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The Spectrum of the Anisotropic Transfer Equation

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The discrete values of k, for which the equation of transfer in a homogeneous medium with an arbitrary phase function has a solution proportional to exp $(\pm k\tau)$, where τ is optical depth, are studied. Various forms of the characteristic equation, from which k can be solved, are given. The simple relation $g_n(k^{-1}) \to 0$ for $n \to \infty$, where $g_n(x)$ are the Kuščer polynomia, is recommended for practical computation. The relation by which the albedo for simple scattering, $\omega_0 = a$, depends on k when the form of the scattering pattern is given, is derived both for linearly anisotropic scattering ($N = 1$) and for the Henyey-Greenstein scattering functions. Knowledge of the multiple values of k for one a, which may be read from the graphs presented, is helpful in estimating the domain of practical validity of the diffusion approximation.

Key words: radiative transfer — characteristic equation

1. Introduction

A host of papers in the recent and not-too-recent literature (see e.g. four important books: Chandrasekhar, 1950; Busbridge, 1960; Sobolev, 1963; Case and Zweifel, 1968) have discussed the values of the "characteristic exponent", or the "inverse diffusion length" k, which occurs in solutions of the transfer equation proportional to exp $(-k\tau)$. Here τ is optical depth. The equation from which k may be solved is usually called the "characteristic equation" and sometimes (incorrectly) the "dispersion equation". After restating the problem in Section 2, we shall try to answer the practical question how to find most rapidly accurate values of the eigenvalues k (Section 3). Multiple values of k occur with a fixed albedo if the scattering diagram is strongly anisotropic (Section 6).

2. The Integral Equation

Consider a homogeneous medium with light scattering governed by a phase function

$$\Phi(\cos\alpha) = \sum_{n=0}^{N} \omega_n P_n(\cos\alpha)\,, \tag{1}$$

where $P_n(\cos\alpha)$ = Legendre polynomium of the first kind; ω_n is a given set of coefficients; $\omega_0 = a$ = single scattering albedo, called in neutron scattering the number of secondaries; $\omega_1 = 3\,ag$; $g = \langle\cos\alpha\rangle$ = anisotropy coefficient = mean value of $\cos\alpha$ determined with $\Phi(\cos\alpha)$ as the weight function; N = a given number so that $\omega_n = 0$ for $n > N$. Practical phase functions may have $N = \infty$, but even then $\omega_n \to 0$ sufficiently rapidly with $n \to \infty$ to make the distinction between infinite N and finite N academic.

In the following, we shall write sums with the symbol $\sum_n$. These sums are finite, as in Eq. (1), if N is finite and the terms contain ω_n as a coefficient. They are infinite series, as in Eq. (11), if ω_n is not a coefficient.

Let a direction be defined along which we measure optical depth τ, so that the intensity of a light beam travelling in the positive τ-direction is attenuated as $e^{-\tau}$. Let θ be the angle of any direction with the positive τ-direction and write $u = \cos\theta$. Consider a radiation field with the intensity, independent of azimuth, $I(\tau, u)$. The radiation scattered at depth τ then is proportional to the source function

$$J(\tau, u) = 1/2 \int_{-1}^{1} h(u, v)\, I(\tau, v)\, dv\,, \tag{2}$$

where

$$h(u, v) = \frac{1}{2\pi}\int_0^{2\pi} \Phi[uv + (1-u^2)^{1/2}(1-v^2)^{1/2}\cos\varphi]\, d\varphi\,. \tag{3}$$

An equivalent and more convenient form is

$$h(u, v) = \sum_n \omega_n P_n(u)\, P_n(v)\,. \tag{4}$$

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The equation of radiative transfer reads

$$u\,\frac{\partial I(\tau, u)}{\partial \tau} = -I(\tau, u) + J(\tau, u)\,. \tag{5}$$

The simplest problems of radiative transfer in plane-parallel, azimuth-independent geometry require the simultaneous solution of Eqs. (2) and (5) with the proper boundary conditions at top and bottom surface. In this paper we deal only with solutions of (2) and (5) of the form

$$I(\tau,u) = \frac{J(\tau, u)}{1-ku} = C e^{-k\tau} P(u)\,. \tag{6}$$

We shall conveniently take $k \geqq 0$ throughout; the equivalent solutions with opposite sign can be obtained by inverting the signs of τ and u. The solution (6) automatically satisfies Eq. (5) and Eq. (2) gives the integral equation

$$(1-ku)\,P(u) = \frac{1}{2}\int_{-1}^{1} h(u,v)\,P(v)\,dv\,. \tag{7}$$

It is seen that k is an eigenvalue and $P(u)$ the corresponding eigenfunction. The spectrum for $\omega_0 < 1$ is known to consist of one or more discrete values k_j in the range $0 < k_j < 1$ with non-singular eigenfunctions and the continuum of eigenvalues $k > 1$ with singular eigenfunctions. If $\omega_0 = 1$, one eigenvalue is $k = 0$.

The reason for studying this spectrum is twofold. First, a method suggested by van Kampen, rediscovered by Case and worked out for arbitrary anisotropic phase functions by a number of further authors (e.g. McCormick and Kuščer, 1966; Shultis and Kaper, 1969) requires the knowledge of the complete spectrum, the orthogonality theorems for the eigenfunctions, the proof of the completeness, the expansion of the solution in terms of these eigenfunctions, and the determination of the coefficients from the boundary conditions. This is more readily said than done. We may refer to the cited papers for further detail.

The second reason is that it is often sufficient to define a "diffusion domain" as any range of τ inside an extended medium which is far from boundaries and from primary source layers and to assume that the solution in a "diffusion domain" is described with practical precision by the superposition of two "diffusion streams", one in the positive and one in negative τ-direction. Here a "diffusion stream in the positive τ-direction" is called a solution of the form (6), where k is the smallest eigenvalue and $P(u)$ the corresponding eigenfunction. The effect of all other eigenvalues, discrete or continuous is lumped together into certain empirical functions. This idea has been worked out to a practical and accurate method of computation (van de Hulst, 1968a, b). The corrections correspond to solutions which are damped out more rapidly near the boundaries and become numerically insignificant in the diffusion domain. Knowledge of the next-higher value of k will certainly be helpful to estimate the depth of the transition region.

3. Convergence of the Kuščer Polynomia

Let k be any eigenvalue, $\gamma = k^{-1}$ and

$$h_n = 2n + 1 - \omega_n\,. \tag{8}$$

Kuščer (1955) defined the set of polynomia, starting with $g_0(x) = 1$, $g_1(x) = h_0 x$, and continuing by the recurrence relation

$$h_n\, x\, g_n(x) = (n+1) g_{n+1}(x) + n g_{n-1}(x)\,. \tag{9}$$

An explicit expression for $g_n(x)$ is

$$g_n(x) = \frac{1}{n!}\begin{vmatrix} h_0 x & 1 & & & \\ 1 & h_1 x & 2 & & \\ & 2 & \cdots & & \\ & & \cdots & & n-1 \\ & & & n-1 & h_{n-1} x \end{vmatrix} \tag{10}$$

Adopting for the solution of (7) an infinite expansion in terms of Legendre polynomia we readily find that the coefficients satisfy the relation (9) with $x = \gamma$ so that

$$P(u) = \sum_n (2n+1) g_n(\gamma) P_n(u)\,, \tag{11}$$

which also fixes the normalization $g_0(\gamma) = 1$. During this derivation we obtain the finite sum

$$(1-ku)\,P(u) = \sum_n \omega_n g_n(\gamma) P_n(u)\,. \tag{12}$$

The derivation can be valid only if the infinite series (11) converges for $-1 \leqq u \leqq 1$. A necessary condition, which we shall later find to be also a sufficient condition, is:

$$g_n(\gamma) \to 0 \quad \text{for} \quad n \to \infty\,. \tag{13}$$

We observe that for $n > N$, we have $\omega_n = 0$, $h_n = 2n + 1$, so that Eq. (9) is then identical to the recurrence relation for the Legendre functions. If, for a fixed argument $x > 1$, the values $g_m(x)$ and $g_{m+1}(x)$ are given, these can always be written as a linear combination of the Legendre functions of

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the first kind $P_n(x)$ and of the second kind $Q_n(x)$, of the corresponding orders m and $m+1$. The recurrence relation then states that this must be true for all $n \geqq N$ and hence we have

$$g_n(x) = A(x) P_n(x) + B(x) Q_n(x) \quad (n \geqq N) . \tag{14}$$

Since only $Q_n(\gamma)$ satisfies the condition (13) this leads to $A(\gamma) = 0$ and

$$g_n(\gamma) = B Q_n(\gamma) , \tag{15}$$

where B is a constant valid for the root γ.

Let us now examine the ratio

$$r_n(x) = g_n(x)/g_{n-1}(x) , \tag{16}$$

defined for $n \geqq 1$. Eq. (9) can be translated into a recursion formula for increasing n:

$$r_{n+1}(x) = \frac{h_n x}{n+1} - \frac{n}{(n+1)\, r_n(x)} \tag{17}$$

or for decreasing n:

$$r_n(x) = \frac{n}{-(n+1)\, r_{n+1}(x) + h_n x} \tag{18}$$

If r_n has a limit for $n \to \infty$, then this limit r must satisfy the quadratic equation

$$r = 2x - r^{-1} , \tag{19}$$

which follows from (17) because $\omega_n \to 0$. We shall denote the two roots by

$$r = x - (x^2-1)^{1/2} \quad \text{and} \quad r^{-1} = x + (x^2-1)^{1/2} , \tag{20}$$

where $x > 1$, $r < 1$. It is known that for $n \to \infty$ the first term in (14) increases as r^{-n}, the second term decreases as r^{+n}.

The practical experience, in computing $g_n(x)$ by means of the recurrence scheme (9) for an x which is not precisely the root γ, is that after an initial convergence the values blow up. This is explained by the fact that in (14) the coefficient $A(x)$ may be small but the first term will always dominate for large n, unless we have the exact root for which $A(\gamma) = 0$. If we do have this root, the series (11) converges about as a geometric series with ratio r so that condition (13) is also a sufficient condition.

Trying a power series in terms of n^{-1} in (17) or (18) we readily find that

$$r_n(\gamma) = r\{1 - (2n)^{-1} + O(n^{-2})\} . \tag{21}$$

Figure 1 shows four illustrations of this asymptotic behaviour. The corresponding form of $g_n(\gamma)$, which can be verified by substitution of (22) into (16), is

$$g_n(\gamma) = C n^{-1/2} r^n \{1 + O(n^{-1})\} , \tag{22}$$

where C is a constant.

The following remark is of practical importance in the numerical work. If x is close to γ and $r_n(x) = r_n(\gamma) + \varepsilon_n$, where the error ε_n is small (in a certain range of n), then Eqs. (17) or (18) give

$$\varepsilon_{n+1} = r^{-2} \varepsilon_n . \tag{23}$$

This shows that the errors increase in the forward scheme (17) but decrease, by a factor r^2, in the retrograde scheme (18). Practical tests show that the retrograde scheme stabilizes itself very rapidly indeed. It is not even necessary to start with a good estimate (which Eq. (21) can provide) but starting from $r_m = 1$ or $r_m = 0$, where m may for instance be 20 or 10, is equally good. The choice $r_m = 0$ corresponds to putting $g_m(x) = 0$, i.e., to solving x as a zero of the determinant in Eq. (10) with $n = m$. It is not surprising that this should give roots very nearly equal to the correct ones.

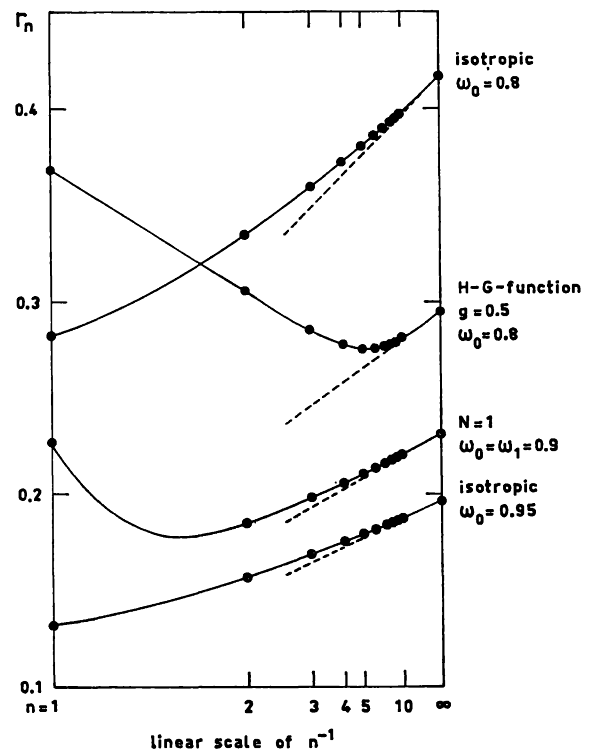

Fig. 1. Ratio between successive values of the Kuščer polynomia for the main root γ in four different examples

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4. Forms of the Characteristic Equation

The preceding discussion results in the following recommendation for finding the roots $\gamma = k^{-1}$. Choose an $x > 1$; start at a sufficiently large n with a reasonable estimate for r_n, for instance based on (20) and (21); use the retrograde scheme (18) to find, in $n-1$ steps, $r_1(x)$ and note the result. Then vary x and repeat until a value $x = \gamma$ is found for which

$$r_1(\gamma) = h_0 \gamma \,. \tag{24}$$

This recipe, which of course permits many variations, *replaces* the necessity to write and solve the characteristic equation.

Most earlier authors, working with the assumption that $N =$ finite, have tacitly decided that there would be no point to consider orders $n > N$. With this restriction, Eq. (13) cannot be used and it is necessary, instead, to write a characteristic equation. Some forms may be mentioned here.

(a) Using the exact ratio

$$r_{N+1}(\gamma) = Q_{N+1}(\gamma)/Q_N(\gamma) \tag{25}$$

as a starting value of the retrograde steps described above, and imposing condition (24), we find the continued fraction

$$h_0\gamma = \cfrac{1}{h_1\gamma - \cfrac{4}{h_2\gamma - \cfrac{9}{\cdots\cdots\cdots\cdots \atop h_{N-1}\gamma - \cfrac{N^2}{h_N\gamma - (N+1)\,Q_{N+1}(\gamma)/Q_N(\gamma)}}}} \tag{26}$$

which is an exact, though weird form of the characteristic equation.

(b) A more conventional form is obtained by substituting form (12) at both sides of Eq. (7) and equating the coefficients of $P_j(u)$. We then obtain

$$g_j(\gamma) = \sum_n \omega_n A_{jn}(\gamma) g_n(\gamma) \,. \tag{27}$$

Here

$$A_{jn}(z) = 1/2 \int_{-1}^{1} \frac{P_j(x)\, P_n(x)\, dx}{1 - x/z} = \begin{cases} z P_j(z)\, Q_n(z), & j \geqq n \\ z Q_j(z)\, P_n(z), & j \leqq n \,. \end{cases} \tag{28}$$

In particular, for $j = 0$, (28) becomes

$$A_{0n}(z) = z Q_n(z) \tag{29}$$

and (27) becomes

$$1 = \sum_n \omega_n \gamma g_n(\gamma) Q_n(\gamma) \,. \tag{30}$$

This is the simplest form of the characteristic equation, which strangely enough is not given in most books. For isotropic scattering ($N = 0$) it leads to the well known result

$$1 = \omega_0 \gamma Q_0(\gamma) = \frac{\omega_0 \gamma}{2} \ln \frac{\gamma + 1}{\gamma - 1} = \frac{\omega_0}{2k} \ln \frac{1 + k}{1 - k} \,. \tag{31}$$

(c) The most familiar form of the characteristic equation is found by again taking (27) for $j = 0$, and by using Waller's (1946) identity

$$R(z) \int_{-1}^{1} \frac{P_n(x)\, dx}{z - x} = \int_{-1}^{1} \frac{R(x)\, P_n(x)\, dx}{z - x} \,, \tag{32}$$

which is valid if $R(x)$ is a polynomium of degree $\leqq n$. Since $g_n(x)$ has the same degree as $P_n(x)$ we find at once

$$1 = \sum_n \frac{\omega_n}{2} \int_{-1}^{1} \frac{P_n(\mu)\, g_n(\mu)\, d\mu}{1 - \mu/\gamma} \tag{33}$$

which, upon introduction of the characteristic function

$$\Psi(\mu) = 1/2 \sum_n \omega_n P_n(\mu) g_n(\mu) \tag{34}$$

may also be written as

$$1 = \int_{-1}^{1} \frac{\Psi(\mu)\, d\mu}{1 - k\mu} \,. \tag{35}$$

5. Solution of ω_0 for Fixed ω_n ($n \geqq 1$)

It is often convenient to discuss the spectrum of the integral equation (7) not in terms of the eigenvalues $k = \gamma^{-1}$ belonging to a given set of numbers $\omega_0 \ldots \omega_N$, but to solve the inverse problem, namely to solve for one open parameter in the set $\omega_0 \ldots \omega_N$ for a given k.

Busbridge (1967) has posed a very simple problem in this class. She supposes that ω_n for $n \geqq 1$ is given and wishes to find ω_0. The solution is explicitly given in Eq. (26). Upon replacing γ by k^{-1} this gets a form which we write out completely for $N = 3$:

$$\omega_0 = 1 - \cfrac{k^2}{h_1 - \cfrac{4k^2}{h_2 - \cfrac{9k^2}{h_3 - 4k\, Q_4(k^{-1})/Q_3(k^{-1})}}} \,. \tag{36}$$

Evidently, the result is a unique value of ω_0. It can also be written in the form of a power series in k^2, in which the coefficient of k^{2j} contains only the coef-

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ficients $\omega_1 \ldots \omega_j$. The first few terms are

$$\omega_0 = 1 - \frac{1}{h_1} k^2 - \frac{4}{h_1^2 h_2} k^4 - \left(\frac{6}{h_1^3 h_2^2} + \frac{36}{h_1^2 h_2^2 h_3} \right) k^6 + \ldots . \quad (37)$$

The coefficients up to that of k^4 were given by Busbridge (1967). Results equivalent to (36) and (37) may also be derived from (30).

6. Solution of the Albedo a for a Scattering Diagram of Fixed Form

The simple problem posed and answered in Section 5 is not the most significant problem in its class. A physically more useful problem emerges when we write

$$\omega_n = a b_n , \quad (38)$$

where $b_0 = 1$ and $b_n (n = 1 \ldots N)$ is a given set of coefficients, and then ask for a as a function of k. This means that the scattering pattern has a fixed shape, and that only the albedo for single scattering, $a = \omega_0$, is varied. It is clear that Eq. (26), though still correct, does not at once give the answer, because all h_n contain the unknown a. This also opens the possibility that more than one solution exists.

From (10), (8) and (38) we see that $g_n(\gamma)$ is a polynomial of degree n in a. Consequently, for finite N, Eq. (30) must have $N + 1$ roots a. For $N = 0$ this is the single root defined by (31); the properties have been amply discussed in the literature on radiative transfer (e.g. Case, De Hoffman, Placzek, 1953; Grosjean, 1963).

We shall first briefly review the results for $N = 1$. Here a follows from the quadratic equation

$$x(1-a)^2 + \{3 - x - 2kQ_2(\gamma)/Q_1(\gamma)\}(1-a) - k^2 = 0 , \quad (39)$$

where the phase function is defined in a traditional notation by $\omega_0 = a$, $\omega_1 = ax$ and where again $\gamma = k^{-1}$. It is seen that the two roots $a_{0,1}$ belonging to the same value of k are related by

$$(1 - a_0)(1 - a_1) = - k^2/x . \quad (40)$$

Figure 2 shows these roots for $x = 1$, i.e., for the extreme case of linearly anisotropic scattering, which has often been used as a practising example. The

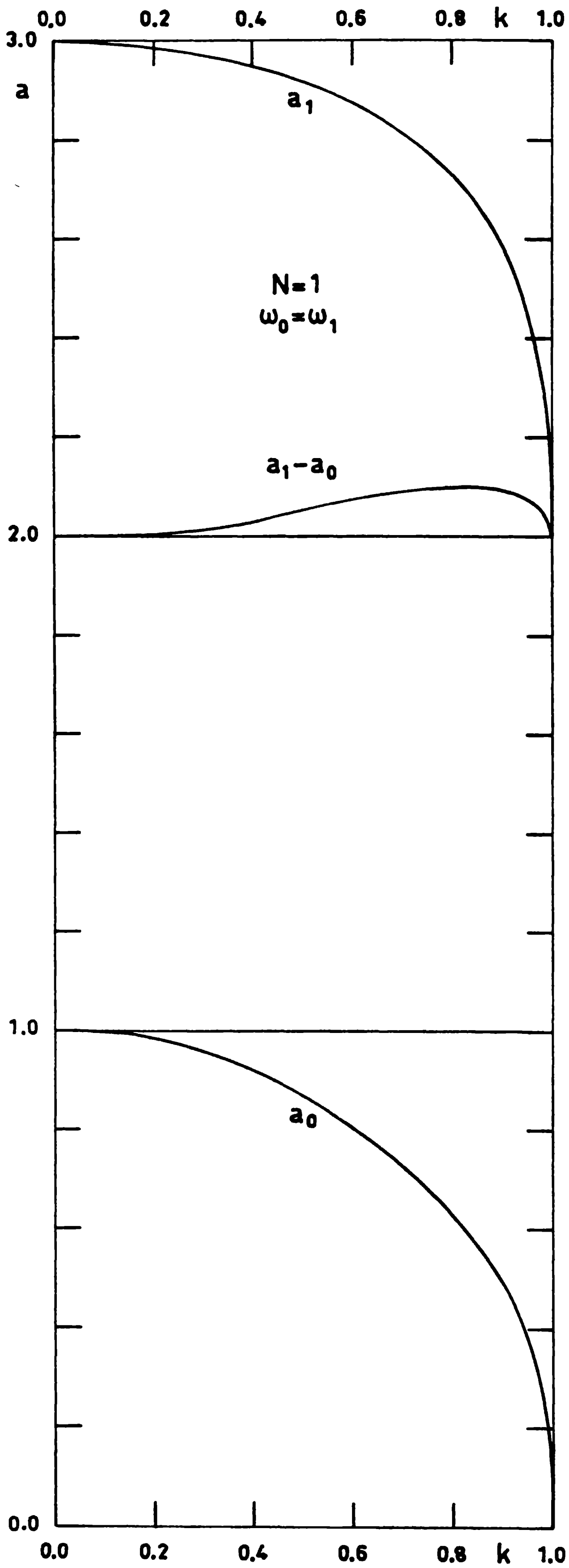

Fig. 2. Two values of the albedo, a_0 and a_1, satisfy the characteristic equation for a given value of k for the linearly anisotropic phase function defined by $\omega_0 = \omega_1$ ($N = 1$)

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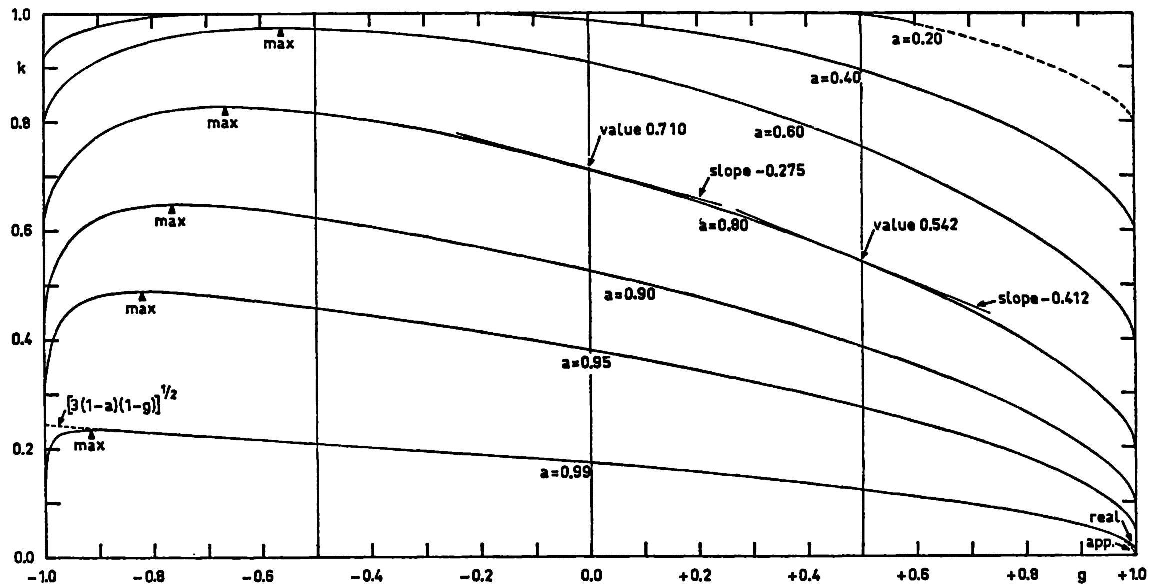

Fig. 3. Relation between a and k in the main root for the Henyey-Greenstein functions over the full range of anisotropy factors g

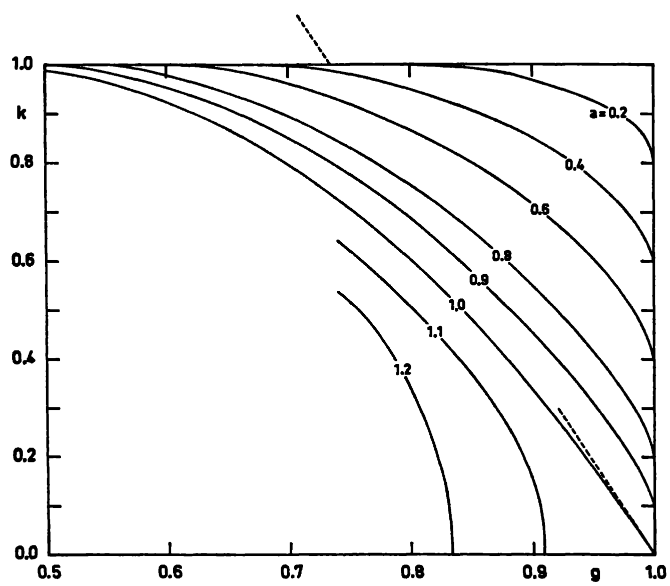

Fig. 4. Relation between a and k in the second root for Henyey-Greenstein functions with strong forward scatter

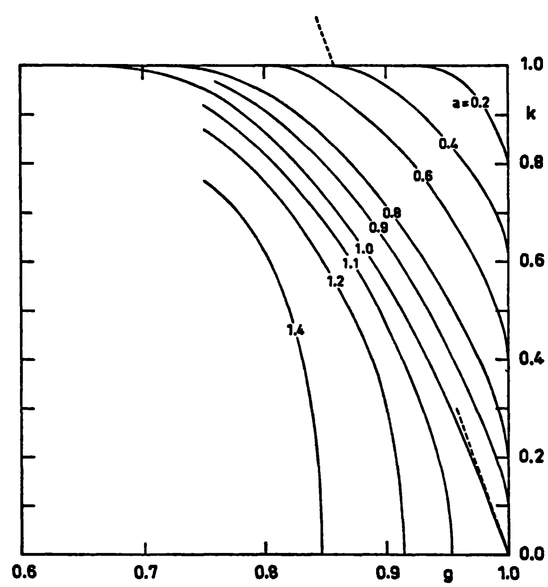

Fig. 5. As Fig. 4, third root

values of the lower root, a_0, were taken from Kaper *et al.* (1970). They define a curve rather similar to that for $N = 0$. The values a_1 were then found from Eq. (40); this curve starts for $k = 0$ at $a_1 = 3$ and finishes for $k = 1$ at $a_1 = 2$ with a vertical tangent. Further properties may be derived from Eq. (39).

The obvious generalization of this result for any finite N is that $N + 1$ real, non-negative values of a correspond to one k. We shall not prove this conjecture, but simply remark that at $k = 0$ the $N + 1$ non-trivial solutions of (12) are defined by

$$h_j = 0 \,, g_j = 1 \,, g_n = 0 \quad (n \neq j \,, j = 0 \text{ --- } N). \quad (41)$$

We shall now show some detailed results on these multiple solutions for one particular example with $N = \infty$, namely the Henyey-Greenstein phase func-

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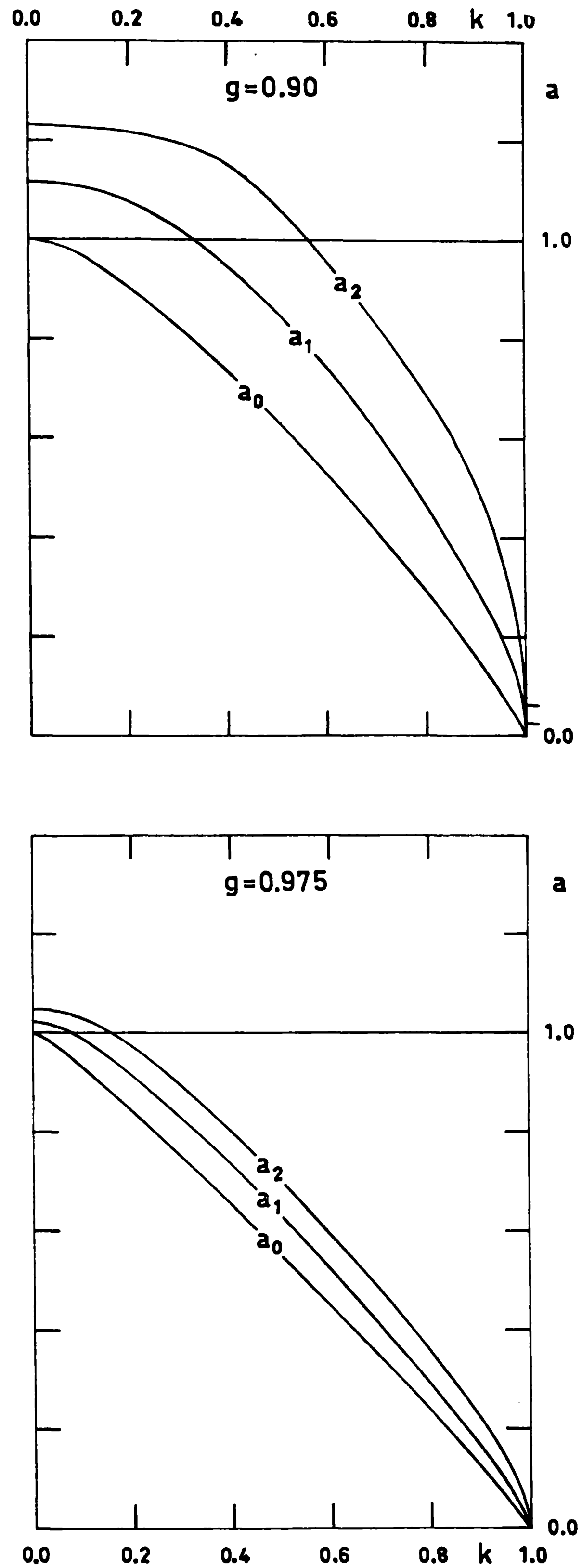

tion, defined by

$$\omega_n = (2n+1) a g^n , \tag{42}$$

where $-1 \leqq g \leqq 1$. This phase function has been employed in many transfer computations by van de Hulst, Irvine and others and many properties of the spectrum of eigenvalues are known from the work of Grosjean (1963) and Vanmassenhove (1967); see also Vanmassenhove and Grosjean (1967).

Figures 3 to 5 show the three smallest values of k for given combinations (a, g). A variety of numerical methods have been used; they are all based on the condition (13) or on one of the forms of the characteristic equation explained above. All three roots go to the limit $k = 1 - a$ for $g \to 1$. For any $a \leqq 1$ the second root exists only if $g > 0.50$ (approximately) and the third root if $g > 0.71$ (approximately). A similar situation exists for $g < 0$, i.e. for predominantly backward scattering. All roots go to $k = (1 - a^2)^{1/2}$ for $g \to 1$. We do not present further details because these values of g do not find much application.

The three roots are jointly shown for two particular values of g in Fig. 6. The starting points at $k = 0$ are at $a = 1$, $a = g^{-1}$, and $a = g^{-2}$, in accordance with (8), (41) and (42).

By analogy with Fig. 2 we expect that each root reaches a finite value a in the limit $k = 1$. These values are found along the top of Figs. 4 and 5 and along the right edge of the drawings in Fig. 6.

To find these limits precisely we may observe that (30) or (35) require in the limit $k = 1$ that

$$2\,\Psi(1) = \sum_n \omega_n g_n(1) = 0 , \tag{43}$$

which, together with (9) or (10) and (42) fixes the relation between a and g for each root at $k = 1$. Vanmassenhove (1967, Table 4) has computed a few values. Let $a_j(g)$ be the j-th root belonging to a value of g; the main root is $a_0 = 0$. We find it convenient to use the products $a_j g^j$ because it can be shown that these approach for $g = 0$ the finite limit $j/(2j+1)$. The combined available values are

$g =$	0	0.1	0.3	0.5	0.7
$a_1 g =$	0.333	0.374	0.411	0.33	0.15
$a_2 g^2 =$	0.400	0.412	0.439	0.46	0.33
$a_3 g^3 =$	0.429	—	—	0.47	0.45

Fig. 6. Two examples showing the relations between a and k in the first three roots for a Henyey-Greenstein phase function with fixed anisotropy

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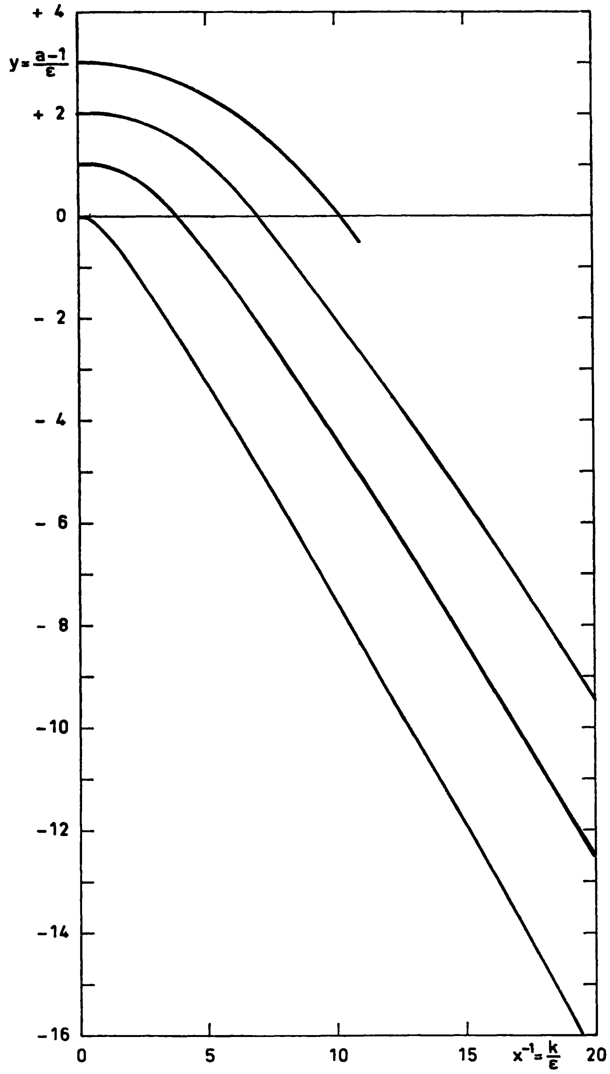

Fig. 7. Final form of the curves of Fig. 6 when $g \to 1$ and the coordinates are expanded accordingly: $y = (a-1)/(1-g)$, $x^{-1} = k/(1-g)$

It appears likely that near $g = 1$ the approximate behaviour is $a_1 = 2.4(1-g)^2$, and similarly for a_2, but the coefficient is uncertain and the matter has not been pursued. It should be noted that knowledge of the exact $a_j(g)$ relations for $k = 1$ would not help much in drawing the curves in Figs. 4 and 5 because of the horizontal tangents.

The behaviour of the main root near the point $k = 1$, $a = 0$ for an arbitrary phase function has been studied in detail by Maslennikov and Sushkevich (1964).

Finally, we have looked what happens to the curves in Fig. 6 if we let $g \to 1$. The answer is shown in Fig. 7. If we define

$$y = \frac{a-1}{1-g}, \quad x = \frac{k}{1-g} \tag{44}$$

and then let $g \to 1$, the curves from Fig. 6 approach those of Fig. 7. We may compute x as an eigenvalue for which the set of equations

$$(2n+1)(n-y)x^{-1}g_n = (n+1)g_{n+1} + n g_{n-1} \tag{45}$$

has a solution satisfying $g_n \to 0$ for $n \to \infty$. This equation and this condition follow at once from (9) and (13). A computation showed that the value $y = 0$ is reached for $x = 3.7900$, 6.9830, 10.1466, etc. It may be noted that these zeros differ little from the zeros of the Bessel function $J_1(x)$.

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