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STUDIES OF THE SPHERICAL HARMONICS METHOD IN NEUTRON TRANSPORT THEORY

Walter Kofink

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STUDIES OF THE SPHERICAL HARMONICS METHOD IN NEUTRON TRANSPORT THEORY

Walter Kofink

Page	Line	Errata
i	Title	*for* Milne's Problem *read* Milne Problem
1	Title	*for* Milne's problem *read* Milne problem
2	2	*for* T. C. Mark *read* J. C. Mark
2	ref 1	*for* T. C. Mark *read* J. C. Mark
13	equation (21)	should read:

$$f_{00}(\zeta) = \frac{\sinh(\Delta - \zeta)/\lambda_0}{\sinh \Delta/\lambda_0} + \sum_s \alpha_s e^{\zeta/\lambda_s} \qquad (\zeta \leqq 0) \tag{21}$$

14	ref 5	*for* T. C. Mark *read* J. C. Mark
19	17	*for* methods in a special *read* methods is a special
21	11	*for* $\mu = \cos \Theta$ *read* $\mu = \cos \theta$
22		the second line of equation (42) should read:

$$= 2N\lambda_0^2(c + a\lambda_0^2)p(-\mu)p\ (\mu) \sum_{j=1}^{(L+1)/2} \frac{1 + (a/c)\delta(\lambda_a)\mu_j}{(\mu - \mu_j)(\lambda_0^2 - \mu_j^2)r(-\mu_j)p'(\mu_j)} \tag{42}$$

27	equation (53)	*for* $4\pi\Sigma\alpha_k$ *read* $4\pi \sum_k \alpha_k$
28	equation (55)	*for* $\frac{4\pi}{3} f_{10}(\zeta)$ *read* $\frac{4\pi}{3} f_{10}(0)$
29	equation (58)	should read:

$$\lambda_0^2 \approx \frac{1 + \frac{4}{5}\gamma_a + \frac{108}{175}\gamma_a^2\gamma_t}{3\gamma_a\gamma_t} \tag{58}$$

44	9	*for* formula (15) *read* formula (32)
44	11	*for* equation (15) *read* equation (32)
47	9	*for* spacial *read* special
47	equation (A30)	should read:

$$A = G\left[(\lambda_0 + \lambda_a)r(\lambda_a)p(-\lambda_a) + (\lambda_0 - \lambda_a)r(-\lambda_a)p(\lambda_a)\right] \tag{A30}$$

47	equation (A31)	should read:

$$B = G\left[(\lambda_0 - \lambda_a)r(\lambda_a)p(-\lambda_a) + (\lambda_0 + \lambda_a)r(-\lambda_a)p(\lambda_a)\right] \tag{A31}$$

51	9	*after* interpolation formula with *add* $\lambda = -\mu$

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STUDIES OF THE SPHERICAL HARMONICS METHOD IN NEUTRON TRANSPORT THEORY

I. The Relation Between P_L- and Gauss Quadrature Solutions of the Milne Problem

Walter Kofink

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Studies of the Spherical Harmonics Method in Neutron Transport Theory:

I. The relation between P_L- and Gauss quadrature solutions of the Milne problem.

Walter Kofink*

Introduction

The fact that the Gauss quadrature (denoted here as the Chandrasekhar-Wick [C-W] -) method and the spherical harmonics method of dealing with the monoenergetic transport equation are closely related, has been often pointed out in the literature. However, contrary to some statements which have been made, the two are not identical -- basically the C-W method, as applied to the Milne problem, is a non-analytic approximation, whereas all functions used in the spherical harmonics method are continuous. It is the purpose of this paper to examine in detail the relation between the two methods. The Milne problem with p-wave scattering will be used as a convenient example for the analysis. Incidental to these considerations will be derived completely general spherical harmonics solution to the Milne problem, and a comparison with the Gauss quadrature solutions will be given. In a following report it will be shown how these approximate results, in the limit, give the rigorous results of the Wiener-Hopf method of solution of the Milne problem.

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Previous general solutions of the Milne problem by application of the spherical harmonics method have been given by J. C. Mark,[1] by B. Carlson,[2] and by M. C. Wang and E. Guth.[3] The considerations which follow are more general than those of previous authors, first, in that the scattering is assumed anisotropic, and second, in that the relation with the Gauss quadrature method is shown more clearly.

1. The P_L-approximation

Suppose a medium which occupies the region $z \leq 0$ has s- and p-wave scattering of neutrons and has total macroscopic cross section $\Sigma = \Sigma_a + \Sigma_s$ where Σ_a and Σ_s are the cross sections for absorption and scattering. The anisotropy of the scattering is covered by a transport cross section Σ_t. The x,y-plane is a plane boundary between the medium and the vacuum at $z \geq 0$.

Transport theory yields the integro-differential equation

$$\mu \frac{\partial f(z,\mu)}{\partial z} + \Sigma f(z,\mu) = \frac{1}{2}\Sigma_s \int_{-1}^{+1} f(z,\mu')\,d\mu' + \frac{3}{2}(\Sigma - \Sigma_t)\mu \int_{-1}^{+1} f(z,\mu')\mu'\,d\mu' ,$$

where $\mu = \cos\vartheta$ and ϑ is the angle between the positive z-axis and the direction of the directed flux $f(z,\mu)$. At $z = -\infty$ there is an infinite source of neutrons. It is convenient, to introduce dimensionless quantities $\zeta = \Sigma z$ for the coordinate, $\gamma_a = \Sigma_a/\Sigma$, $\gamma_t = \Sigma_t/\Sigma$ and later $c = 1 - \gamma_a = \Sigma_s/\Sigma$, $a = 3\gamma_a(1-\gamma_t)$. The Boltzmann equation takes then the form

$$\mu \frac{\partial f(\zeta,\mu)}{\partial \zeta} + f(\zeta,\mu) = \frac{1}{2}(1-\gamma_a)\int_{-1}^{+1} f(\zeta,\mu')\,d\mu' + \frac{3}{2}(1-\gamma_t)\mu \int_{-1}^{+1} f(\zeta,\mu')\mu'\,d\mu'. \qquad (1)$$

1 J. C. Mark, The Spherical Harmonics Method I (CRT-340), II (CRT-338).
2 B. Carlson, Neutron Diffusion-Spherical Harmonics Theory (MDDC-236).
3 M. C. Wang and E. Guth, Phys. Rev. 84, 1092 (1951).

Applying now the spherical harmonics method, by assuming first that

$$f(\xi,\mu) = \sum_{\ell=0}^{\infty} f_{\ell 0}(\xi)\, P_\ell(\mu) \,, \tag{2}$$

one finds for the partial fluxes $\left[4\pi f_{00}(\xi) = \text{density},\ \frac{4\pi}{3} f_{10}(\xi) = \text{current in } z\text{-direction},\ f_{20}(\xi),\ f_{30}(\xi), \cdots\right]$ the following <u>infinite</u> system of differential equations - $\left(' = \partial/\partial\xi \right)$ - :

$$\begin{array}{lllllll}
\ell = 0 & : & \frac{1}{3} f_{10}' & & + \gamma_a f_{00} & = & 0 \\
\ell = 1 & : & \frac{2}{5} f_{20}' & + f_{00}' & + \gamma_t f_{10} & = & 0 \\
\ell = 2 & : & \frac{3}{7} f_{30}' & + \frac{2}{3} f_{10}' & + f_{20} & = & 0 \\
\ell = 3 & : & \frac{4}{9} f_{40}' & + \frac{3}{5} f_{20}' & + f_{30} & = & 0 \\
\vdots & & & & & & \\
\ell & : & \frac{\ell+1}{2\ell+3} f_{\ell+1,0}' & + \frac{\ell}{2\ell-1} f_{\ell-1,0}' & + f_{\ell 0} & = & 0 \\
\vdots & & & & & &
\end{array} \tag{3}$$

The general equation ℓ holds for $\ell \geq 2$; the first two equations for $\ell = 0, 1$, however, are changed or "disturbed" if $\gamma_a \neq 1$ and $\gamma_t \neq 1$. One may describe the vacuum as far as its effect on the medium is concerned, as a perfect absorber without scattering, i.e. $\gamma_a = 1$, $\gamma_t = 1$ in the vacuum. In this case the general equation holds for all $\ell \geq 0$, because $f_{-1,0}(\xi) = 0$; its solution in this case will be simpler than in the general case.

In the L-approximation of the spherical harmonics method one cuts the infinite system of differential equations after the Lth-equation and demands

that only the spherical harmonics up to and including P_L shall be used in the series (2) as an approximation. This implies that $f_{L+1,0}(\xi) = 0$, $f_{L+2,0}(\xi) = 0$, $f_{L+3,0}(\xi) = 0, \ldots$. The first of these equations, $f_{L+1,0}(\xi) = 0$, turns out to be equivalent to the characteristic equation, which determines the various modes of partial solutions of the finite system left after the truncation of the infinite system of differential equations. To put the remaining $f_{L+2,0}(\xi), f_{L+3,0}(\xi), \ldots = 0$ is a process, which is, properly taken, <u>inconsistent with the infinite system of differential equations</u>, because these later harmonics are related to the non-vanishing $f_{L,0}(\xi)$ by a recursion formula which keeps them different from zero until $\ell \to \infty$.

The supposition

$$f_{\ell 0}(\xi) = (2\ell+1)\, g_\ell(\lambda)\, e^{-\xi/\lambda} \qquad (\ell \geq 2) \tag{4}$$

in the ℓth equation of (3) yields a recursion formula for the g_ℓ's

$$(\ell+1)\, g_{\ell+1}(\lambda) + \ell\, g_{\ell-1}(\lambda) - (2\ell+1)\lambda\, g_\ell(\lambda) = 0$$

which is identical with the recursion formula of the Legendre functions of the 1.and 2.kind. Therefore, putting

$$f_{\ell 0}(\xi) = (2\ell+1)\left[A(\lambda)\, P_\ell(\lambda) + B(\lambda)\, Q_\ell(\lambda)\right] e^{-\xi/\lambda} \tag{5}$$

with 2 arbitrary functions $A(\lambda)$ and $B(\lambda)$, independent of ℓ, one is able to fulfill the set of differential equations (3) for $2 \leq \ell \leq \infty$. The parameter λ is arbitrary until now and the solution $f_{\ell 0}$ above is a

partial solution only. From the Legendre function of second kind[4]

$$Q_\ell(\lambda) = P_\ell(\lambda)\, Q_0(\lambda) - W_{\ell-1}(\lambda) \quad \text{with} \quad Q_0(\lambda) = \frac{1}{2}\log\frac{1+\lambda}{1-\lambda} \quad (|\lambda|<1)$$

one must use only the non-singular part $W_{\ell-1}(\lambda)$, in order to avoid solutions which are singular at $\lambda = \pm 1$. $W_{\ell-1}$ satisfies the same recursion formula as P_ℓ with the index on W lowered by 1; this is evident since Q_ℓ and P_ℓ satisfy the recursion relation and Q_0, being independent of ℓ, does not disturb the recursion. Hence, one adopts simply the pure polynomial

$$f_{\ell 0}(f) = (2\ell+1)\left[A(\lambda)\, P_\ell(\lambda) + B(\lambda)\, W_{\ell-1}(\lambda)\right] e^{-f/\lambda} \tag{6}$$

as a partial solution for $\ell \geq 2$. The functions $A(\lambda)$ and $B(\lambda)$ are to be determined by a calculation of $f_{20}(f)$ and $f_{30}(f)$ as a consequence of the first two "disturbed" equations for $\ell = 0$ and $\ell = 1$. Supposing

$$f_{00}(f) = e^{-f/\lambda}$$

one obtains from equations (3) for

$$\ell = 0 : \qquad f_{10}(f) = 3\gamma_a \lambda\, e^{-f/\lambda}$$

$$\ell = 1 : \qquad f_{20}(f) = 5\left[-\frac{1}{2} + \frac{3}{2}\gamma_a\gamma_t\lambda^2\right] e^{-f/\lambda}$$

$$\ell = 2 : \qquad f_{30}(f) = 7\left[-\left(\frac{5}{6} + \frac{2}{3}\gamma_a\right)\lambda + \frac{5}{2}\gamma_a\gamma_t\lambda^3\right] e^{-f/\lambda}$$

A comparison of these $f_{20}(f)$ and $f_{30}(f)$ with those of equation (6) yields

$$\begin{aligned} A(\lambda) &= 1 + 3\gamma_a(1-\gamma_t)\lambda^2 &&= 1 + a\lambda^2 \\ B(\lambda) &= -\lambda\left[1 - \gamma_a + 3\gamma_a(1-\gamma_t)\lambda^2\right] &&= -\lambda(c + a\lambda^2). \end{aligned} \tag{7}$$

4 E. Jahnke and F. Emde, Tables of Functions, 4th Ed. Ch. VII.

If we characterize the vacuum by $\gamma_a = 1$ and $\gamma_t = 1$, $B_{vac}(\lambda)$ vanishes and we have only the Legendre polynomials of 1. kind with the coefficients $A_{vac}(\lambda) = 1$. Hence, the vacuum is described by the <u>simplest</u> solutions. The usual Milne problem has vacuum on one side; but one may see that the solutions above are adapted to two or even more media with arbitrary different γ_a, γ_t's.

This method of connecting the solutions $f_{\ell 0}(\xi)$ with a supposed partial solution $f_{00}(\xi)$ was already used by B. Carlson in the case of isotropic scattering.

2. Scattering involving higher atomic angular momenta

Let us interrupt briefly the course of further calculations to show that this method of determination of $A(\lambda)$ and $B(\lambda)$ may be extended to d,f,g,.....-wave scattering. Then we shall have more "disturbed" equations in the system (3). We deal with d-wave scattering by putting a factor γ_d before f_{20} in equation $\ell = 2$, with f-wave scattering by putting a factor γ_f before f_{30} in equation $\ell = 3$, and so on.

If $\bar{\ell}$ is the first "undisturbed" equation with a factor 1 before $f_{\bar{\ell}0}$ namely $\ell = \bar{\ell}$:

$$\frac{\bar{\ell}+1}{2\bar{\ell}+3} f'_{\bar{\ell}+1,0} + \frac{\bar{\ell}}{2\bar{\ell}-1} f'_{\bar{\ell}-1,0} + f_{\bar{\ell}0} = 0$$

then $A(\lambda)$ and $B(\lambda)$ have to be determined from the equations

$$\frac{f_{\bar{\ell}0}}{(2\bar{\ell}+1) f_{00}} = A(\lambda) P_{\bar{\ell}}(\lambda) + B(\lambda) W_{\bar{\ell}-1}(\lambda)$$

$$\frac{f_{\bar{\ell}+1}}{(2\bar{\ell}+3) f_{00}} = A(\lambda) P_{\bar{\ell}+1}(\lambda) + B(\lambda) W_{\bar{\ell}}(\lambda) .$$

After the application of the relation

$$P_{\bar{\ell}}(\lambda)\, W_{\bar{\ell}}(\lambda) - P_{\bar{\ell}+1}(\lambda)\, W_{\bar{\ell}-1}(\lambda) = \frac{1}{\bar{\ell}+1}$$

the solution of these equations acquires the simple form

$$A(\lambda) = \frac{\bar{\ell}+1}{f_{00}} \left\{ \frac{1}{2\bar{\ell}+1} f_{\bar{\ell}0}\, W_{\bar{\ell}}(\lambda) - \frac{1}{2\bar{\ell}+3} f_{\bar{\ell}+1,0}\, W_{\bar{\ell}-1}(\lambda) \right\}$$

$$B(\lambda) = -\frac{\bar{\ell}+1}{f_{00}} \left\{ \frac{1}{2\bar{\ell}+1} f_{\bar{\ell}0}\, P_{\bar{\ell}+1}(\lambda) - \frac{1}{2\bar{\ell}+3} f_{\bar{\ell}+1,0}\, P_{\bar{\ell}}(\lambda) \right\}. \tag{8}$$

In a straightforward calculation one has to find $f_{\bar{\ell}0}/f_{00}$ and $f_{\bar{\ell}+1,0}/f_{00}$ from the "disturbed" system $\ell = 0$ until $\ell = \bar{\ell}-1$ and the two subsequent "undisturbed" equations $\ell = \bar{\ell}$ and $\ell = \bar{\ell}+1$. Putting the result in equations (8) one finds $A(\lambda)$ and $B(\lambda)$ in the extended case.

In the special case $\bar{\ell} = 3$ with γ_d as a factor before f_{20} in the equation $\ell = 2$ of the system (3) one obtains

$$A(\lambda) = 1 + a\lambda^2 + b\left[-3\lambda^2 + 9\left(1 - c - \frac{a}{3}\right)\lambda^4\right]$$

$$B(\lambda) = -\lambda\left\{ c + a\lambda^2 + b\left[1 - 3\left(2 - c - \frac{a}{3}\right)\lambda^2 + 9\left(1 - c - \frac{a}{3}\right)\lambda^4\right]\right\} \tag{9}$$

where the additional terms with the factor

$$b = \frac{5}{4}(1 - \gamma_d) \tag{10}$$

show the influence of the d-wave scattering. One recognizes that every further "disturbed" equation increases the degree in λ of $A(\lambda)$ and $B(\lambda)$ by 2. The degree of the characteristic equation in P_L-approximation, however, always remains $L+1$ in λ, because it is independent of the constant factors $\gamma_a, \gamma_t, \gamma_d, \ldots$. Consequently, some relations exist between the

coefficients of all powers of λ^2 in $A(\lambda)$ and $-B(\lambda)/\lambda$ with the exception of the power λ^0. If one writes in our special case $\bar{\ell}=3$ $A(\lambda)$ and $B(\lambda)$ as polynomials of λ^2

$$A(\lambda) = A_1 + A_2\lambda^2 + A_3\lambda^4, \qquad -\frac{B(\lambda)}{\lambda} = B_1 + B_2\lambda^2 + B_3\lambda^4,$$

one obtains in this way the relations

$$B_3 = A_3, \qquad B_2 = A_2 - \frac{1}{3}A_3$$

and the characteristic equation for the $\ell=3$ case (the analog of the following equation (12)) contains

$$A_1 - B_1 - \frac{1}{5}A_3 - \frac{1}{3}B_2 = \left(1 - c - \frac{a}{3}\right)\left(1 - \frac{4}{5}b\right) = \gamma_a\gamma_t\gamma_d$$

as coefficient of its highest power λ^{L+1}.

Presumably this coefficient will be simply the product of all γ's in the general case of arbitrary $\bar{\ell} < L-1$ also.

3. The characteristic equation

We return to the case $\bar{\ell}=2$, i.e. to our main course. The partial solutions $f_{00}(\xi)$, $f_{10}(\xi)$ and $f_{\ell 0}(\xi)$ for $\ell \geq 2$, when put in equation (2), give a partial solution $f(\xi,\mu;\lambda)$ of the infinite system (3) of differential equations, characterized by an arbitrary parameter λ. A general solution could be constructed by superposition of a dense distribution of such solutions

$$f(\xi,\mu) = \int \alpha(\lambda)\, f(\xi,\mu;\lambda)\, d\lambda$$

where $\alpha(\lambda)$ should be chosen so as to satisfy the boundary conditions. This process of satisfying the boundary conditions is reduced to an <u>algebraic</u> problem by cutting the infinite system (3) after a finite L in the spherical harmonics method. Then $L+1$ equations remain, the last one being

$$\frac{L+1}{2L+3} f'_{L+1,0} + \frac{L}{2L-1} f'_{L-1,0} + f_{L0} = 0 \tag{11}$$

In the P_L-approximation, however, $f_{L+1,0}$ is not allowed to appear; this is only the case if one selects the λ's of the partial solutions (5) in such a manner, that $f_{L+1,0}(\lambda_k)$ with these special λ_k's vanishes. Therefore, the characteristic equation in L-approximation is

$$f_{L+1,0}(\lambda_k) = A(\lambda_k) P_{L+1}(\lambda_k) + B(\lambda_k) W_L(\lambda_k) = 0$$

i.e.

$$(1+a\lambda_k^2) P_{L+1}(\lambda_k) - \lambda_k (c+a\lambda_k^2) W_L(\lambda_k) = 0 . \tag{12}$$

This is an algebraic equation of degree $L+1$, because the coefficients of the higher powers cancel. If L is odd, $L+1$ is even and the equation is of degree $\frac{L+1}{2}$ in λ_k^2; hence, one has $\frac{L+1}{2}$ pairs of roots $\lambda_k, -\lambda_k$. In case L is even, $L+1$ is odd, a root $\lambda=0$ appears. This event is uncomfortable and the following treatment is for <u>odd L</u> only.

4. <u>The solutions on the vacuum and the medium side</u>

Having obtained the $f_{\ell 0}(\xi)$'s, we put them in equation (2) and obtain the solutions for $f(z,\mu)$.

(a) On the <u>vacuum side</u> ξ has a different meaning in comparison with

the medium side; it is $\xi = \Xi z$ with an arbitrarily chosen cross section for absorption $\Xi_a = \Xi$; $\Xi_s = 0$. After the calculation one may put $\Xi_a = \infty$, but this is not essential. The solution on this side, $z \geqslant 0$, is in P_L-approximation

$$f(z,\mu) = \sum_{j=1}^{(L+1)/2} \left[\beta_j \, e^{-\xi/\mu_j} \sum_{\ell=0}^{L} (2\ell+1) P_\ell(\mu_j) P_\ell(\mu)\right]$$

$$= (L+1) \, P_{L+1}(\mu) \sum_{j=1}^{(L+1)/2} \beta_j \, \frac{P_L(\mu_j)}{\mu - \mu_j} \, e^{-\xi/\mu_j} \qquad (13)$$

with arbitrary constants β_j , which are found later from the boundary conditions at $z = 0$. The characteristic equation is

$$P_{L+1}(\mu_j) = 0 , \qquad (14)$$

from which we keep the positive roots μ_j $\left(j = 1, 2, \cdots \frac{L+1}{2}\right)$. One has to take positive roots only because $f(z,\mu)$ should tend to zero for $z = +\infty$; hence the solution satisfies the boundary condition of the Milne problem at $z = \infty$. From the second expression for $f(z,\mu)$ in equation (13) one sees immediately that it has zeros in the directions $\mu = -\mu_j$ for all $z \geqslant 0$. Hence we fulfill the condition of no backward flux into the medium only in $\frac{L+1}{2}$ discrete backward cones in the P_L-approximation. This result is valid for $z = 0$ also and is essential for establishing the boundary conditions on the medium side. $f(\xi,\mu)$ has no poles in the forward directions $\mu = +\mu_j$, because the denominator $\mu - \mu_j$ cancels against an equal factor in $P_{L+1}(\mu) = (2L+2)!/\{2^{L+1}[(L+1)!]^2\} \prod_{j=1}^{(L+1)/2} (\mu - \mu_j)(\mu + \mu_j)$

In the directions of the cones $\mu = +\mu_j$ we have a finite flux for $z \geqslant 0$

$$f(z,+\mu_j) = (L+1)\beta_j\, P'_{L+1}(\mu_j)\, P_L(\mu_j)\, e^{-\zeta/\mu_j} = (L+1)^2 \beta_j \frac{[P_L(\mu_j)]^2}{1-\mu_j^2}\, e^{-\zeta/\mu_j}.$$

(b) The solution on the <u>medium side</u>, which must satisfy the boundary conditions at $z=0$ later, is in P_L-approximation, $z \leq 0$, $\zeta = \Sigma z$,

$$f(z,\mu) = \sum_{K=\bar{0},0,1,2,\ldots}^{(L-1)/2} \Big[\alpha_K e^{\zeta/\lambda_K} \Big\{ 1 - 3\gamma_a \lambda_K \mu + \sum_{\ell=2}^{L} (2\ell+1)\Big((1+a\lambda_K^2)\, P_\ell(-\lambda_K) + \lambda_K (c+a\lambda_K^2)\, W_{\ell-1}(-\lambda_K)\Big) P_\ell(\mu)\Big\}\Big] \tag{15}$$

with arbitrary constants α_K. Instead of counting the roots from $1, 2, \cdots \frac{L+1}{2}$ in the sum (15), the largest root λ_0 is distinguished from the others λ_1, $\lambda_2, \lambda_3, \cdots \lambda_{\frac{L-1}{2}}$, because it, being essentially the diffusion length, plays a somewhat different role in the Milne problem, which contains an infinite source at $z = -\infty$, than the other roots. To represent this fact, the sum contains one term with the coefficient $\alpha_{\bar{0}}$ and the root $\lambda_{\bar{0}} = -\lambda_0$. The exponential factor $\exp(\zeta/\lambda_{\bar{0}}) = \exp(-\zeta/\lambda_0)$ in this case tends to infinity for $\zeta \to -\infty$. It is the slowest decreasing solution with negative λ's, if one follows the positive z-direction from the source at $z = -\infty$, because λ_0 is the largest root of (12). Therefore, (15) already satisfies the boundary condition of the Milne problem at $z = -\infty$ and the extra term $K = \bar{0}$ is chosen to give the asymptotic behavior of $f(\zeta,\mu)$ at $\zeta = -\infty$.

By applying Christoffels' sum formulae -- see Appendix I -- on the sum over ℓ in equation (15) and by using the characteristic equation (12)

one may give the equation (15) a simpler form —— $(z \leq 0)$ ——

$$f(z,\mu) = \sum_{k=\bar{0},0,1,\dots}^{(L-1)/2} \alpha_k \lambda_k \, e^{z/\lambda_k} \left\{ -a\lambda_k + \frac{c+a\lambda_k^2}{\lambda_k+\mu} \left[1 - \frac{P_{L+1}(\mu)}{P_{L+1}(-\lambda_k)} \right] \right\} . \tag{16}$$

One recognizes immediately from equation (15) that $f(z,\mu)$ is a <u>polynomial in μ of at most the degree L in μ</u>. The equivalent expression (16) has no poles in the directions $\mu = -\lambda_k$; the denominators $\lambda_k + \mu$ are removable again by developing $P_{L+1}(\mu) - P_{L+1}(-\lambda_k)$ in a power series of $\mu + \lambda_k$.

In the following we always denote by $\sum_k$ a sum over $k = \bar{0}, 0, 1, \dots \frac{L-1}{2}$ and we take an index s for summing only over $s = 1, 2, \dots \frac{L-1}{2}$ after removing the 2 summands with $k = \bar{0}, 0$.

If we separate $f(z,\mu) = f^{I}(z,\mu) + f^{II}(z,\mu)$ into two parts

$$f^{I}(z,\mu) = \sum_k \alpha_k \lambda_k \, e^{z/\lambda_k} \left\{ -a\lambda_k + \frac{c+a\lambda_k^2}{\lambda_k+\mu} \right\} \tag{17}$$

and

$$f^{II}(z,\mu) = -\sum_k \alpha_k \lambda_k \, e^{z/\lambda_k} \, \frac{c+a\lambda_k^2}{\lambda_k+\mu} \, \frac{P_{L+1}(\mu)}{P_{L+1}(-\lambda_k)} \tag{18}$$

we have in $f^{I}(z,\mu)$ the result, which would be found by applying the Gauss quadrature method to the problem according to C-W for <u>positive</u> μ. $f^{I}(z,\mu)$ has poles, however, in the $\frac{L+1}{2}$ <u>negative</u> directions $\mu = -\lambda_k$ and must be replaced in the C-W method by another expression using the original integral equation. $f^{II}(z,\mu)$ is zero for $\mu = \mu_j$; therefore the fluxes according to both methods coincide in the $\frac{L+1}{2}$ positive directions $\mu = \mu_j$ for all $z \leq 0$.

The addition of $f^{II}(z,\mu)$ removes the poles of $f^{I}(z,\mu)$ at $\mu = -\lambda_k$ again; the spherical harmonics method unlike the Gauss quadrature method yields in $f(z,\mu)$ a continuous expression for all μ's but at the cost of a poorer approximation compared with the Gauss quadrature method.

Considering now the boundary at $z = 0$ we remark that $f(0,\mu)$ from equation (16) for $z \leq 0$ contains the $\frac{L+3}{2}$ unknown constants α_k and from equation (13) for $z \geq 0$ the $\frac{L+1}{2}$ unknown constants β_j. Therefore one of the α_k's is still available for the normalization of the asymptotic behavior of $f(z,\mu)$ at $z = -\infty$. We impose on the first 2 coefficients the condition $\alpha_{\bar{0}} + \alpha_0 = 1$. This means that we choose the solution for the density $4\pi f_{00}(\zeta)$ in the following manner $(\zeta \leq 0)$

$$f_{00}(\zeta) = \cosh \zeta/\lambda_0 - (\alpha_{\bar{0}} - \alpha_0) \sinh \zeta/\lambda_0 + \sum_s \alpha_s e^{\zeta/\lambda_s}$$

or

$$= \cosh \zeta/\lambda_0 - \frac{\lambda_0}{\delta} \sinh \zeta/\lambda_0 + \sum_s \alpha_s e^{\zeta/\lambda_s} \qquad (19)$$

with the <u>linear extrapolation distance</u> $\delta = \lambda_0/(\alpha_{\bar{0}} - \alpha_0)$. The <u>distance of the extrapolated endpoint</u> Δ is related to δ by the equation

$$\Delta = \frac{\lambda_0}{2} \log \frac{\lambda_0 + \delta}{\lambda_0 - \delta} . \qquad (20)$$

An alternate representation of $f_{00}(\zeta)$ is therefore

equation (21) should read:

$$f_{00}(\zeta) = \frac{\sinh(\Delta - \zeta)/\lambda_0}{\sinh \Delta/\lambda_0} + \sum_s \alpha_s e^{\zeta/\lambda_s} \quad (\zeta \leq 0) \qquad (21) \qquad (21)$$

δ and Δ are dimensionless quantities which are to be multiplied by Σ^{-1} in order to obtain the extrapolation distances in centimeters. The $\sum_s$ is the transient part, which does not contribute to the asymptotic behavior

at $z = -\infty$, because the λ_s are much smaller than λ_0.

5. A short comparison with the Gauss quadrature method[5]

The characteristic equation in the spherical harmonics method was shown to be $(1+a\lambda_k^2)P_{L+1}(\lambda_k) - \lambda_k(c+a\lambda_k^2)W_L(\lambda_k) = 0$ $W_L(\lambda_k)$ may be represented[6] by

$$W_L(\lambda_k) = \frac{1}{2}\int_{-1}^{+1} \frac{P_{L+1}(\lambda_k) - P_{L+1}(u)}{\lambda_k - u}\, du \tag{22}$$

The integrand is a polynomial of degree L in u; hence the integral is given correctly by the Gauss quadrature method, which is here used only as a mathematical aid to give another correct expression for $W_L(\lambda_k)$:

$$W_L(\lambda_k) = \frac{1}{2}\sum_{j=\pm 1}^{\pm(L+1)/2} a_j \frac{P_{L+1}(\lambda_k) - P_{L+1}(\mu_j)}{\lambda_k - \mu_j} = \frac{1}{2}\sum_{j=\pm 1}^{\pm(L+1)/2} a_j \frac{P_{L+1}(\lambda_k)}{\lambda_k - \mu_j} \tag{23}$$

- because $P_{L+1}(\mu_j) = 0$ —, where

$$a_j = \frac{1}{P'_{L+1}(\mu_j)}\int_{-1}^{+1} \frac{P_{L+1}(u)\,du}{u-\mu_j} = -2\,\frac{Q_{L+1}(\mu_j)}{P'_{L+1}(\mu_j)} = 2\,\frac{W_L(\mu_j)}{P'_{L+1}(\mu_j)}\,,$$

Putting the last value of a_j in equation (23) one obtains the formula

$$W_L(\lambda_k) = P_{L+1}(\lambda_k)\sum_{j=\pm 1}^{\pm(L+1)/2} \frac{W_L(\mu_j)}{(\lambda_k-\mu_j)P'_{L+1}(\mu_j)}\,,$$

5 A similar comparison has been made by G. C. Mark I.
6 A. Erdélyi, etc., Higher Transcendental Functions, Vol. I, p. 154, Eq. (31).

which could be found by an application of the Lagrange interpolation formula also. With equation (23) the characteristic equation may be written in the form

$$\left[1 + a\lambda_k^2 - \lambda_k (c + a\lambda_k^2) \frac{1}{2} \sum_{j=\pm 1}^{\pm (L+1)/2} \frac{a_j}{\lambda_k - \mu_j} \right] P_{L+1}(\lambda_k) = 0 ,$$

where the factor $P_{L+1}(\lambda_k)$ is different from zero as long as $c \neq 0$, $a \neq 0$. Hence, the <u>characteristic equation of the spherical harmonics method is also</u>

$$1 + a\lambda_k^2 - \lambda_k (c + a\lambda_k^2) \frac{1}{2} \sum_{j=\pm 1}^{\pm (L+1)/2} \frac{a_j}{\lambda_k - \mu_j} = 0 . \tag{24}$$

The same equation will now be derived with the C-W-method. The original Boltzmann equation was

$$\mu \frac{\partial f(\xi,\mu)}{\partial \xi} + f(\xi,\mu) = \frac{1}{2}(1-\gamma_a) \int_{-1}^{+1} f(\xi,\mu')\, d\mu' + \frac{3}{2}(1-\gamma_t)\mu \int_{-1}^{+1} \mu' f(\xi,\mu')\, d\mu' .$$

Integrating this equation over μ from -1 to +1 one gets

$$\frac{\partial}{\partial \xi} \int_{-1}^{+1} \mu f(\xi,\mu)\, d\mu + \int_{-1}^{+1} f(\xi,\mu)\, d\mu$$

$$= \frac{1}{2}(1-\gamma_a) \int_{-1}^{+1} f(\xi,\mu')\, d\mu' \int_{-1}^{+1} d\mu + \frac{3}{2}(1-\gamma_t) \int_{-1}^{+1} \mu' f(\xi,\mu')\, d\mu' \int_{-1}^{+1} \mu\, d\mu .$$

The last integral over μ vanishes and one finds the relation

$$\frac{\partial}{\partial \xi} \int_{-1}^{+1} \mu f(\xi,\mu)\, d\mu = -\gamma_a \int_{-1}^{+1} f(\xi,\mu)\, d\mu \tag{25}$$

between the two integrals on the right side of the Boltzmann equation. This is an essential equation for solving the anisotropic case with the C-W-method. If one assumes now a partial solution with an arbitrary constant λ_r

$$f(\xi,\mu) \sim g(\mu)\, e^{-\xi/\lambda_r}$$

one has

$$\frac{\partial f}{\partial \xi} \sim -\frac{1}{\lambda_r}\, g(\mu)\, e^{-\xi/\lambda_r}$$

and from equation (25)

$$\int_{-1}^{+1} \mu f(\xi,\mu)\, d\mu = \gamma_a \lambda_r \int_{-1}^{+1} f(\xi,\mu)\, d\mu .$$

Hence, the Boltzmann equation yields

$$\begin{aligned}\left(-\frac{\mu}{\lambda_r}+1\right) g(\mu) &= \left[\tfrac{1}{2}(1-\gamma_a) + \tfrac{3}{2}\gamma_a(1-\gamma_t)\lambda_r\mu\right] \int_{-1}^{+1} g(\mu)\, d\mu \\ &= \tfrac{1}{2}(c + a\lambda_r\mu)\, C\end{aligned} \tag{26}$$

$$\text{with} \quad C = \int_{-1}^{+1} g(\mu)\, d\mu = \text{const.}$$

and one obtains the solution

$$g(\mu) = \frac{C}{2}\, \frac{\lambda_r}{\lambda_r - \mu}\, (c + a\lambda_r\mu) \tag{27}$$

as a μ-dependent amplitude of the partial solution $f(\xi,\mu)$ above. The expression (27) for $g(\mu)$ shows a pole at $\mu = \lambda_r$. In conformity with the physical conditions of the Milne problem one supposes therefore $g(\mu) = 0$ for positive μ and equal to (27) for negative μ at $\xi = 0$. Equations (26) and (27) are consistent only for certain λ_r's , which one gets by carrying out the integral

$$C = \int_{-1}^{+1} g(\mu)\, d\mu = \frac{C}{2} \int_{-1}^{0} \frac{\lambda_r (c + a\lambda_r \mu)}{\lambda_r - \mu}\, d\mu .$$

Hence, it follows a transcendental characteristic equation for the λ_r's :

$$1 + a\lambda_r^2 - \lambda_r (c + a\lambda_r^2) \log \frac{1+\lambda_r}{\lambda_r} = -1. \qquad (27a)$$

Selecting the λ_r's as roots of this equation, C in (27) may be considered as an arbitrary constant. For $\xi \neq 0$, however, the backward scattering has to be considered and the divergence of the integral would become manifest.

Therefore, one replaces the integral equation (26) by a system of linear equations, evaluating the integral <u>in L-approximation</u> by Gauss quadrature method and using instead the exact λ_r of equation (27a) another λ_K

$$\left(-\frac{\mu_i}{\lambda_K} + 1\right) g(\mu_i) = \frac{1}{2}(c + a\lambda_K \mu_i) \sum_{j=\pm 1}^{\pm(L+1)/2}{}' a_j\, g(\mu_j) \qquad (28)$$

$$\left(i = \pm 1, \pm 2, \dots \pm \frac{L+1}{2}\right)$$

The μ_j's are also in the Gauss quadrature method the roots of $P_{L+1}(\mu_j) = 0$ and we have here $L+1$ linear equations for the determination of the $g(\mu_j)$ which depend on λ_K by equation (27). Therefore, one obtains by introduction of $g(\mu)$ from equation (27) the characteristic equation of the C-W method for those possible λ_K , for which the system of linear equations

(28) has a solution. This gives

$$1 = \frac{1}{2}\sum_{j=\pm 1}^{\pm(l+1)/2} a_j \frac{\lambda_k}{\lambda_k - \mu_j}(c + a\lambda_k/\mu_j) \equiv \frac{1}{2}\sum_{j=\pm 1}^{\pm(l+1)/2} a_j \lambda_k \left[-a\lambda_k + \frac{c + a\lambda_k^2}{\lambda_k - \mu_j}\right]$$

$$\equiv -\frac{a}{2}\lambda_k^2 \sum_{j=\pm 1}^{\pm(l+1)/2} a_j + \frac{1}{2}\lambda_k (c + a\lambda_k^2) \sum_{j=\pm 1}^{\pm(l+1)/2} \frac{a_j}{\lambda_k - \mu_j} \; ;$$

because $\sum_{j=\pm 1}^{\pm(l+1)/2} a_j = 2$, we get finally the characteristic equation in the C-W method

$$1 + a\lambda_k^2 - \lambda_k (c + a\lambda_k^2)\frac{1}{2}\sum_{j=\pm 1}^{\pm(l+1)/2} \frac{a_j}{\lambda_k - \mu_j} = 0 \qquad (29)$$

which is identical with equation (24).

In the C-W method[7] one has now to assume a superposition of partial solutions -- for the negative z of our medium with the opposite sign of the λ_k's --

$$f_{C-W}(z,\mu) = \sum_k g_{-k}(\mu)\, e^{z/\lambda_k} = \sum_k \alpha_k \lambda_k \frac{c - a\lambda_k\mu}{\lambda_k + \mu}\, e^{z/\lambda_k}$$

$$\equiv \sum_k \alpha_k \lambda_k\, e^{z/\lambda_k}\left[-a\lambda_k + \frac{c + a\lambda_k^2}{\lambda_k + \mu}\right] \qquad (30)$$

where the α_k's replace the different constants $\frac{1}{2}C_k$'s of equation (27) for the set of $-\lambda_k$'s ; as before they must be determined from the boundary condition at $z = 0$. One recognizes the identity of the C-W expression (30) and the first part $f^{I}(z,\mu)$ of the spherical harmonics method equation

7 S. Chandrasekhar, Radiative Transfer, Oxford 1950.

(17).

6. Completion of the solution

For the fluxes at the boundary $z = 0$ we have two expressions: equation (16) on the medium side and equation (13) on the vacuum side

$$f(0,\mu) = \sum_k \alpha_k \lambda_k \left\{ -a\lambda_k + \frac{c + a\lambda_k^2}{\lambda_k + \mu} \left[1 - \frac{P_{L+1}(\mu)}{P_{L+1}(-\lambda_k)} \right] \right\}$$
$$= (L+1)\, P_{L+1}(\mu) \sum_{j=1}^{(L+1)/2} \beta_j \frac{P_L(\mu_j)}{\mu - \mu_j} . \qquad (31)$$

They must be equal for every μ between $-1 \leq \mu \leq 1$; it can be shown by a suitable application of the Lagrange interpolation formula to the medium side of this equation, that the β_j's can always be chosen in such a way to fit this condition. To determine the remaining $\frac{L+1}{2}$ α_k's (this means for instance $\alpha_0 - \alpha_0 = \frac{\lambda_0}{\delta}, \alpha_1, \alpha_2, \ldots\ldots, \alpha_{\frac{L-1}{2}}$) it is sufficient to remark that the vacuum side expression vanishes at $\mu = -\mu_j$. Hence the medium side expression has to vanish at the same points; this yields $\frac{L+1}{2}$ inhomogeneous linear equations for the remaining $\frac{L+1}{2}$ α_k's:

$$\sum_k \alpha_k \lambda_k \left\{ -a\lambda_k + \frac{c + a\lambda_k^2}{\lambda_k - \mu_j} \right\} = 0 \qquad \left(j = 1, 2, \ldots\ldots, \frac{L+1}{2} \right). \qquad (32)$$

Because $P_{L+1}(-\mu_j) = 0$ in equation (31) the C-W method and spherical harmonics method lead to the same equations (32) for the coefficients α_k. The appearance of the μ_j's in both methods is a special feature of the Milne problem and other problems with a vacuum on one side. In these cases the replacement of the vacuum by a perfect absorber leads in P_L

approximation to the use of the pure Legendre polynomials of the 1. kind on the vacuum side, whereas they are introduced as a mathematical substitute in the C-W method on the medium side.

The calculation of the coefficients α_K is carried out in the Appendix II. In solving the system (32) of linear equations one is led to the introduction of "half Legendre polynomials" which have only the positive roots μ_j of (14) and λ_s $\left(s = 1, 2, \ldots \frac{L-1}{2}\right)$ of (12), namely

$$p(\lambda) = \prod_{j=1}^{(L+1)/2} (\lambda - \mu_j) \qquad \text{and} \qquad r(\lambda) = \prod_{s=1}^{(L-1)/2} (\lambda - \lambda_s) \tag{33}$$

excluding the largest root λ_0 of (12) from $r(\lambda)$. Intimately connected with the extrapolation distances δ and Δ is the following function of λ

$$\delta(\lambda) = \lambda \, \frac{r(\lambda)\, p(-\lambda) + r(-\lambda)\, p(\lambda)}{r(\lambda)\, p(-\lambda) - r(-\lambda)\, p(\lambda)} \, . \tag{34}$$

One may use this function for a shorter representation of the coefficients α_K.

After introducing two further abbreviations

$$\lambda_a = i\sqrt{\frac{c}{a}} \tag{35}$$

and for a common factor of the α_K's independent of K

$$N = \frac{r(\lambda_0)\, r(-\lambda_0)}{r(\lambda_0)\, p(-\lambda_0) + r(-\lambda_0)\, p(\lambda_0)} \; \frac{\delta(\lambda_0)}{\delta(\lambda_0) + \frac{a}{c}\lambda_0^2\, \delta(\lambda_a)} \, , \tag{36}$$

the solution α_k of equation (32) may be written

$$\alpha_{\bar{0}} = N\left[1 + \frac{a}{c}\lambda_0\,\delta(\lambda_a)\right]\frac{p(-\lambda_0)}{r(-\lambda_0)} \tag{37}$$

$$\alpha_0 = N\left[1 - \frac{a}{c}\lambda_0\,\delta(\lambda_a)\right]\frac{p(\lambda_0)}{r(\lambda_0)} \tag{38}$$

$$\alpha_s = N\left[1 - \frac{a}{c}\lambda_s\,\delta(\lambda_a)\right]\frac{c + a\lambda_0^2}{c + a\lambda_s^2}\;\frac{2\lambda_0^2\,p(\lambda_s)}{\lambda_s(\lambda_s^2 - \lambda_0^2)\,r'(\lambda_s)} \tag{39}$$

$$\left(s = 1, 2, \ldots \frac{L-1}{2}\right).$$

The extrapolation distances are -- see equations (19) and (20) --

$$\delta = \frac{\delta(\lambda_0) + \frac{a}{c}\lambda_0^2\,\delta(\lambda_a)}{1 + \frac{a}{c}\,\delta(\lambda_a)\,\delta(\lambda_0)} \tag{40}$$

and

$$\Delta = \lambda_0\left[\tanh^{-1}\frac{\delta(\lambda_0)}{\lambda_0} + \tanh^{-1}\frac{a}{c}\lambda_0\,\delta(\lambda_a)\right]$$

Introducing the coefficients α_k in equation (16) one obtains the solution for the directed flux $f(z,\mu)$ in every direction $\mu = \cos\theta$ and on every plane $z = \xi/\Sigma$ of the medium in P_L-approximation for the Milne problem with anisotropic scattering and absorption. The case of fission, with production of neutrons having the same energy as the neutrons which induced the fission, is covered by the formalism by putting $\gamma_a < 0$.

At the boundary $z = 0$ the l. part of $f(0,\mu)$ namely $f^{I}(0,\mu)$ i.e. the C-W part for positive μ -- equation (17) with the coefficients (37)-(39) -- can be summed up to a closed expression by a calculation carried out in

the Appendix III:

$$f^{I}(0,\mu) = 2N(c+a\lambda_0^2)\left[1+\frac{a}{c}\delta(\lambda_a)\mu\right]\frac{\lambda_0^2}{\lambda_0^2-\mu^2}\,\frac{p(-\mu)}{r(-\mu)} \qquad (41)$$

This expression has poles at $\mu = -\lambda_s$. Remembering that $f(0,\mu)$ is a polynomial of degree L in μ <u>coinciding with $f^{I}(0,\mu)$</u> at the points $\mu = \mu_j$ and having <u>zeros</u> at the points $\mu = -\mu_j$ one is able to apply the Lagrange interpolation formula to construct this polynomial, which represents the directed flux at the boundary according to the <u>spherical harmonics method</u> and which is regular for all μ $(-1 \leq \mu \leq 1)$:

$$f(0,\mu) = \sum_{j=1}^{(L+1)/2} \frac{f^{I}(0,\mu_j)\,P_{L+1}(\mu)}{(\mu-\mu_j)\,P'_{L+1}(\mu_j)}$$

the second line of equation (42) should read:

$$= 2N\lambda_0^2(c+a\lambda_0^2)p(-\mu)p(\mu)\sum_{j=1}^{(L+1)/2}\frac{1+(a/c)\delta(\lambda_a)\mu_j}{(\mu-\mu_j)(\lambda_0^2-\mu_j^2)r(-\mu_j)p'(\mu_j)} \qquad (42)$$

(42)

By comparison of equation (42) with the second expression of equation (13) for $\xi = 0$ finally the coefficients β_j of the vacuum side representation are obtained

$$\beta_j = \frac{f^{I}(0,\mu_j)}{(L+1)\,P_L(\mu_j)\,P'_{L+1}(\mu_j)} = \frac{2N\lambda_0^2(c+a\lambda_0^2)\left[1+\frac{a}{c}\delta(\lambda_a)\mu_j\right]p(-\mu_j)}{(L+1)\,P_L(\mu_j)\,P'_{L+1}(\mu_j)\,(\lambda_0^2-\mu_j^2)\,r(-\mu_j)}\,. \qquad (43)$$

S. Chandrasckhar introduced in his book "Radiative Transfer," p. 127, a function $H(\mu)$, to which the functions $p(\mu)$ and $r(\mu)$ here are related by the equation

$$H(\mu) = \frac{\lambda_0 \lambda_1 \cdots \lambda_{(l-1)/2}}{\mu_1 \mu_2 \cdots \mu_{(l+1)/2}} \frac{-p(-\mu)}{(\lambda_0+\mu)\, r(-\mu)}$$

$$= \frac{-1}{\sqrt{1-c-(a/3)}} \frac{p(-\mu)}{(\lambda_0+\mu)\, r(-\mu)} = \frac{\lambda_0}{\lambda_0+\mu} \frac{r(0)}{p(0)} \frac{p(-\mu)}{r(-\mu)} ,$$

$$\left(\text{Remark: } 1-c-\frac{a}{3} = \gamma_a \gamma_t\right)$$

7. Investigation of $f^{II}(0,\mu)$

The representation of $f(0,\mu)$ given in equation (42) has the form of equation (13) for $z=0$, or of the second term on the right side of equation (31), both of which were derived from a consideration of the vacuum side. Therefore it was possible also to deduce from formula (42) the coefficients β_j (equation 43) of the vacuum side representation of $f(0,\mu)$. We obtain the medium side representation if we put the α_k's of equations (37)-(39) in the first term on the right side of equation (31) or in equation (16) for $z=0$. Then we get the medium side representation, which is rather lengthy.

The connection between medium side and vacuum side representation is quickly obtained by an application of the Lagrange interpolation formula to the medium side representation of $f^{II}(0,\mu)$. To this end we construct the function $f(\lambda) = 1-\beta\lambda$ with the use of its values at the

$L+2$ points $\lambda_j = (-\lambda_0, \lambda_0, \lambda_1, \ldots, \lambda_{\frac{L-1}{2}}, -\mu_1, -\mu_2, \ldots, -\mu_{\frac{L+1}{2}})$ at which the polynomial $R(\lambda) = (\lambda^2 - \lambda_0^2)\, r(\lambda)\, p(-\lambda)$ has its zeros. Then the Lagrange interpolation formula

$$\frac{f(\lambda)}{R(\lambda)} = \sum_{\text{all } \lambda_j\text{'s}} \frac{f(\lambda_j)}{(\lambda - \lambda_j)\, R'(\lambda_j)} \tag{44}$$

gives for $\lambda = -\mu$

$$\frac{1+\beta\mu}{(\mu^2-\lambda_0^2)\, r(-\mu)\, p(\mu)} = -\Bigg\{ \frac{1+\beta\lambda_0}{(\lambda_0-\mu)\, 2\lambda_0\, r(-\lambda_0)\, p(\lambda_0)} + \frac{1-\beta\lambda_0}{(\lambda_0+\mu)\, 2\lambda_0\, r(\lambda_0)\, p(-\lambda_0)}$$
$$+ \sum_{s=1}^{(L-1)/2} \frac{1-\beta\lambda_s}{(\lambda_s+\mu)(\lambda_s^2-\lambda_0^2)\, r'(\lambda_s)\, p(-\lambda_s)}$$
$$+ \sum_{j=1}^{(L+1)/2} \frac{1+\beta\mu_j}{(\mu-\mu_j)(\lambda_0^2-\mu_j^2)\, r(-\mu_j)\, p'(\mu_j)} \Bigg\} \tag{45}$$

Now $f^{II}(0,\mu)$ in medium side representation (See equation (18))

$$f^{II}(0,\mu) = -\sum_k \alpha_k \lambda_k \frac{c+a\lambda_k^2}{\lambda_k+\mu} \frac{P_{L+1}(\mu)}{P_{L+1}(-\lambda_k)} = -\sum_k \alpha_k \lambda_k \frac{c+a\lambda_k^2}{\lambda_k+\mu} \frac{p(\mu)\, p(-\mu)}{p(\lambda_k)\, p(-\lambda_k)}$$

with the coefficients α_k from equations (37) - (39)

$$= -N\lambda_0 (c+a\lambda_0^2)\, p(\mu)\, p(-\mu) \Bigg\{ \frac{1+\frac{a}{c}\delta(\lambda_a)\lambda_0}{(\lambda_0-\mu)\, r(-\lambda_0)\, p(\lambda_0)} + \frac{1-\frac{a}{c}\delta(\lambda_a)\lambda_0}{(\lambda_0+\mu)\, r(\lambda_0)\, p(-\lambda_0)}$$
$$+ 2\lambda_0 \sum_{s=1}^{(L-1)/2} \frac{1-\frac{a}{c}\delta(\lambda_a)\lambda_s}{(\lambda_s+\mu)(\lambda_s^2-\lambda_0^2)\, r'(\lambda_s)\, p(-\lambda_s)} \Bigg\} \tag{46}$$

is simply proportional to the first 3 terms on the right side of equation (45) with the constant $\beta = \frac{a}{c}\,\delta(\lambda_a)$. Hence by comparison with equation (45) we may write $f^{II}(0,\mu)$ of equation (46) also in the following form

$$f^{II}(0,\mu) = N\cdot 2\lambda_0^2(c+a\lambda_0^2)\,p(\mu)\,p(-\mu)\cdot$$

$$\cdot\left\{\frac{1+\frac{a}{c}\delta(\lambda_a)\mu}{(\mu^2-\lambda_0^2)\,r(-\mu)\,p(\mu)} + \sum_{j=1}^{(L+1)/2}\frac{1+\frac{a}{c}\delta(\lambda_a)\mu_j}{(\mu-\mu_j)(\lambda_0^2-\mu_j^2)\,r(-\mu_j)\,p'(\mu_j)}\right\}$$

$$\equiv -2N(c+a\lambda_0^2)\left[1+\frac{a}{c}\delta(\lambda_a)\mu\right]\frac{\lambda_0^2}{\lambda_0^2-\mu^2}\;\frac{p(-\mu)}{r(-\mu)}$$

$$+2N\lambda_0^2(c+a\lambda_0^2)\,p(\mu)\,p(-\mu)\sum_{j=1}^{(L+1)/2}\frac{1+\frac{a}{c}\delta(\lambda_a)\mu_j}{(\mu-\mu_j)(\lambda_0^2-\mu_j^2)\,r(-\mu_j)\,p'(\mu_j)}\;. \qquad (47)$$

The first term on the right side of the last equation is $-f^{I}(0,\mu)$ in the form of equation (41) again. Hence we have extracted by the use of the Lagrange formula the "pole-part" $-f^{I}(0,\mu)$ of $f^{II}(0,\mu)$. The second term is the result of the spherical harmonics method $f(0,\mu)$ in the vacuum side representation of equation (42) again. Keeping equation (46) and (47) together we have the relation between the two representations of $f(0,\mu)$ on the medium side (M. S.) and on the vacuum side (V. S.):

$$f(0,\mu) = N\cdot 2\lambda_0^2(c+a\lambda_0^2)\left\{\frac{1+\frac{a}{c}\delta(\lambda_a)\mu}{\lambda_0^2-\mu^2}\;\frac{p(-\mu)}{r(-\mu)} + \right.$$

$$+ p(\mu)\, p(-\mu) \Big[\frac{1+\frac{a}{c}\,\delta(\lambda_a)\,\lambda_0}{2(\lambda_0-\mu)\, r(-\lambda_0)\, p(\lambda_0)} + \frac{1-\frac{a}{c}\,\delta(\lambda_a)\,\lambda_0}{2(\lambda_0+\mu)\, r(\lambda_0)\, p(-\lambda_0)}$$

$$+ \sum_{s=1}^{(L-1)/2} \frac{1-\frac{a}{c}\,\delta(\lambda_a)\,\lambda_s}{(\lambda_s+\mu)(\lambda_s^2-\lambda_0^2)\, r'(\lambda_s)\, p(-\lambda_s)} \Big] \Big\} \qquad (M.S.) \qquad (48)$$

$$= N \cdot 2\lambda_0^2 (c+a\lambda_0^2)\, p(\mu)\, p(-\mu) \sum_{j=1}^{(L+1)/2} \frac{1+\frac{a}{c}\,\delta(\lambda_a)\,\mu_j}{(\mu-\mu_j)(\lambda_0^2-\mu_j^2)\, r(-\mu_j)\, p'(\mu_j)} \qquad (V.S.) \qquad (49)$$

8. Density and current

We may replace $\lambda_k(c+a\lambda_k^2)$ in equation (16) with the help of characteristic equation (12)

$$\lambda_k(c+a\lambda_k^2) = \frac{(1+a\lambda_k^2)\, P_{L+1}(\lambda_k)}{W_L(\lambda_k)}$$

and obtain another sometimes convenient formula for $f(z,\mu)$, $z \leq 0$, L odd:

$$f(z,\mu) = \sum_k \alpha_k\, e^{z/\lambda_k} \Big\{ -a\lambda_k^2 + \frac{1+a\lambda_k^2}{W_L(\lambda_k)} \, \frac{P_{L+1}(\lambda_k) - P_{L+1}(-\mu)}{\lambda_k+\mu} \Big\} . \qquad (50)$$

Because

$$W_L(\lambda_k) = \frac{1}{2} \int_{-1}^{+1} \frac{P_{L+1}(\lambda_k) - P_{L+1}(-\mu)}{\lambda_k+\mu}\, d\mu$$

we obtain quickly from (50) the <u>density</u> $(z \leq 0)$

$$\rho(z) = 2\pi \int_{-1}^{+1} f(\xi,\mu)\,d\mu = 4\pi \sum_k \alpha_k e^{\xi/\lambda_k} \Big\{ -a\lambda_k^2 \cdot \frac{1}{2}\int_{-1}^{+1} d\mu$$

$$+ \frac{1+a\lambda_k^2}{W_L(\lambda_k)} \frac{1}{2} \int_{-1}^{+1} \frac{P_{L+1}(\lambda_k) - P_{L+1}(-\mu)}{\lambda_k + \mu}\, d\mu \Big\}$$

$$= 4\pi \sum_k \alpha_k e^{\xi/\lambda_k} = 4\pi f_{00}(\xi) = \frac{4\pi}{c} f^{I}(z,0). \qquad (51)$$

At the boundary $z = 0$ the density $\rho(0) = 4\pi \sum_k \alpha_k$ is related to the 1. part of directed flux $f^{I}(0,0)$ in the direction $\mu = 0$ which is according to equation (17) and equation (41).

$$f^{I}(0,0) = c \sum_k \alpha_k = 2N(c + a\lambda_0^2)\frac{p(0)}{r(0)}. \qquad (52)$$

Hence the density at the boundary in the spherical harmonics method is

$$\rho(0) = 4\pi \sum_k \alpha_k = 8\pi N\left(1 + \frac{a}{c}\lambda_0^2\right)\frac{p(0)}{r(0)}. \qquad (53)$$

This equation relates also the density at $z = 0$ with the normalization factor N and could be used for a change in normalization from N to unit density. The normalization with N results from the choice in equation (19).

Also the current $j(z)$ for $z \leq 0$ is quickly obtained with the help of equation (50):

$$j(z) = 2\pi \int_{-1}^{+1} \mu\, f(z,\mu)\, d\mu$$

$$= 4\pi \sum_k \alpha_k e^{\xi/\lambda_k} \left\{ -a\lambda_k^2 \cdot \frac{1}{2}\int_{-1}^{+1} \mu\, d\mu + \frac{1+a\lambda_k^2}{W_L(\lambda_k)} \frac{1}{2}\int_{-1}^{+1} \mu \frac{P_{L+1}(\lambda_k) - P_{L+1}(-\mu)}{\lambda_k + \mu} d\mu \right\}$$

$$= 4\pi \sum_k \alpha_k e^{\xi/\lambda_k} \frac{1+a\lambda_k^2}{W_L(\lambda_k)} \cdot \frac{1}{2}\int_{-1}^{+1} d\mu \left[P_{L+1}(\lambda_k) - P_{L+1}(-\mu) - \lambda_k \frac{P_{L+1}(\lambda_k) - P_{L+1}(-\mu)}{\lambda_k + \mu} \right]$$

$$= 4\pi \sum_k \alpha_k e^{\xi/\lambda_k} \frac{1+a\lambda_k^2}{W_L(\lambda_k)} \left[P_{L+1}(\lambda_k) - \lambda_k W_L(\lambda_k) \right]$$

$$= 4\pi \sum_k \alpha_k e^{\xi/\lambda_k} \frac{1+a\lambda_k^2}{W_L(\lambda_k)} \left[\frac{c+a\lambda_k^2}{1+a\lambda_k^2} - 1 \right] \lambda_k W_L(\lambda_k) \quad \text{with (12)}$$

$$= 4\pi(c-1) \sum_k \alpha_k \lambda_k e^{\xi/\lambda_k} = -4\pi \gamma_a \sum_k \alpha_k \lambda_k e^{\xi/\lambda_k} = \frac{4\pi}{3} f_{10}(\xi). \qquad (54)$$

For $z = 0$ we have the current at the boundary

$$j(0) = 2\pi \int_{-1}^{+1} \mu\, f(0,\mu)\, d\mu = \frac{4\pi}{3} f_{10}(0) = -4\pi \gamma_a \sum_k \alpha_k \lambda_k$$

$$= -\frac{16\pi N \gamma_a \lambda_0^2\, p(\lambda_a)\, p(-\lambda_a)}{\lambda_a \left[r(\lambda_a)\, p(-\lambda_a) - r(-\lambda_a)\, p(\lambda_a) \right]}. \qquad (55)$$

The last result is obtained by a further application of the Lagrange interpolation formula (see Appendix IV). Equation (55) might also be used to change the normalization to unit current in z-direction.

9. Special cases

(a) No absorption: $\gamma_a = 0$.

For no absorption the quantities $c = 1-\gamma_a \to 1$ and $a = 3\gamma_a(1-\gamma_t) = 0$ whatever finite value γ_t may have. The first two equations of the system (3) show that in the limit $\gamma_a = 0$

$$f_{00}(\xi) = 1 - \frac{\xi}{\delta} + \sum_s \alpha_s e^{\xi/\lambda_s} \tag{56}$$

$$f_{10}(\xi) = \frac{1}{\delta\gamma_t} \tag{57}$$

This means that the asymptotic part of $f_{00}(\xi)$ degenerates into a straight line and that $f_{10}(\xi)$ is a constant and does not contain the transients s. The $f_{\ell 0}(\xi)$ for $\ell \geq 2$ contain instead only transients and no asymptotic part. The square of the largest root of the characteristic equation (12) may be estimated to

$$\cancel{\lambda_0^2 \approx \frac{1+\frac{4}{5}\gamma_a + \frac{108}{175}\gamma_a(1-\gamma_t)}{3\gamma_a\gamma_t}} \qquad \boxed{\lambda_0^2 \approx \frac{1+\frac{4}{5}\gamma_a + \frac{108}{175}\gamma_a^2\gamma_t}{3\gamma_a\gamma_t}} \tag{58}$$

in the general case. In the limit $\gamma_a = 0$ and arbitrary γ_t this expression goes to infinity, or precisely

$$3\gamma_a\gamma_t\lambda_0^2 \to 1 \tag{59}$$

Also $\lambda_a = i\sqrt{\frac{c}{a}}$ goes to infinity $\lambda_a \to i\infty$; $\frac{a}{c}\lambda_0^2 = \frac{3\gamma_a(1-\gamma_t)}{1-\gamma_a}\lambda_0^2 \to \frac{1-\gamma_t}{\gamma_t}$; $1+\frac{a}{c}\lambda_0^2 \to \frac{1}{\gamma_t}$. A development of $\delta(\lambda)$ in a power series of $1/\lambda$ shows

$$\delta(\lambda) = M_1 - \Lambda_1 + \frac{1}{\lambda^2}\left[M_3 - M_2M_1 + M_1\Lambda_1(M_1-\Lambda_1) + \Lambda_1\Lambda_2 - \Lambda_3\right] + \frac{1}{\lambda^4}(\cdots) + \cdots, \tag{60}$$

where

$$M_1 = \sum_{j=1}^{(L+1)/2} \mu_j , \quad M_2 = \sum_{\substack{j,k \\ j<k}}^{(L+1)/2} \mu_j \mu_k , \quad M_3 = \sum_{\substack{j,k,l \\ j<k<l}}^{(L+1)/2} \mu_j \mu_k \mu_l , \quad \ldots$$

$$\Lambda_1 = \sum_{s=1}^{(L-1)/2} \lambda_s , \quad \Lambda_2 = \sum_{\substack{s,t \\ s<t}}^{(L-1)/2} \lambda_s \lambda_t , \quad \Lambda_3 = \sum_{\substack{s,t,u \\ s<t<u}}^{(L-1)/2} \lambda_s \lambda_t \lambda_u , \quad \ldots \tag{61}$$

are the primitive symmetrical functions of the roots μ_j and λ_s.

For $|\lambda| = \infty$ only the 1 term of the series (60) remains; hence we have in the special case $\gamma_a = 0$, $\lambda_0 \to \infty$, $\lambda_a \to i\infty$

$$\delta(\lambda_0) = \delta(\lambda_a) \to M_1 - \Lambda_1 \tag{62}$$

$$\frac{r(\lambda_0)\, r(-\lambda_0)}{r(\lambda_0)\, p(-\lambda_0) + r(-\lambda_0)\, p(\lambda_0)} \to -\frac{1}{2(M_1 - \Lambda_1)}$$

$$N \to -\frac{\gamma_t}{2(M_1 - \Lambda_1)} . \tag{63}$$

The two extrapolated distances become equal: $\delta = \Delta \to (M_1 - \Lambda_1)/\gamma_t$; the coefficients $\alpha_{\bar{0}}$ and α_0 diverge, but in the development of the first term of $f_{00}(\xi)$

$$\alpha_{\bar{0}}\, e^{-\xi/\lambda_0} + \alpha_0\, e^{\xi/\lambda_0} = \alpha_{\bar{0}} + \alpha_0 - \frac{\alpha_{\bar{0}} - \alpha_0}{\lambda_0}\xi + \frac{1}{2}\frac{1}{\lambda_0^2}(\alpha_{\bar{0}} + \alpha_0)\xi^2 + \ldots \to 1 - \frac{\alpha_{\bar{0}} - \alpha_0}{\lambda_0}\xi$$

only the sum $\alpha_{\bar{0}} + \alpha_0 = 1$ and $\dfrac{\alpha_{\bar{0}} - \alpha_0}{\lambda_0} \to \dfrac{\gamma_t}{M_1 - \Lambda_1} = \dfrac{1}{\delta}$ play a role.

In this way one gets systematically equation (56) again

$$f_{00}(\xi) \to 1 - \frac{\xi}{\delta} + \sum_s \alpha_s\, e^{\xi/\lambda_s} = 1 - \frac{\gamma_t \xi}{M_1 - \Lambda_1} + \sum_s \alpha_s\, e^{\xi/\lambda_s} .$$

For $f_{10}(\xi) = 3\gamma a \{ \alpha_{\bar{0}} \lambda_0 e^{-\xi/\lambda_0} - \alpha_0 \lambda_0 e^{\xi/\lambda_0} \} - 3\gamma a \sum_s \alpha_s \lambda_s e^{\xi/\lambda_s}$

$$= \{ 3\gamma a \lambda_0 (\alpha_{\bar{0}} - \alpha_0) - 3\gamma a \xi + \frac{3\gamma a}{2\lambda_0} (\alpha_{\bar{0}} - \alpha_0) \xi^2 + \cdots \} - 3\gamma a \sum_s \alpha_s \lambda_s e^{\xi/\lambda_s}$$

only the first term remains after the limiting process

$$f_{10}(\xi) \longrightarrow 3\gamma a \lambda_0^2 \frac{\alpha_{\bar{0}} - \alpha_0}{\lambda_0} \rightarrow \frac{1}{\delta \cdot \gamma_t} = \frac{1}{M_1 - \Lambda_1} ,$$

which is equation (57) again. The asymptotic part plays no role in the higher $f_{\ell 0}$'s, but the coefficients α_s of the transients behave regularly since

$$\alpha_s \longrightarrow \frac{p(\lambda_s)}{(M_1 - \Lambda_1) \lambda_s \gamma'(\lambda_s)} \tag{64}$$

The characteristic equation (12) is now only of the degree $L-1$, because 2 roots $\lambda_0, -\lambda_0$ are infinite, and (12) becomes

$$P_{L+1}(\lambda_s) - \lambda_s W_L(\lambda_s) = 0 \qquad (\pm\lambda_1, \pm\lambda_2, \ldots \pm\lambda_{\frac{L-1}{2}}) \tag{65}$$

(As in (12), the largest coefficient in this equation vanishes.) One recognizes in (65) the independence of the λ_s of γ_t, and (64) shows that the α_s are also independent of γ_t. Only $\delta = \Delta$ depends on γ_t. The same is the case with directed fluxes through the boundary. The Gauss quadrature method gives

$$f^I(0,\mu) = \frac{-p(-\mu)}{(M_1 - \Lambda_1)\gamma(-\mu)} \qquad (\mu \geq 0) , \tag{66}$$

[the - sign compensates one - sign in $p(-\mu)$, which contains one (-1) - factor more than $r(-\mu)$], and the spherical harmonics method

$$f(0,\mu) = -\frac{p(-\mu)\,p(\mu)}{M_1 - \Lambda_1} \sum_{j=1}^{(L+1)/2} \frac{1}{(\mu-\mu_j)\,r(-\mu_j)\,p'(\mu_j)} . \qquad (67)$$

(b) <u>Isotropic scattering, absorption:</u> $\gamma_a \neq 0,\ \gamma_t = 1.$ (L finite).

In this case $c = 1-\gamma_a$ is different from 1, but $a = 3\gamma_a(1-\gamma_t) = 0$ The root λ_0 of (12) will remain finite $\lambda_0^2 \approx \frac{1+\frac{4}{5}\gamma_a}{3\gamma_a}$ (see equation (58)). $\lambda_a = i\sqrt{\frac{c}{a}}$ however, is still infinite as $\lambda_a \to i\infty$. Hence one obtains by equation (62) $\delta(\lambda_a) = M_1 - \Lambda_1$. The other quantities become

$$\frac{a}{c}\lambda_0^2 \to 0, \qquad N \to N_1 = \frac{r(\lambda_0)\,r(-\lambda_0)}{r(\lambda_0)\,p(-\lambda_0) + r(-\lambda_0)\,p(\lambda_0)},$$

$$\alpha_{\bar{c}} = N_1 \frac{p(-\lambda_0)}{r(-\lambda_0)}, \quad \alpha_0 = N_1 \frac{p(\lambda_0)}{r(\lambda_0)}, \quad \alpha_s = N_1 \frac{2\lambda_0^2\,p(\lambda_s)}{\lambda_s(\lambda_s^2-\lambda_0^2)\,r'(\lambda_s)}, \qquad (68)$$

$$\delta = \delta(\lambda_0), \quad \Delta = \lambda_0 \tanh^{-1}\frac{\delta(\lambda_0)}{\lambda_0}. \qquad \left(s = 1, 2, \ldots \frac{L-1}{2}\right)$$

The directed flux at the boundary according to the Gauss quadrature method is

$$f^{I}(0,\mu) = 2N_1 c \frac{\lambda_0^2}{\lambda_0^2-\mu^2}\,\frac{p(-\mu)}{r(-\mu)} \qquad (\mu \geq 0) \qquad (69)$$

and according to the spherical harmonics method

$$f(0,\mu) = 2N_1 c\lambda_0^2\,p(-\mu)\,p(\mu) \sum_{\mu=1}^{(L+1)/2} \frac{1}{(\mu-\mu_j)(\lambda_0^2-\mu_j^2)\,r(-\mu_j)\,p'(\mu_j)} . \qquad (70)$$

Appendix I. Calculation of the sum over ℓ in equation (15)

With $W_{\ell-1} = P_\ell Q_0 - Q_\ell$ we have[4]

$$\sum_{\ell=2}^{L} (2\ell+1)\left[(1+a\lambda_k^2)P_\ell(-\lambda_k) + \lambda_k(c+a\lambda_k^2)W_{\ell-1}(-\lambda_k)\right] P_\ell(\mu)$$

$$= \sum_{\ell=2}^{L} (2\ell+1)\left\{\left[1+a\lambda_k^2+\lambda_k(c+a\lambda_k^2)Q_0(-\lambda_k)\right] P_\ell(-\lambda_k)P_\ell(\mu)\right.$$

$$\left. - \lambda_k(c+a\lambda_k^2)Q_\ell(-\lambda_k)P_\ell(\mu)\right\}$$

$$= \sum_{\ell=0}^{L} (2\ell+1)\{\cdots\}$$

$$-\left[\left(1+a\lambda_k^2+\lambda_k(c+a\lambda_k^2)Q_0(-\lambda_k)\right)(1-3\lambda_k\mu) + \lambda_k(c+a\lambda_k^2)\left(Q_0(-\lambda_k)+3\mu Q_1(-\lambda_k)\right)\right]$$

$$= \left(\sum_{\ell=0}^{L}(2\ell+1)\{\cdots\}\right) - 1 + 3\gamma_a\lambda_k\mu - a\lambda_k^2 \quad \text{with} \begin{cases} P_0 = 1, \quad P_1 = \mu, \quad 1-c = \gamma_a, \\ Q_1(-\lambda_k) = -\lambda_k Q_0(-\lambda_k) - 1. \end{cases}$$

Hence, we obtain for the whole curly bracket in equation (15)

$$1 - 3\gamma_a\lambda_k\mu + \sum_{\ell=2}^{L}(2\ell+1)\{\cdots\}$$

$$= -a\lambda_k^2 + \left[1+a\lambda_k^2+\lambda_k(c+a\lambda_k^2)Q_0(-\lambda_k)\right]\sum_{\ell=0}^{L}(2\ell+1)P_\ell(-\lambda_k)P_\ell(\mu)$$

$$- \lambda_k(c+a\lambda_k^2)\sum_{\ell=0}^{L}(2\ell+1)Q_\ell(-\lambda_k)P_\ell(\mu). \qquad (A1)$$

Now we use the Christoffel formulae (see Erdélyi, Higher Transcendental Functions, p. 162; equations (20) and (31)) to calculate the two sums

$$\sum_{\ell=0}^{L}(2\ell+1)P_\ell(-\lambda_k)P_\ell(\mu) = \frac{L+1}{\mu+\lambda_k}\left[P_{L+1}(\mu)P_L(-\lambda_k) - P_L(\mu)P_{L+1}(-\lambda_k)\right]$$

and

$$\sum_{\ell=0}^{L}(2\ell+1)Q_\ell(-\lambda_k)P_\ell(\mu) = \frac{1}{\mu+\lambda_k}\left\{(L+1)\left[P_{L+1}(\mu)Q_L(-\lambda_k) - P_L(\mu)Q_{L+1}(-\lambda_k)\right] - 1\right\}.$$

Putting these values in equation (A1) and replacing the Q's with the aid of the W's one gets

$$1 - 3/a\, \lambda_k \mu + \sum_{\ell=2}^{L} (2\ell+1) \{\cdots\} = -a\lambda_k^2 + \frac{\lambda_k (c + a\lambda_k^2)}{\mu + \lambda_k}$$

$$+ \frac{L+1}{\mu+\lambda_k} \Big\{ \big[(1+a\lambda_k^2) P_L(-\lambda_k) + \lambda_k (c + a\lambda_k^2) W_{L-1}(-\lambda_k) \big] P_{L+1}(\mu)$$

$$- \big[(1+a\lambda_k^2) P_{L+1}(-\lambda_k) + \lambda_k (c + a\lambda_k^2) W_L(-\lambda_k) \big] P_L(\mu) \Big\}.$$

The coefficient of $P_L(\mu)$ in the last term vanishes because it is the characteristic equation (12) for $\lambda = -\lambda_k$. One may replace $1 + a\lambda_k^2$ in the coefficient of $P_{L+1}(\mu)$ by its value in the characteristic equation

$$1 + a\lambda_k^2 = -\lambda_k (c + a\lambda_k^2) \frac{W_L(-\lambda_k)}{P_{L+1}(-\lambda_k)} ,$$

and one obtains

$$1 - 3/a\, \lambda_k \mu + \sum_{\ell=2}^{L} (2\ell+1) \{\cdots\} = -a\lambda_k^2 + \frac{\lambda_k (c + a\lambda_k^2)}{\mu + \lambda_k}$$

$$- \frac{\lambda_k (c + a\lambda_k^2)}{\mu + \lambda_k} \frac{P_{L+1}(\mu)}{P_{L+1}(-\lambda_k)} (L+1) \big[P_L(-\lambda_k) W_L(-\lambda_k) - P_{L+1}(-\lambda_k) W_{L-1}(-\lambda_k) \big].$$

The last bracket in this expression is a constant $= 1/(L+1)$.

Hence we get finally for the expression

$$1 - 3/a\, \lambda_k \mu + \sum_{\ell=2}^{L} (2\ell+1) \left[(1 + a\lambda_k^2)\, P_\ell(-\lambda_k) + \lambda_k (c + a\lambda_k^2)\, W_{\ell-1}(-\lambda_k) \right] P_\ell(\mu)$$

$$= -a\lambda_k^2 + \frac{\lambda_k (c + a\lambda_k^2)}{\mu + \lambda_k} \left[1 - \frac{P_{L+1}(\mu)}{P_{L+1}(-\lambda_k)} \right] \qquad (A\ 2)$$

$$\equiv \frac{\lambda_k}{\mu + \lambda_k} \left\{ c - a\lambda_k \mu - (c + a\lambda_k^2) \frac{P_{L+1}(\mu)}{P_{L+1}(-\lambda_k)} \right\}.$$

For odd L is $P_{L+1}(-\lambda) = P_{L+1}(\lambda)$, therefore the choice of the sign of λ is arbitrary in $P_{L+1}(\lambda)$.

Appendix II. Calculation of the coefficients a_K

In the following the solution of the equations (32)

$$f(0,-\mu_j) = \sum_{K=\bar{0},0,1,2,\cdots}^{(L-1)/2} \alpha_K \lambda_K \left\{ -a\lambda_K + \frac{c+a\lambda_K^2}{\lambda_K-\mu_j} \right\} = 0 \quad \left(j=1,2,\cdots \frac{L+1}{2}\right) \tag{32}$$

and $\alpha_{\bar{0}} + \alpha_0 = 1$

will be carried out in 2 ways, (a) <u>a straightforward way</u> and (b) <u>a shorter way</u>. Both ways show different interesting features.

(a) <u>The straightforward way</u>

We take equation (32) for i and j and subtract $f(0,-\mu_i) - f(0,-\mu_j) = 0$ for two arbitrary $i,j = 1,2,\cdots \frac{L+1}{2}$, $(i \neq j)$. Then we get rid of the term $-a\lambda_K$ in the curly bracket of (32):

$$\sum_K \alpha_K \lambda_K (c+a\lambda_K^2)\left[\frac{1}{\lambda_K-\mu_i} - \frac{1}{\lambda_K-\mu_j}\right] = (\mu_i-\mu_j)\sum_K \frac{\alpha_K\lambda_K(c+a\lambda_K^2)}{(\lambda_K-\mu_j)(\lambda_K-\mu_i)} = 0 \quad (i \neq j) \tag{A 3}$$

Originally we have $\frac{L+3}{2}$ unknown coefficients $\alpha_{\bar{0}}, \alpha_0, \alpha_1, \cdots \alpha_{\frac{L-1}{2}}$; this number is reduced by 1, however, in view of our condition of normalization $\alpha_{\bar{0}} + \alpha_0 = 1$. By the subtraction above one loses one linear independent equation, which may be represented by the sum of the equations (32) over $j = 1, 2, \cdots \frac{L+1}{2}$:

$$\sum_{j=1}^{(L+1)/2} f(0,-\mu_j) = \sum_K \sum_j \alpha_K \lambda_K \left\{ -a\lambda_K + \frac{c+a\lambda_K^2}{\lambda_K-\mu_j} \right\} = 0 \tag{A 4}$$

With the introduction of the polynomial $p(\lambda) = \prod_{j=1}^{(L+1)/2} (\lambda - \mu_j)$, its logarithmic derivative $\frac{p'(\lambda)}{p(\lambda)} = \sum_{j=1}^{(L+1)/2} \frac{1}{\lambda - \mu_j}$ and new variables b_K for equation (A3)

$$\alpha_K \lambda_K (c + a\lambda_K^2) = b_K \, p(\lambda_K) \qquad \left(K = \bar{0}, 0, 1, \cdots \frac{L-1}{2}\right) \tag{A5}$$

one may write both equations

$$\sum_K b_K \left[\prod_{\ell=1}^{(L+1)/2} {}^{(\ell \neq i,j)} (\lambda_K - \mu_j) \right] = 0 \tag{A6}$$

$$\left(i,j = 1, 2, \cdots \frac{L+1}{2} \; ; \; i \neq j\right)$$

and

$$\sum_K \alpha_K \lambda_K \left[-\frac{L+1}{2} a \lambda_K + (c + a\lambda_K^2) \frac{p'(\lambda_K)}{p(\lambda_K)} \right] = 0 \tag{A7}$$

Let us consider first the set of $\frac{1}{2} \frac{L+1}{2} \cdot \frac{L-1}{2}$ equations (A6). They are equivalent to $\frac{L-1}{2}$ linear independent equations only; one recognizes this fact again by the following process: A power development of the product

$$\prod_{\ell=1}^{(L+1)/2} {}^{(\ell \neq i,j)} (\lambda_K - \mu_\ell)$$

in powers of λ_K yields

$$\sum_K \Big\{ b_K \lambda_K^{(L-3)/2} - \Big(\sum_\ell {}^{(\ell \neq i,j)} \mu_\ell\Big) b_K \lambda_K^{(L-5)/2} + \Big(\sum_{\substack{\ell,\ell' \\ \ell<\ell'}} {}^{(\ell,\ell' \neq i,j)} \mu_\ell \mu_{\ell'}\Big) b_K \lambda_K^{(L-7)/2}$$

$$- + - + \cdots + (-1)^{(L-3)/2} \Big(\prod_\ell {}^{(\ell \neq i,j)} \mu_\ell\Big) b_K \Big\} = 0 \tag{A8}$$

A sufficient way to satisfy these equations for every choice of i, j is to put to zero every term in the power development

$$\sum_K b_K \lambda_K^m = 0 \qquad \left(m = 0, 1, 2, \ldots \frac{L-3}{2}\right) \tag{A 9}$$

Then we have a simpler system of $\frac{L-1}{2}$ linear independent equations again for the $\frac{L-1}{2}$ unknown variables $b_1, b_2, \ldots b_{\frac{L-1}{2}}$; if we regard the variables $b_{\bar{0}}$ and b_0 as known quantities just for a moment:

$$\sum_{s=1}^{(L-1)/2} b_s \lambda_s^m = -\left(b_{\bar{0}} \lambda_{\bar{0}}^m + b_0 \lambda_0^m\right) \qquad \left(m = 0, 1, \ldots \frac{L-3}{2}\right) \tag{A 10}$$

The solution of this system is with $r(\lambda) = \prod_{j=1}^{(L-1)/2} (\lambda - \lambda_j)$ and $r'(\lambda_s) = \prod_{j=1}^{(L-1)/2} {}^{(j \neq s)} (\lambda_s - \lambda_j)$:

$$b_s = \frac{1}{r'(\lambda_s)} \left\{ \frac{r(\lambda_{\bar{0}})\, b_{\bar{0}}}{\lambda_s - \lambda_{\bar{0}}} + \frac{r(\lambda_0)\, b_0}{\lambda_s - \lambda_0} \right\} \qquad \left(s = 1, 2, \ldots \frac{L-1}{2}\right) \tag{A 11}$$

or remembering $\lambda_{\bar{0}} = -\lambda_0$ and the relation (A5) between the α_k's and b_k's

$$\alpha_s = \frac{\lambda_0 (c + a \lambda_0^2)}{\lambda_s (c + a \lambda_s^2)} \; \frac{p(\lambda_s)}{r'(\lambda_s)} \left\{ \frac{\alpha_0\, r(\lambda_0)}{(\lambda_s - \lambda_0)\, p(\lambda_0)} - \frac{\alpha_{\bar{0}}\, r(-\lambda_0)}{(\lambda_s + \lambda_0)\, p(-\lambda_0)} \right\} \tag{A 12}$$

This equation relates the coefficients α_s to the coefficients $\alpha_{\bar{0}}$ and α_0. Putting these values of α_s in equation (A7) we obtain a relation between $\alpha_{\bar{0}}$ and α_0 ; this relation together with the normalization condition $\alpha_{\bar{0}} + \alpha_0 = 1$ determines $\alpha_{\bar{0}}$ and α_0 completely. To solve equation (A7) we

separate the two terms in the bracket and sum over

$$1)\quad -\frac{L+1}{2}\, a \sum_k \alpha_k \lambda_k^2 \qquad \text{and} \qquad 2)\ \sum_k \alpha_k \lambda_k (c + a\lambda_k^2)\, \frac{p'(\lambda_k)}{p(\lambda_k)}$$

with the aid of the slightly extended Lagrange interpolation formula

$$f(\lambda) = R(\lambda)\left[\sum_j \frac{f(\lambda_j)}{(\lambda-\lambda_j)\, R'(\lambda_j)} + r_0\right] \tag{A 13}$$

if $f(\lambda)$ and $R(\lambda)$ are polynomials of the same degree in λ. r_0 is a constant to be determined.

(1) We consider first, using (A12)

$$a\sum_k \alpha_k \lambda_k^2 = a(\alpha_{\bar{0}} + \alpha_0)\lambda_0^2 + a\sum_s \alpha_s \lambda_s^2 = a\lambda_0^2 + a\sum_s \alpha_s \lambda_s^2$$

$$= a\lambda_0^2 + \frac{\lambda_0(c + a\lambda_0^2)}{p(\lambda_0)\, p(-\lambda_0)} \sum_s \frac{\left[(\lambda_s+\lambda_0)\alpha_0\, r(\lambda_0)\, p(-\lambda_0) - (\lambda_s-\lambda_0)\alpha_{\bar{0}}\, r(-\lambda_0)\, p(\lambda_0)\right]\lambda_s\, p(\lambda_s)}{(\lambda_s^2-\lambda_0^2)(\lambda_s^2+\frac{c}{a})\, r'(\lambda_s)} \tag{A 14}$$

If one chooses

$$f(\lambda) = \left[(\lambda+\lambda_0)\alpha_0\, r(\lambda_0)\, p(-\lambda_0) - (\lambda-\lambda_0)\alpha_{\bar{0}}\, r(-\lambda_0)\, p(\lambda_0)\right]\lambda\, p(\lambda)$$

and

$$R(\lambda) = (\lambda-\lambda_0)(\lambda^2-\lambda_a^2)\, r(\lambda) \qquad \text{with } \lambda^2-\lambda_a^2 = \lambda^2 + \frac{c}{a}, \qquad \lambda_a = i\sqrt{\frac{c}{a}}$$

both polynomials $f(\lambda)$ and $R(\lambda)$ are of the same degree $\frac{L+5}{2}$ in λ. Therefore one has to find r_0 in the interpolation formula (A13) by comparison of the coefficients of the largest power of λ; it is

$$r_0 = \alpha_0\, r(\lambda_0)\, p(-\lambda_0) - \alpha_{\bar{0}}\, r(-\lambda_0)\, p(\lambda_0).$$

Then a straightforward application of (A13) at the points

$$\lambda_j = \left(-\lambda_a, \lambda_a, \lambda_0, \lambda_1, \ldots, \lambda_{\frac{L-1}{2}}\right)$$

yields

$$a \sum_k \alpha_k \lambda_k^2$$

$$= \frac{\lambda_0}{p(\lambda_0)p(-\lambda_0)} \Big\{ (c+a\lambda_0^2)\big(\alpha_0\, r(\lambda_0)\, p(-\lambda_0) - \alpha_{\bar{0}}\, r(-\lambda_0)\, p(\lambda_0)\big)$$

$$+ \frac{a}{2}\left[(\lambda_0-\lambda_a)\alpha_0\, r(\lambda_0)p(-\lambda_0) + (\lambda_0+\lambda_a)\alpha_{\bar{0}}\, r(-\lambda_0)p(\lambda_0)\right] \frac{p(-\lambda_a)}{r(-\lambda_a)}$$

$$+ \frac{a}{2}\left[(\lambda_0+\lambda_a)\alpha_0\, r(\lambda_0)\, p(-\lambda_0) + (\lambda_0-\lambda_a)\alpha_{\bar{0}}\, r(-\lambda_0)\, p(\lambda_0)\right] \frac{p(\lambda_a)}{r(\lambda_a)} \Big\} \qquad (A15)$$

(2) We consider secondly

$$\sum_k \alpha_k \lambda_k (c+a\lambda_k^2) \frac{p'(\lambda_k)}{p(\lambda_k)} \equiv \lambda_0 (c+a\lambda_0^2)\left[\alpha_0 \frac{p'(\lambda_0)}{p(\lambda_0)} - \alpha_{\bar{0}} \frac{p'(-\lambda_0)}{p(-\lambda_0)}\right]$$

$$+ \sum_s \alpha_s \lambda_s (c+a\lambda_s^2) \frac{p'(\lambda_s)}{p(\lambda_s)} . \qquad (A16)$$

Putting α_s from equation (A12) in the last sum one obtains

$$\sum_s \alpha_s \lambda_s (c+a\lambda_s^2) \frac{p'(\lambda_s)}{p(\lambda_s)}$$

$$= \frac{\lambda_0 (c+a\lambda_0^2)}{p(\lambda_0)\, p(-\lambda_0)} \sum_s \frac{\left[(\lambda_s+\lambda_0)\alpha_0\, r(\lambda_0)p(-\lambda_0) - (\lambda_s-\lambda_0)\alpha_{\bar{0}}\, r(-\lambda_0)p(\lambda_0)\right] p'(\lambda_s)}{(\lambda_s^2-\lambda_0^2)\, r'(\lambda_s)}$$

$$(A17)$$

To this expression one has to apply the same kind of interpolation

formula (A13) with

$$f(\lambda) = \left[(\lambda+\lambda_0)\,\alpha_0\, r(\lambda_0)\, p(-\lambda_0) - (\lambda-\lambda_0)\,\alpha_{\bar{0}}\, r(-\lambda_0)\, p(\lambda_0)\right] p'(\lambda)$$

and

$$R(\lambda) = (\lambda-\lambda_0)\, r(\lambda)$$

at the points $\lambda_j = (\lambda_0, \lambda_1, \cdots, \lambda_{\frac{L-1}{2}})$. Both polynomials $f(\lambda)$ and $R(\lambda)$ are again of the same degree $(L+1)/2$ in λ . The coefficient of the largest power $\lambda^{(L-1)/2}$ of $p'(\lambda)$ is $(L+1)/2$; hence we find by comparison of the largest powers of $f(\lambda)$ and $R(\lambda)$

$$r_1 = \frac{L+1}{2}\left(\alpha_0\, r(\lambda_0)\, p(-\lambda_0) - \alpha_{\bar{0}}\, r(-\lambda_0)\, p(\lambda_0)\right).$$

A straightforward application of the interpolation formula gives now

$$\sum_s \frac{\left[(\lambda_s+\lambda_0)\,\alpha_0\, r(\lambda_0)\, p(-\lambda_0) - (\lambda_s-\lambda_0)\,\alpha_{\bar{0}}\, r(-\lambda_0)\, p(\lambda_0)\right] p'(\lambda_s)}{(\lambda_s^2-\lambda_0^2)\, r'(\lambda_s)}$$

$$= \frac{L+1}{2}\left(\alpha_0\, r(\lambda_0)\, p(-\lambda_0) - \alpha_{\bar{0}}\, r(-\lambda_0)\, p(\lambda_0)\right)$$

$$+ \alpha_{\bar{0}}\, p(\lambda_0)\, p'(-\lambda_0) - \alpha_0\, p(-\lambda_0)\, p'(\lambda_0). \qquad (A18)$$

Putting the constituents together in $\sum_K$ all terms with $p'(\lambda_0)$ and $p'(-\lambda_0)$ cancel; one obtains the simple result for the second sum

$$\sum_K \alpha_K\, \lambda_K (c + a\lambda_K^2)\, \frac{p'(\lambda_K)}{p(\lambda_K)}$$

$$= \frac{L+1}{2}\, \frac{\lambda_0 (c + a\lambda_0^2)}{p(\lambda_0)\, p(-\lambda_0)} \left[\alpha_0\, r(\lambda_0)\, p(-\lambda_0) - \alpha_{\bar{0}}\, r(-\lambda_0)\, p(\lambda_0)\right]. \qquad (A19)$$

Both sums (1) and (2) together yield now

$$\sum_k \alpha_k \lambda_k \left[-\frac{L+1}{2} a \lambda_k + (c + a\lambda_k^2) \frac{p'(\lambda_k)}{p(\lambda_k)} \right] = - \frac{(L+1) a \lambda_0}{4 p(\lambda_0) p(-\lambda_0) r(\lambda_a) r(-\lambda_a)} \cdot$$

$$\cdot \Big\{ \left[(\lambda_0 - \lambda_a) \alpha_0 r(\lambda_0) p(-\lambda_0) + (\lambda_0 + \lambda_a) \alpha_{\bar{0}} r(-\lambda_0) p(\lambda_0) \right] r(\lambda_a) p(-\lambda_a)$$

$$+ \left[(\lambda_0 + \lambda_a) \alpha_0 r(\lambda_0) p(-\lambda_0) + (\lambda_0 - \lambda_a) \alpha_{\bar{0}} r(-\lambda_0) p(\lambda_0) \right] r(-\lambda_a) p(\lambda_a) \Big\} = 0 \qquad (A\,20)$$

For $a \neq 0$ the curly bracket $\{ \cdots \} = 0$ gives now the required relation between $\alpha_{\bar{0}}$ and α_0. In the case of $\gamma_t = 1$, $a = 0$ we have to split a in two factors $\sqrt{a}$, because $\lim_{\gamma_t \to 1} \lambda_0 \sqrt{a} \to 1 + \frac{2}{5}\gamma_a + \cdots$ remains finite and different from zero, and to multiply the curly bracket with a factor $\sqrt{a}$ also for compensation of the denominator in $\lambda_a = i\sqrt{\frac{c}{a}}$. Correct in all cases is the quotient

$$\frac{\alpha_{\bar{0}}}{\alpha_0} = - \frac{r(\lambda_0) p(-\lambda_0)}{r(-\lambda_0) p(\lambda_0)} \; \frac{(\lambda_0 - \lambda_a) r(\lambda_a) p(-\lambda_a) + (\lambda_0 + \lambda_a) r(-\lambda_a) p(\lambda_a)}{(\lambda_0 + \lambda_a) r(\lambda_a) p(-\lambda_a) + (\lambda_0 - \lambda_a) r(-\lambda_a) p(\lambda_a)}$$

$$= \frac{r(\lambda_0) p(-\lambda_0)}{r(-\lambda_0) p(\lambda_0)} \; \frac{\lambda_a F_-(\lambda_a) - \lambda_0 F_+(\lambda_a)}{\lambda_a F_-(\lambda_a) + \lambda_0 F_+(\lambda_a)} \qquad (A\,21)$$

with the notation $F_\pm(\lambda) \equiv r(\lambda) p(-\lambda) \pm r(-\lambda) p(\lambda)$. $\qquad (A\,22)$

Finally we use the normalization condition $\alpha_{\bar{0}} + \alpha_0 = 1$ or $\frac{1}{\alpha_0} = 1 + \frac{\alpha_{\bar{0}}}{\alpha_0}$ to obtain

$$\alpha_0 = \frac{\lambda_a F_-(\lambda_a) + \lambda_0 F_+(\lambda_a)}{\lambda_a F_+(\lambda_0) F_-(\lambda_a) - \lambda_0 F_-(\lambda_0) F_+(\lambda_a)} \; r(-\lambda_0) p(\lambda_0) \qquad (A\,23)$$

and

$$\alpha_{\bar{0}} = \frac{\lambda_a F_-(\lambda_a) - \lambda_0 F_+(\lambda_a)}{\lambda_a F_+(\lambda_0) F_-(\lambda_a) - \lambda_0 F_-(\lambda_0) F_+(\lambda_a)} \; r(\lambda_0)\, p(-\lambda_0) \qquad (A\,24)$$

The introduction of the function

$$\delta(\lambda) = \lambda \; \frac{r(\lambda)\,p(-\lambda) + r(-\lambda)\,p(\lambda)}{r(\lambda)\,p(-\lambda) - r(-\lambda)\,p(\lambda)} \equiv \lambda \, \frac{F_+(\lambda)}{F_-(\lambda)} \qquad (34)$$

has the advantage of a simple behaviour for $|\lambda| \to \infty$, as was shown in equation (60). It leads to a finite limit

$$\lim_{|\lambda| \to \infty} \delta(\lambda) = M_1 - \Lambda_1 = \sum_{j=1}^{(L+1)/2} \mu_j - \sum_{s=1}^{(L-1)/2} \lambda_s$$

or

$$\lim_{a \to 0} \delta(\lambda_a) = \lim_{a \to 0} \delta\left(i\sqrt{\frac{c}{a}}\right) = M_1 - \Lambda_1 \quad \text{also.}$$

Finally this way of calculation of the coefficients α_k shows by equation (A9) that

$$\sum_k b_k \lambda_k^m = \sum_k \alpha_k \frac{c + a\lambda_k^2}{p(\lambda_k)} \lambda_k^{m+1} = 0 \qquad \text{for } m = 0, 1, \dots \frac{L-3}{2},$$

or for any arbitrary polynomial $f(\lambda)$ of degree $\leq \frac{L-3}{2}$ in λ

$$\sum_k \alpha_k \lambda_k \; \frac{(c + a\lambda_k^2) f(\lambda_k)}{p(\lambda_k)} = 0. \qquad (A\,25)$$

Examples for such $f(\lambda)$'s are $p''(\lambda)$, $r'(\lambda)$ etc.

A further result is contained in equation (A15), if one considers that the sum of the 2. and 3. term of (A15) vanish in consequence of equation (A20),

namely the simple value for the sum

$$\sum_k \alpha_k \lambda_k^2 = \frac{\lambda_0 (c + a\lambda_0^2)\left(\alpha_0 \, r(\lambda_0) p(-\lambda_0) - \alpha_{\bar{0}} \, r(-\lambda_0) p(\lambda_0)\right)}{a \, p(\lambda_0) p(-\lambda_0)}$$

$$= -2N\lambda_0^2 \left(1 + \frac{a}{c}\lambda_0^2\right) \delta(\lambda_a) \qquad (A26)$$

after introduction of $\alpha_{\bar{0}}$ (equation 37) and α_0 (equation 38). $\sum_k \alpha_k \lambda_k^2$ is related to the second moment of the directed flux at the boundary.

(b) <u>The shorter way</u>

A short calculation of the coefficients α_k uses the Lagrange interpolation formula as a generalization of a method, which was used first by Wick.[8] To this end we try to reconstruct formula (~~25~~ 32) by a convenient interpolation, which allows one to read off the coefficients directly by comparison of the constructed equation with equation (~~28~~ 32). To do that, we represent the polynomial $f(\lambda) = (C + D\lambda)\, p(\lambda)$ of the degree $\frac{L+3}{2}$ in λ twice -- <u>first</u> by its values at the $\frac{L+5}{2}$ points $\lambda_j = (-\lambda_a, \lambda_a, \lambda_0, \lambda_1 \cdots \lambda_{\frac{L-1}{2}})$ using the polynomial $R_1(\lambda) = (\lambda^2 - \lambda_a^2)(\lambda - \lambda_0)\, r(\lambda)$ of the degree $\frac{L+5}{2}$ in λ in the Lagrange interpolation formula

$$f(\lambda) = R(\lambda) \sum_j \frac{f(\lambda_j)}{(\lambda - \lambda_j)\, R'(\lambda_j)}$$

where λ_j runs over the series of points mentioned above and with $R(\lambda) = R_1(\lambda)$; <u>secondly</u> we repeat this process replacing the point λ_0 by $-\lambda_0$ without a change of the other points. This means, we use this time $R(\lambda) = R_2(\lambda) = (\lambda^2 - \lambda_a^2)(\lambda + \lambda_0)\, r(\lambda)$ in the Lagrange formula.

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8 G. C. Wick, ZS. f. Physik <u>120</u>, 202 (1943).

(1) $R(\lambda) = R_1(\lambda)$ yields (C,D are constants)

$$\frac{(C+D\lambda)\,p(\lambda)}{(\lambda^2-\lambda_a^2)(\lambda-\lambda_0)\,r(\lambda)}$$

$$= \frac{(C-D\lambda_a)\,p(-\lambda_a)}{(\lambda+\lambda_a)\,2\lambda_a(\lambda_a+\lambda_0)\,r(-\lambda_a)} + \frac{(C+D\lambda_a)\,p(\lambda_a)}{(\lambda-\lambda_a)\,2\lambda_a(\lambda_a-\lambda_0)\,r(\lambda_a)}$$

$$+ \frac{(C+D\lambda_0)\,p(\lambda_0)}{(\lambda-\lambda_0)(\lambda_0^2-\lambda_a^2)\,r(\lambda_0)} + \sum_{s=1}^{(L-1)/2} \frac{(C+D\lambda_s)\,p(\lambda_s)}{(\lambda-\lambda_s)(\lambda_s^2-\lambda_a^2)(\lambda_s-\lambda_0)\,r'(\lambda_s)} \,. \qquad (A\,27)$$

(2) $R(\lambda) = R_2(\lambda)$ yields

$$\frac{(C+D\lambda)\,p(\lambda)}{(\lambda^2-\lambda_a^2)(\lambda+\lambda_0)\,r(\lambda)}$$

$$= \frac{(C-D\lambda_a)\,p(-\lambda_a)}{(\lambda+\lambda_a)\,2\lambda_a(\lambda_a-\lambda_0)\,r(-\lambda_a)} + \frac{(C+D\lambda_a)\,p(\lambda_a)}{(\lambda-\lambda_a)\,2\lambda_a(\lambda_a+\lambda_0)\,r(\lambda_a)}$$

$$+ \frac{(C-D\lambda_0)\,p(-\lambda_0)}{(\lambda+\lambda_0)(\lambda_0^2-\lambda_a^2)\,r(-\lambda_0)} + \sum_{s=1}^{(L-1)/2} \frac{(C+D\lambda_s)\,p(\lambda_s)}{(\lambda-\lambda_s)(\lambda_s^2-\lambda_a^2)(\lambda_s+\lambda_0)\,r'(\lambda_s)} \,. \qquad (A\,28)$$

Both formulae differ only in the sign of λ_0.

Now we choose the following special values in both equations: $\lambda = \mu_j$, for which $p(\lambda)$ is $p(\mu_j) = 0$ and the left sides of both equations vanish; further we put C = c and D = aμ_j. Then we multiply the first equation by a constant A, the second by a constant B and add both together. We obtain

$$B \frac{p(-\lambda_0)}{(\lambda_0^2-\lambda_a^2)\, r(-\lambda_0)} \frac{c-a\lambda_0\mu_j}{\lambda_0+\mu_j} - A \frac{p(\lambda_0)}{(\lambda_0^2-\lambda_a^2)\, r(\lambda_0)} \frac{c+a\lambda_0\mu_j}{\lambda_0-\mu_j}$$

$$+ \sum_{s=1}^{(L-1)/2} \left(\frac{-A}{\lambda_s-\lambda_0} + \frac{-B}{\lambda_s+\lambda_0} \right) \frac{p(\lambda_s)}{(\lambda_s^2-\lambda_a^2)\, r'(\lambda_s)} \frac{c+a\lambda_s\mu_j}{\lambda_s-\mu_j}$$

$$= - \left\{ \frac{(c-a\lambda_a\mu_j)\, p(-\lambda_a)}{(\mu_j+\lambda_a)\, 2\lambda_a\, r(-\lambda_a)} \left(\frac{A}{\lambda_a+\lambda_0} + \frac{B}{\lambda_a-\lambda_0} \right) \right.$$

$$\left. + \frac{(c+a\lambda_a\mu_j)\, p(\lambda_a)}{(\mu_j-\lambda_a)\, 2\lambda_a\, r(\lambda_a)} \left(\frac{A}{\lambda_a-\lambda_0} + \frac{B}{\lambda_a+\lambda_0} \right) \right\}. \qquad (A29)$$

We compare this equation with equation (32), which after separation of the terms with the indices $\bar{o}$ and o may be written in the following form

$$\alpha_{\bar{o}}\, \lambda_0 \frac{c-a\lambda_0\mu_j}{\lambda_0+\mu_j} + \alpha_0 \lambda_0 \frac{c+a\lambda_0\mu_j}{\lambda_0-\mu_j} + \sum_{s=1}^{(L-1)/2} \alpha_s \lambda_s \frac{c+a\lambda_s\mu_j}{\lambda_s-\mu_j} = 0, \qquad (32)$$

$$\left(j = 1, 2, \cdots \frac{L+1}{2} \right)$$

and we recognize that they would be comparable, if the right side of (A29) could be put to zero. This, however, is possible, because the constants A and B are still arbitrary constants and because it turns out that A and B can be chosen independent of j. This will be shown now: the right side

of (A29) may be written

$$-\frac{A}{2\lambda_a}\left\{\frac{(c-a\lambda_a\mu_j)\,p(-\lambda_a)}{(\mu_j+\lambda_a)(\lambda_a+\lambda_0)\,r(-\lambda_a)}+\frac{(c+a\lambda_a\mu_j)\,p(\lambda_a)}{(\mu_j-\lambda_a)(\lambda_a-\lambda_0)\,r(\lambda_a)}\right\}$$

$$-\frac{B}{2\lambda_a}\left\{\frac{(c-a\lambda_a\mu_j)\,p(-\lambda_a)}{(\mu_j+\lambda_a)(\lambda_a-\lambda_0)\,r(-\lambda_a)}+\frac{(c+a\lambda_a\mu_j)\,p(\lambda_a)}{(\mu_j-\lambda_a)(\lambda_a+\lambda_0)\,r(\lambda_a)}\right\}$$

$$=\frac{a}{2(\lambda_0^2-\lambda_a^2)\,r(\lambda_a)\,r(-\lambda_a)}\Big\{A\big[(\lambda_0-\lambda_a)\,r(\lambda_a)\,p(-\lambda_a)+(\lambda_0+\lambda_a)\,r(-\lambda_a)\,p(\lambda_a)\big]$$

$$-B\big[(\lambda_0+\lambda_a)\,r(\lambda_a)\,p(-\lambda_a)+(\lambda_0-\lambda_a)\,r(-\lambda_a)\,p(\lambda_a)\big]\Big\}$$

That μ_j is only contained in the curly bracket on the left side of the equation above as a <u>factor</u> $c+a\mu_j^2=a(\mu_j^2-\lambda_a^2)$ in this formula one owes to the fact that $c+a\lambda_a^2=c+a(-\frac{c}{a})=0$, by reason of which the originally occurring terms $(c+a\lambda_a^2)\mu_j$ vanish. Hence <u>A and B do not depend on the special μ_j chosen</u> on the left side of (A29), and the right side of equation (A29) will vanish for

equation (A30) should read:

$$A = G\left|(\lambda_0+\lambda_a)r(\lambda_a)p(-\lambda_a)+(\lambda_0-\lambda_a)r(-\lambda_a)p(\lambda_a)\right| \qquad (A30)$$

equation (A31) should read:

$$B = G\left|(\lambda_0-\lambda_a)r(\lambda_a)p(-\lambda_a)+(\lambda_0+\lambda_a)r(-\lambda_a)p(\lambda_a)\right| \qquad (A31)$$

with an arbitrary constant G, which has to be determined later from our supposition of normalization $\alpha_{\bar{0}}+\alpha_0=1$.

After that the equations (32) and (A29) are in form suitable for comparison, which shows

$$\alpha_{\bar{0}}\lambda_0 = \frac{B\,p(-\lambda_0)}{(\lambda_0^2-\lambda_a^2)\,r(-\lambda_0)}, \qquad \alpha_0\lambda_0 = \frac{-A\,p(\lambda_0)}{(\lambda_0^2-\lambda_a^2)\,r(\lambda_0)},$$

$$\alpha_s\lambda_s = -\left[\frac{A}{\lambda_s-\lambda_0} + \frac{B}{\lambda_s+\lambda_0}\right]\frac{p(\lambda_s)}{(\lambda_s^2-\lambda_a^2)\,r'(\lambda_s)} \qquad (A\,32)$$

One may use the first two equations to remove A and B from the last, whereupon one obtains a sometimes useful short representation of the coefficients α_s of the transients in terms of $\alpha_{\bar{0}}$ and α_0

$$\alpha_s = \frac{\lambda_0(c+a\lambda_0^2)}{\lambda_s(c+a\lambda_s^2)}\,\frac{p(\lambda_s)}{r'(\lambda_s)}\left\{\frac{\alpha_0\,r(\lambda_0)}{(\lambda_s-\lambda_0)\,p(\lambda_0)} - \frac{\alpha_{\bar{0}}\,r(-\lambda_0)}{(\lambda_s+\lambda_0)\,p(-\lambda_0)}\right\} \qquad (A\,12)$$

$$\left(s = 1, 2, \ldots \frac{L-1}{2}\right).$$

From the normalization condition

$$\alpha_{\bar{0}} + \alpha_0 = \frac{B\,r(\lambda_0)\,p(-\lambda_0) - A\,r(-\lambda_0)\,p(\lambda_0)}{\lambda_0(\lambda_0^2-\lambda_a^2)\,r(\lambda_0)\,r(-\lambda_0)} = 1 \qquad (A\,33)$$

one may find now the constant G, using the abbreviations (A22)

$$G = \frac{\lambda_0(\lambda_0^2-\lambda_a^2)\,r(\lambda_0)\,r(-\lambda_0)}{\lambda_0\,F_-(\lambda_0)\,F_+(\lambda_a) - \lambda_a\,F_+(\lambda_0)\,F_-(\lambda_a)} \qquad (A\,34)$$

We put this expression for G in the equations for the constants A, B

$$A = \frac{\lambda_0 (\lambda_0^2 - \lambda_a^2)\, r(\lambda_0)\, r(-\lambda_0) \left[\lambda_0 F_+(\lambda_a) + \lambda_a F_-(\lambda_a) \right]}{\lambda_0 F_-(\lambda_0) F_+(\lambda_a) - \lambda_a F_+(\lambda_0) F_-(\lambda_a)} \qquad (A\ 35)$$

$$B = \frac{\lambda_0 (\lambda_0^2 - \lambda_a^2)\, r(\lambda_0)\, r(-\lambda_0) \left[\lambda_0 F_+(\lambda_a) - \lambda_a F_-(\lambda_a) \right]}{\lambda_0 F_-(\lambda_0) F_+(\lambda_a) - \lambda_a F_+(\lambda_0) F_-(\lambda_a)} \qquad (A\ 36)$$

and in the equations for the coefficients $\alpha_{\bar{0}}$, α_0, α_s

$$\alpha_{\bar{0}} = \frac{\left[\lambda_a F_-(\lambda_a) - \lambda_0 F_+(\lambda_a) \right] r(\lambda_0)\, p(-\lambda_0)}{\lambda_a F_+(\lambda_0) F_-(\lambda_a) - \lambda_0 F_-(\lambda_0) F_+(\lambda_a)}$$

$$\alpha_0 = \frac{\left[\lambda_a F_-(\lambda_a) + \lambda_0 F_+(\lambda_a) \right] r(-\lambda_0)\, p(\lambda_0)}{\lambda_a F_+(\lambda_0) F_-(\lambda_a) - \lambda_0 F_-(\lambda_0) F_+(\lambda_a)} \qquad (A\ 37)$$

$$\alpha_s = \frac{\left[\lambda_a F_-(\lambda_a) + \lambda_s F_+(\lambda_a) \right] r(\lambda_0)\, r(-\lambda_0)}{\lambda_a F_+(\lambda_0) F_-(\lambda_a) - \lambda_0 F_-(\lambda_0) F_+(\lambda_a)} \; \frac{c + a\lambda_0^2}{c + a\lambda_s^2} \; \frac{2\lambda_0^2\, p(\lambda_s)}{(\lambda_s^2 - \lambda_0^2)\, \lambda_s\, r'(\lambda_s)}$$

and finally in the equation for the linear extrapolation distance

$$\delta \equiv \frac{\lambda_0}{\alpha_{\bar{0}} - \alpha_0} = \lambda_0 \; \frac{\lambda_0 F_-(\lambda_0) F_+(\lambda_a) - \lambda_a F_+(\lambda_0) F_-(\lambda_a)}{\lambda_0 F_+(\lambda_0) F_+(\lambda_a) - \lambda_a F_-(\lambda_0) F_-(\lambda_a)} \qquad (A\ 38)$$

After that the solution is complete; the corresponding quantities are equal to those of the equations (37), (38), (39), if one remembers the abbreviations (34), (35), and (36).

Appendix III. Summation of the C-W part $f^{I}(0,\mu)$

(1) The sum, which has to be carried out is

$$f^{I}(0,\mu) = \sum_{k=\bar{0},0,1,\ldots}^{(L-1)/2} \alpha_k \lambda_k \left\{ -a\lambda_k + \frac{c+a\lambda_k^2}{\lambda_k+\mu} \right\} \tag{17}$$

The first part of this sum was found already -- see equation (A26) --

$$-a\sum_k \alpha_k \lambda_k^2 = \frac{\lambda_0(c+a\lambda_0^2)}{p(\lambda_0)\,p(-\lambda_0)}\left[\alpha_{\bar{0}}\, r(-\lambda_0)\,p(\lambda_0) - \alpha_0\, r(\lambda_0)\,p(-\lambda_0)\right] . \tag{A 39}$$

The second part is

$$\sum_k \alpha_k \lambda_k \frac{c+a\lambda_k^2}{\lambda_k+\mu} = \alpha_{\bar{0}}\lambda_0 \frac{c+a\lambda_0^2}{\lambda_0-\mu} + \alpha_0\lambda_0 \frac{c+a\lambda_0^2}{\lambda_0+\mu} + \sum_{s=1}^{(L-1)/2} \alpha_s\lambda_s \frac{c+a\lambda_s^2}{\lambda_s+\mu} . \tag{A 40}$$

By introduction of the values of α_s from equation (A12) in the last sum one obtains

$$\sum_{s=1}^{(L-1)/2} \alpha_s\lambda_s \frac{c+a\lambda_s^2}{\lambda_s+\mu}$$

$$= \frac{\lambda_0(c+a\lambda_0^2)}{p(\lambda_0)\,p(-\lambda_0)} \sum_{s=1}^{(L-1)/2} \frac{\left[(\lambda_s+\lambda_0)\alpha_0\, r(\lambda_0)\,p(-\lambda_0) - (\lambda_s-\lambda_0)\alpha_{\bar{0}}\, r(-\lambda_0)\,p(\lambda_0)\right] p(\lambda_s)}{(\lambda_s+\mu)(\lambda_s^2-\lambda_0^2)\, r'(\lambda_s)} .$$

Numerator and denominator in the sum are both of degree $\frac{L+3}{2}$ in λ_s.

An application of the extended Lagrange interpolation formula (A13) with

$$f(\lambda) = [(\lambda+\lambda_0)\,\alpha_0\, r(\lambda_0)\, p(-\lambda_0) - (\lambda-\lambda_0)\,\alpha_{\bar{0}}\, r(-\lambda_0)\, p(\lambda_0)]\; p(\lambda)$$

and

$$R(\lambda) = (\lambda^2 - \lambda_0^2)\, r(\lambda)$$

at the $\frac{L+3}{2}$ points $\lambda_j = (-\lambda_0, \lambda_0, \lambda_1, \ldots \lambda_{\frac{L-1}{2}})$ requires a comparison of the largest powers $\lambda^{(L+3)/2}$ on both sides of the equation to find

$$r_0 = \alpha_0\, r(\lambda_0)\, p(-\lambda_0) - \alpha_{\bar{0}}\, r(-\lambda_0)\, p(\lambda_0)$$

Then a straightforward application of the interpolation formula with $\lambda = -\mu$ yields

$$\sum_s \frac{[(\lambda_s+\lambda_0)\alpha_0\, r(\lambda_0)\, p(-\lambda_0) - (\lambda_s-\lambda_0)\alpha_{\bar{0}}\, r(-\lambda_0)\, p(\lambda_0)]\; p(\lambda_s)}{(\lambda_s+\mu)(\lambda_s^2-\lambda_0^2)\, r'(\lambda_s)}$$

$$= \alpha_0\, r(\lambda_0)\, p(-\lambda_0) - \alpha_{\bar{0}}\, r(-\lambda_0)\, p(\lambda_0) + p(\lambda_0)\, p(-\lambda_0)\left(\frac{\alpha_{\bar{0}}}{\mu-\lambda_0} - \frac{\alpha_0}{\mu+\lambda_0}\right)$$

$$+ \frac{[(\mu-\lambda_0)\alpha_0\, r(\lambda_0)\, p(-\lambda_0) - (\mu+\lambda_0)\alpha_{\bar{0}}\, r(-\lambda_0)\, p(\lambda_0)]\; p(-\mu)}{(\mu^2-\lambda_0^2)\, r(-\mu)} .$$

Hence, one obtains by addition of all parts of the sum (17) the Gauss quadrature part of the directed flux on the boundary:

$$f^{I}(0,\mu) = \frac{\lambda_0(c+a\lambda_0^2)}{p(\lambda_0)\,p(-\lambda_0)}\; \frac{(\lambda_0+\mu)\, r(-\lambda_0)\, p(\lambda_0)\,\alpha_{\bar{0}} + (\lambda_0-\mu)\, r(\lambda_0)\, p(-\lambda_0)\,\alpha_0}{\lambda_0^2-\mu^2}\; \frac{p(-\mu)}{r(-\mu)} . \tag{A41}$$

Introduction of $\alpha_{\bar{0}}$ and α_0 from equations (A23,24) completes the expression

$$f^{I}(0,\mu) = \frac{2\lambda_0^2(c+a\lambda_0^2)\,r(\lambda_0)\,r(-\lambda_0)}{\lambda_a F_+(\lambda_0)F_-(\lambda_a) - \lambda_0 F_-(\lambda_0)F_+(\lambda_a)} \; \frac{\lambda_a F_-(\lambda_a) - \mu F_+(\lambda_a)}{\lambda_0^2-\mu^2} \; \frac{p(-\mu)}{r(-\mu)} \, . \tag{A 42}$$

Finally the use of $\delta(\lambda)$ equation (37), λ_a equation (38) and N equation (39) leads to the form of $f^{I}(0,\mu)$ in equation (41), because $\lambda_a F_-(\lambda_a) - \mu F_+(\lambda_a) = \lambda_a F_-(\lambda_a)\left[1 + \frac{a}{c}\mu\,\delta(\lambda_a)\right]$ and N may be represented also in the following manner

$$N = \frac{r(\lambda_0)\,r(-\lambda_0)\,\lambda_a F_-(\lambda_a)}{\lambda_a F_+(\lambda_0)F_-(\lambda_a) - \lambda_0 F_-(\lambda_0)F_+(\lambda_a)} \, . \tag{A 43}$$

(2) A shorter way to find $f^{I}(0,\mu)$ is connected again with the superposition of A times equation (A27) + B times equation (A28) and the choice of $C = c$ and $D = -a\mu$ in the resulting expression. One gets by this procedure the formula

$$a\,\frac{p(-\mu)}{r(-\mu)}\left(\frac{-A}{\lambda_0+\mu} + \frac{B}{\lambda_0-\mu}\right) = -A\,\frac{(c-a\lambda_0\mu)\,p(\lambda_0)}{(\lambda_0+\mu)(\lambda_0^2-\lambda_a^2)\,r(\lambda_0)} + B\,\frac{(c+a\lambda_0\mu)\,p(-\lambda_0)}{(\lambda_0-\mu)(\lambda_0^2-\lambda_a^2)\,r(-\lambda_0)}$$

$$+\sum_s \frac{(c-a\lambda_s\mu)\,p(\lambda_s)}{(\lambda_s+\mu)(\lambda_s^2-\lambda_a^2)\,r'(\lambda_s)}\left(\frac{A}{\lambda_0-\lambda_s} - \frac{B}{\lambda_0+\lambda_s}\right),$$

where A and B have the values of equations (A30,31). In consequence of (A32)

$$\alpha_{\bar{0}}\lambda_{\bar{0}} = \frac{-B\,p(-\lambda_0)}{(\lambda_0^2-\lambda_a^2)\,r(-\lambda_0)}, \qquad \alpha_0\lambda_0 = \frac{-A\,p(\lambda_0)}{(\lambda_0^2-\lambda_a^2)\,r(\lambda_0)},$$

$$\alpha_s\lambda_s = \left[\frac{A}{\lambda_0-\lambda_s} - \frac{B}{\lambda_0+\lambda_s}\right]\frac{p(\lambda_s)}{(\lambda_s^2-\lambda_a^2)\,r'(\lambda_s)},$$

we have on the right side just

$$\sum_{k=\bar{0},0,1,\ldots}^{(L-1)/2} \alpha_k\lambda_k\,\frac{c-a\lambda_k\mu}{\lambda_k+\mu}$$

which is $f^{I}(0,\mu)$. Hence, again

$$f^{I}(0,\mu) = \left[\frac{aB}{\lambda_0-\mu} - \frac{aA}{\lambda_0+\mu}\right]\frac{p(-\mu)}{r(-\mu)}$$

$$= \frac{2\lambda_0^2(c+a\lambda_0^2)\,r(\lambda_0)\,r(-\lambda_0)}{\lambda_0 F_-(\lambda_0)F_+(\lambda_a)-\lambda_a F_+(\lambda_0)F_-(\lambda_a)}\;\frac{F_+(\lambda_a)\mu-\lambda_a F_-(\lambda_a)}{\lambda_0^2-\mu^2}\;\frac{p(-\mu)}{r(-\mu)}. \qquad \text{(A42)}$$

Appendix IV. Calculation of the current at the boundary

To calculate

$$\sum_{k=\bar{0},0,1,\ldots}^{(L-1)/2} \alpha_k \lambda_k \equiv -\lambda_0 \alpha_{\bar{0}} + \lambda_0 \alpha_0 + \sum_{s=1}^{(L-1)/2} \alpha_s \lambda_s \equiv -(\alpha_{\bar{0}} - \alpha_0)\lambda_0 + \sum_s \alpha_s \lambda_s \qquad (A44)$$

we use equation (A12), which gives the α_s's in terms of $\alpha_{\bar{0}}$ and α_0.

Then we have

$$\sum_s \alpha_s \lambda_s$$

$$= \frac{\lambda_0(c + a\lambda_0^2)}{a\, p(\lambda_0) p(-\lambda_0)} \sum_s \frac{[(\lambda_0+\lambda_s)\alpha_0\, r(\lambda_0) p(-\lambda_0) + (\lambda_0-\lambda_s)\alpha_{\bar{0}}\, r(-\lambda_0) p(\lambda_0)]\, p(\lambda_s)}{(\lambda_s^2-\lambda_0^2)(\lambda_s^2-\lambda_a^2)\, r'(\lambda_s)} . \qquad (A45)$$

We apply the Lagrange interpolation formula in the simple form (44) to a function

$$f(\lambda) = [(\lambda+\lambda_0)\alpha_0\, r(\lambda_0) p(-\lambda_0) + (\lambda_0-\lambda)\, r(-\lambda_0) p(\lambda_0)]\, p(\lambda) \quad \text{of the degree } \frac{L+3}{2}$$

in λ with an aid function $R(\lambda) = (\lambda-\lambda_0)(\lambda^2-\lambda_a^2)\, r(\lambda)$ of degree $\frac{L+5}{2}$ in λ at its $\frac{L+5}{2}$ zeros $\lambda_j = (-\lambda_a, \lambda_a, \lambda_0, \lambda_1, \cdots, \lambda_{\frac{L-1}{2}})$. Then we obtain

$$\frac{[(\lambda_0+\lambda)\alpha_0\, r(\lambda_0) p(-\lambda_0) + (\lambda_0-\lambda)\alpha_{\bar{0}}\, r(-\lambda_0) p(\lambda_0)]\, p(\lambda)}{(\lambda-\lambda_0)(\lambda^2-\lambda_a^2)\, r(\lambda)}$$

$$= \frac{[(\lambda_0-\lambda_a)\alpha_0\, r(\lambda_0) p(-\lambda_0) + (\lambda_0+\lambda_a)\alpha_{\bar{0}}\, r(-\lambda_0) p(\lambda_0)]\, p(-\lambda_a)}{(\lambda+\lambda_a)\, 2\lambda_a(\lambda_0+\lambda_a)\, r(-\lambda_a)}$$

$$- \frac{[(\lambda_0+\lambda_a)\alpha_0\, r(\lambda_0) p(-\lambda_0) + (\lambda_0-\lambda_a)\alpha_{\bar{0}}\, r(-\lambda_0) p(\lambda_0)]\, p(\lambda_a)}{(\lambda-\lambda_a)\, 2\lambda_a(\lambda_0-\lambda_a)\, r(\lambda_a)}$$

$$+\frac{2\lambda_0\alpha_0\, p(\lambda_0)\,p(-\lambda_0)}{(\lambda-\lambda_0)(\lambda_0^2-\lambda_a^2)}+\sum_s \frac{[(\lambda_0+\lambda_s)\alpha_0\, r(\lambda_0)\,p(-\lambda_0)+(\lambda_0-\lambda_s)\alpha_{\bar{0}}\, r(-\lambda_0)\,p(\lambda_0)]\,p(\lambda_s)}{(\lambda-\lambda_s)(\lambda_s-\lambda_0)(\lambda_s^2-\lambda_a^2)\, r'(\lambda_s)}$$

Putting $\lambda=-\lambda_0$ we find the sum $\sum_s$, required above:

$$\sum_s \frac{[(\lambda_0+\lambda_s)\alpha_0\, r(\lambda_0)\,p(-\lambda_0)+(\lambda_0-\lambda_s)\alpha_{\bar{0}}\, r(-\lambda_0)\,p(\lambda_0)]\,p(\lambda_s)}{(\lambda_s^2-\lambda_0^2)(\lambda_s^2-\lambda_a^2)\, r'(\lambda_s)}$$

$$=\frac{p(\lambda_0)\,p(-\lambda_0)}{\lambda_0^2-\lambda_a^2}(\alpha_{\bar{0}}-\alpha_0)+\frac{[(\lambda_0+\lambda_a)\alpha_0\, r(\lambda_0)\,p(-\lambda_0)+(\lambda_0-\lambda_a)\alpha_{\bar{0}}\, r(-\lambda_0)\,p(\lambda_0)]\,p(\lambda_a)}{\lambda_a(\lambda_0^2-\lambda_a^2)\, r(\lambda_a)} \qquad (A46)$$

The last term on the right side is found by an application of the relation (A21) between $\alpha_{\bar{0}}$ and α_0 .

Putting (A45) with (A46) in equation (A44), the first two terms cancel.

We obtain for the sum considered in (A44)

$$\sum_{k=\bar{0},0,1,\ldots}^{(L-1)/2} \alpha_k\lambda_k = \frac{\lambda_0}{\lambda_a}\,\frac{(\lambda_0+\lambda_a)\, r(\lambda_0)\,p(-\lambda_0)\,\alpha_0+(\lambda_0-\lambda_a)\, r(-\lambda_0)\,p(\lambda_0)\,\alpha_{\bar{0}}}{p(\lambda_0)\,p(-\lambda_0)}\;\frac{p(\lambda_a)}{r(\lambda_a)}\,,$$

After introducing α_0 and $\alpha_{\bar{0}}$ (see equations A23,24) we get

$$\sum_{k=\bar{0},0,1,\ldots}^{(L-1)/2} \alpha_k\lambda_k = \frac{2\lambda_0^2\, r(\lambda_0)\, r(-\lambda_0)\,p(\lambda_a)\,[F_+(\lambda_a)+F_-(\lambda_a)]}{r(\lambda_a)[\lambda_a F_+(\lambda_0)F_-(\lambda_a)-\lambda_0 F_-(\lambda_0)F_+(\lambda_a)]}$$

$$=\frac{2\lambda_0^2 N\, p(\lambda_a)}{r(\lambda_a)}\;\frac{F_+(\lambda_a)+F_-(\lambda_a)}{\lambda_a F_-(\lambda_a)} \quad [\text{with } N \text{ of eqn. (A43)}]$$

$$=\frac{4N\lambda_0^2\, p(\lambda_a)\,p(-\lambda_a)}{\lambda_a[r(\lambda_a)\,p(-\lambda_a)-r(-\lambda_a)\,p(\lambda_a)]}\,. \qquad (A47)$$

In the last equation the abbreviations $F_{\pm}(\lambda)$ used in Appendix II were replaced by their definitions, see equation (A22). The last form of equation (A47) was applied to the evaluation of the formula (55) for the current at the boundary $z = 0$.

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