi^2}{4} \frac{\cos \varphi}{r_0 + w_0 \cos \varphi} = r_0 \frac{f + \cos \varphi}{1 + f \cos \varphi} \tag{97}$$

$$w_2 = \frac{\pi^2}{4} \frac{\sin \varphi}{r_0 + w_0 \cos \varphi} = r_0(1-f^2) \frac{\sin \varphi}{1 + f \cos \varphi} \tag{98}$$

with the abbreviation $f = \frac{w_0}{r_0} = - \cos \varphi_1$ . (99)

The differentials are

$$dw_1 = - \frac{w_2 \, d\varphi}{1 + f \cos \varphi}, \quad dw_2 = (1-f^2) \frac{w_1 \, d\varphi}{1 + f \cos \varphi} . \tag{100}$$

The angle $\varphi_1$, belonging to the upper endpoint $w_1 = 0$, $w_2 = \frac{\pi}{2}$, is

$$\varphi_1 = \frac{\pi}{2} + \tan^{-1}\frac{2w_0}{\pi} = \frac{\pi}{2} + \tan^{-1}\left(\frac{2}{\pi}\,\mathrm{cotanh}^{-1}\,\lambda_{0\infty}\right) \equiv \frac{\pi}{2} + \tan^{-1}\left(\frac{1}{\pi}\log\frac{\lambda_{0\infty}+1}{\lambda_{0\infty}-1}\right). \tag{101}$$

$\varphi_1$ lies always between $\frac{\pi}{2}$ and $\pi$. In the case of isotropic scattering without absorption ($c = 1$, $a = 0$) the half ellipse degenerates in a half circle because $w_0$ lies then in the origin of the complex w-plane, and we have $r_0 = \frac{\pi}{2}$ and $\varphi_1 = \frac{\pi}{2}$. In the case of perfect absorption ($c = 0$) on the other hand $w_0$ tends to $\infty$ and $\varphi_1$ to $\pi$.

The advantage of the elliptical way is that we have to calculate only one integral I instead of two integrals $I^{(1)}$ and $I^{(2)}$ in section 7e.

The integrals $\Theta_0$, $\Theta^+$, $\Theta^-$, $\phi_0$, $\phi_a$ and <u>$\chi(\lambda)$ for real $\lambda$'s</u> [see equations (2) and (7)] have in their transformations in the form (74) the quality of accepting in the lower half w-plane the conjugate complex values of those in the upper half w-plane. Hence the integral can be reduced to an integration over $\varphi$ from 0 to $\varphi_1$. They take the following general form

$$I = \frac{\pi}{2r_0}\int_0^{\varphi_1} \frac{T_1\left[R(f+\cos\varphi) - Q\sin\varphi\right] - T_2\left[Q(f+\cos\varphi) + R\sin\varphi\right]}{\Lambda\cdot\left|Ch(\lambda)\right|^2\cdot(1+f\cos\varphi)^2}\,d\varphi \tag{102}$$

with their corresponding functions $T(\lambda) = T_1 + iT_2$ and the functions $\Lambda$, $\left|Ch(\lambda)\right|^2$, R, Q denoted in the equations (77), (79), (85a) and (85b). Using $w_1$ and $w_2$ from (95) and (96) again, one obtains a representation of the integral which contains only the constant f of (99):

$$I = \frac{2}{\pi}\int_0^{\varphi_1} \frac{T_1Z_1 - T_2Z_2}{\Lambda\left|Ch(\lambda)\right|^2(1+f\cos\varphi)}\,d\varphi \tag{103}$$

with

$$Z_1 = (1-f^2)\, w_1 R - w_2 Q \tag{104a}$$

$$Z_2 = (1-f^2)\, w_1 Q + w_2 R \quad . \tag{104b}$$

For the calculation of the transient part $j_t(\zeta)$ of the current-density the corresponding functions $T_1$ and $T_2$ are given for $\chi_1$ by the equations (93b) and (93c) and for $\chi_2$ by the equations (94b) and (94c).

The integral I is only a little more complicated than the integral (92a) because $Z_1/(1+f\cos\varphi)$ and $Z_2/(1+f\cos\varphi)$ replace now R and Q, their representatives of the elliptic path of integration. Furthermore, the interval of integration is extended from $0 \leq \varphi \leq \pi/2$ to $0 \leq \varphi \leq \varphi_1$ $(\pi/2 \leq \varphi_1 \leq \pi)$. We gained, however, the advantage of having to evaluate only <u>one</u> integral for each of the quantities $\Theta_0$, $\Theta^+$, $\Theta^-$, $\phi_0$, $\phi_a$, $\chi(\lambda)$, $\chi_1$ and $\chi_2$. The two different methods of integration may serve as a check of the results.

## ACKNOWLEDGEMENT

The author wishes to thank Dr. Alvin M. Weinberg for several helpful discussions and for the opportunity to spend the summer 1959 at the Oak Ridge National Laboratory.

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