SOME NUMERICAL METHODS FOR THE SOLUTION OF THE EQUATION OF TRANSFER

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Received May 17, 1965

ABSTRACT

In this paper we shall discuss three methods of solution to the equation of radiative transfer. The first method is a numerical extension of a method developed by Chandrasekhar and is included in order to provide a basis of comparison for the other methods. The other two methods were inspired by a desire to consider more general problems in the field of radiative transfer. The second method may be shown to be equivalent to a numerical application of the product calculus of Volterra, while the third method is an application of a general method for the solution of boundary-value problems for ordinary linear differential equations. This latter method enables one to consider problems in which the scattering is anisotropic and a function of optical depth. A discussion of the accuracy of the various methods as compared to the first method is included.

In addition some results based on the first method are presented which indicate that the reddening-curve must be modified if the source presents an appreciable solid angle as seen from the reddening material. The effects of the scattering of radiation from an extended source upon an interstellar absorption line are also discussed.

I. INTRODUCTION

This paper will deal with several methods for the solution of the equation of transfer as formulated by Chandrasekhar (1950). A numerical extension of the method proposed by Chandrasekhar (1950) will be given and used as a basis for determining the accuracy of the other methods described. These other methods will be applied to a larger class of problems than those treated by Chandrasekhar, and sample solutions will be given.

In the first section we will briefly review the method of Chandrasekhar as applied to the problem of isotropic scattering. The second section will deal with an alternate method which allows solutions to be developed for cases where an arbitrary axially symmetric scattering function is given. The third section will demonstrate how the equation may be solved when the scattering is allowed to vary with optical depth. We will discuss the numerical accuracy of these last two methods in light of the solutions given in the first part of this paper. The accuracy of these numerical solutions may be compared with those exact solutions that have been obtained. The numerical solutions have the advantage, however, of being applicable to a large class of transfer problems and boundary conditions and also of specifying the internal radiation field as well as the emergent intensity.

No attempt has been made to discuss the many other excellent approaches to the solution of the transfer equation that exist in the literature, as such a treatment would clearly be beyond the scope of a single paper.

II. THE EQUATION OF TRANSFER AS FORMULATED BY CHANDRASEKHAR

The basic equation of transfer with which we shall deal in this paper is the axially symmetric equation

$$\mu \frac{dI(\tau,\mu)}{d\tau} = I(\tau,\mu) - \tfrac{1}{2}\int_{-1}^{+1} P(\mu,\mu',\tau)\, I(\tau,\mu')\, d\mu' . \tag{1}$$

Chandrasekhar (1950) has shown that the solution to this equation may be approximated by replacing the integral with a Gaussian sum and requiring the equation to hold at the points of the Gaussian division. This leads to a set of simultaneous linear ordinary differential equations.

$$\mu_i \frac{dI(\tau,\mu_i)}{d\tau} = I(\tau,\mu_i) - \tfrac{1}{2}\sum_{j=-n}^{n} P(\mu_j,\mu_i,\tau)\, I(\tau,\mu_j)\, a_j\,. \quad (i = \pm 1,2,3,\ldots \pm n) \tag{2}$$

Here the a_j's are the Gaussian weights appropriate to the points of the Gaussian division μ_j. Anselone (1959) has shown that, as n approaches infinity, the solution to equation (2) approaches the solution to equation (1).

It has been further demonstrated by Chandrasekhar that the solution to equation (2) in the case where P is not a function of μ is given by

$$I(\tau,\mu_i) = \sum_{a=1}^{n} \frac{L_{+a} e^{-k_a \tau}}{1+\mu_i k_a} + \sum_{a=1}^{n} \frac{L_{-a} e^{+k_a \tau}}{1-\mu_i k_a}, \qquad (i = \pm 1, \pm 2, \ldots \pm n) \tag{3}$$

where the $2n$ $L_{\pm a}$'s are determined from the $2n$ boundary condition, $I(\tau_0,+\mu_i)$ and $I(0,-\mu_i)$. The k_a's are determined from the characteristic equation (eq. [6]) for the appropriate value of P.

The solution of equation (2) takes a different form in the special case where P is unity and is

$$I(\tau,\mu_i) = \tfrac{3}{4}F\left(\sum_{a=1}^{n-1} \frac{L_{+a} e^{-k_a \tau}}{\imath+\mu_i k_a} + \sum_{a=1}^{n-1} \frac{L_{-a} e^{+k_a \tau}}{1-\mu_i k_a} + \tau + \mu_i + Q\right). \quad (i = \pm 1,2,3,\ldots \pm n) \tag{4}$$

Here F, Q, and $L_{\pm a}$ are the $2n$ constants of integration specified by the boundary conditions

$$\begin{aligned} &\sum_{a=1}^{n-1} \frac{L_{+a}}{i-\mu_i k_a} + \sum_{a=1}^{n-1} \frac{L_{-a}}{1+\mu_i k_a} - \frac{4I(0,-\mu_i)}{3F} + Q = u_i\,, \qquad (i = 1,2,3,\ldots n) \\ &\sum_{a=1}^{n-1} \frac{L_{+a} e^{-k_a \tau_0}}{1-\mu_i k_a} \sum_{a=1}^{n-1} \frac{L_{-a} e^{+k_a \tau_0}}{1-\mu_i k_a} - \frac{4I(\tau_0+\mu_i)}{3F} + Q = -\tau_0 - \mu_i \quad (i = 1,2,3,\ldots n) \end{aligned} \tag{5}$$

and the k_a's are the roots of the characteristic equation

$$1 = P\sum_{j=1}^{n} \frac{a_j}{1-\mu_j^2 k_j^2}, \tag{6}$$

with P taken to be unity.

It is always possible to find the roots of equation (6) by means of Newton-Raphson iteration techniques and thereby solve equation (5) for the constants of integration. To demonstrate this, consider the function

$$f(k,P) = 1 - P\sum_{j=1}^{n} \frac{a_j}{1-\mu_j^2 k^2}, \tag{7}$$

with $0 < P < 1$, $0 < k < \infty$. Note that $f(k,P)$ will have poles at values of k equal to $1/\mu_j$ and hence will have exactly n such poles. Also note that $f(1/\mu_j + \epsilon,P)$ and $f(1/\mu_j - \epsilon,P)$ have opposite signs. From this it follows that the poles divided the zeros of f. Since

TABLE 1

ROOTS OF THE CHARACTERISTIC FUNCTION $f_n(k,1)$

$n=2$
0 000000
1 972027

$n=3$
0 000000
1 225211
3 202945

$n=4$
0 000000
1 103185
1 591779
4 458086

$n=5$
0 000000
1 059426
1 297814
1 987330
5 721175

$n=6$
0 000000
1 038632
1 183180
1 519150
2 394194
6 987900

$n=7$
0 000000
1 027106
1 125058
1 330224
1 752305
2 806740
8 256597

$n=8$
0 000000
1 020052
1 091143
1 231536
1 991830
3 222568
9 526486

$n=9$
0 000000
1 015422
1 069503
1 172451
1 348533
1 653438
2 235213
3 640471
10 797153

$n=10$
0 000000
1 012222
1 054805
1 133904
1 263385
1 471808
1 822337
2 481124
4 059775
12 068353

$n=12$
0 000000
1 008206
1 036633
1 087898
1.167580
1 285850
1 461193
1 729323
2 167549
2 977720
4 901086
14 611805

$n=14$
0 000000
1 005880
1 026221
1 062311
1 116632
1 194684
1 302621
1 453879
1 670670
1 995226
2 518641
3 478208
5 744648
17 156144

$n=16$
0 000000
1 004414
1 019695
1 046842
1 086403
1 141680
1 216893
1 315372
1 448334
1 630351
1 886543
2 265896
2 873172
3 981925
6 589978
19 701030

$n=18$
0 000000
1 003432
1 015433
1 036112
1 066616
1 108228
1 163010
1 233982
1 325579
1 444458
1 600949
1 811858
2 106332
2 539651
3 229900
4 485851
7 435403
22 246277

$n=20$
0 000000
1 002743
1 012274
1 028846
1 085545
1 127770
1 181417
1 248953
1 333878
1 441246
1 578567
1 757429
1 996629
2 328706
2 815209
3 588119
4 990712
8 281846
24 791774

$n=25$
0 000000
1 001711
1 007688
1 018022
1 032907
1 052657
1 077718
1 108689
1 146359
1 191764
1 246259
1 311636
1 390292
1 485488
1 601754
1 745557
1 926435
2 159041
2 467073
2 891500
3 509737
4 487724
6 256953
10 399661
31 156215

$n=30$
0 000000
1 001166
1 005260
1 012322
1.022437
1 035745
1 052445
1 072798
1 097138
1 125882
1 159558
1 198822
1 244496
1 297619
1 359511
1 431871
1 516913
1 617576
1 737830
1 883172
2 061427
2 284113
2 568909
2 944382
3 459898
4 208720
5 390716
7 525584
12 518918
37 521247

$n=35$
0 000000
1 000844
1 003822
1 008954
1 016280
1 025874
1 037835
1 052297
1.069425
1 089422
1 112538
1 139074
1 169395
1 203942
1 243253
1 287982
1 338931
1 397096
1 463719
1 540370
1 629060
1 732400
1 853844
1 998057
2 171482
2 383288
2 646963
2 983195
3 425414
4 031373
4 910170
6 295601
8 795556
14 638991
43 886616

$n=40$
0 000000
1 000639
1 002901
1 006798
1 012352
1 019602
1 028606
1 039437
1 052188
1 066969
1 083914
1 103184
1 124967
1 149484
1 177000
1 207826
1 242330
1 280950
1 324213
1 372749
1 427323
1 488870
1 558542
1 637774
1 728375
1 832656
1 953619
2 095227
2 262829
2 463814
2 708684
3 012893
3 400137
3 908702
4 604724
5 613135
7 201653
10 066358
16 759569
50 252194

$n=50$
0 000000
1 000401
1 001833
1 004299
1 007807
1 012372
1 018015
1 024764
1 032655
1 041729
1 052037
1 063635
1 076591
1 090981
1 106892
1 124426
1 143695
1 146832
1 187986
1 213326
1 241049
1 271380
1 304579
1 340946
1 380829
1 424638
1 472850
1 526032
1 584854
1 650123
1 722808
1 804093
1 895432
1 998635
2 115977
2 250366
2 405571
2 586569
2 800071
3 055344
3 365561
3 750096
4 238657
4 879237
5 754736
7 021747
9 015829
12 609444
21 001626
62 983724

the first derivative of f with respect to k is always negative in the region between two adjacent poles, the function f will have only one inflection point in this region. As the inflection point will not in general occur at the same value of k for which f is zero, it will be possible to find the root of f by means of Newton-Raphson techniques. That is, if one starts the iterative scheme near a pole so that no inflection point lies between the pole and the root, the iterative sequence will converge to the root. This method was employed to find the roots of $f(k,1)$ for $n = 2, 3, \ldots, 50$ and the results are given in Table 1, while Table 2 contains the results of the solution of characteristic equation for various values of P for the $n = 4$ case.

The accuracy was checked by making use of the relation

$$k_1 k_2 k_3 \ldots k_{n-1} \mu_1 \mu_2 \mu_3 \ldots \mu_n = \sqrt{\tfrac{1}{3}} \tag{8}$$

and for the roots of $f(k,1)$ and $n = 50$ the accuracy was found to be better than four parts in 10^7.

With the roots of equation (6) it is possible to obtain the constants of integration from equation (5).

TABLE 2

ROOTS OF THE CHARACTERISTIC FUNCTION $f_n(k,P)$

P	k_1	k_2	k_3	k_4
1 0 .	0 0000	1 1032	1 5918	4 4581
0 9 .	0 5255	1 1089	1 6136	4 5548
0 8	0 7105	1 1168	1 6426	4 6529
0 7 .	0 8288	1 1276	1 6724	4 7520
0 6	0 9078	1 1423	1 7046	4 8518
0 5	0 9596	1 1609	1 7382	4 9520
0 4 .	0 9924	1 1819	1 7725	5 0524
0 3 .	1 0330	1 2030	1 8066	5 1527
0 2	1 0263	1 2227	1 8400	5 2527
0 1 . ..	1 0352	1 2402	1 8722	5 3524

Substitution of these values into equation (4) then yields the value of the specific intensity at the points of the Gaussian division. An expression for the mean intensity $J(\tau)$ may be found by multiplying equation (4) by the Gaussian weights a_i and summing over all i. This expression may then be substituted into the general solution of the equation of transfer to obtain expressions for the intensity at points other than the points of the Gaussian division. These expressions were derived and evaluated for solutions obtained by this method. Thus, it was possible to compare solutions directly with those given by Chandrasekhar (1950) insofar as the same problems were considered. This also enabled comparisons to be made between the numerical solution and the exact solution obtained by Chandrasekhar for the case of the isotropic scattering conservative semi-infinite atmosphere. Figure 1 shows the error in the emergent intensity for this case.

Insofar as it is necessary to make other numerical comparisons, it will be assumed that the $n = 50$ approximation will represent the exact solution with sufficient accuracy. Figure 2 shows the error incurred in the interior solution for the case described above.

It is interesting to note that the error in the intensity between any two orders of approximation does not depend on μ when the optical depth is large. This is only true for the semi-infinite atmosphere. It is possible to show that the error in $I(\tau, \mu)/F$ for large τ is approximately equal to $\frac{3}{4}$ of the error in Q. In a finite atmosphere this will also be true of the solution when it is optically remote from the boundaries. Since, as n goes to infinity, the approximate solution will approach the true solution and for finite τ the

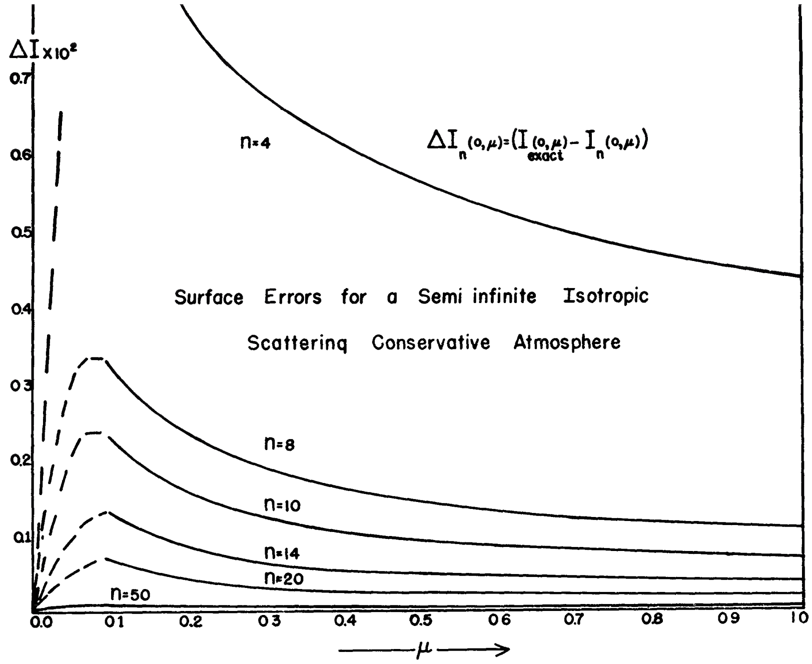

FIG. 1.—Errors in the emergent intensity as a function of μ for various orders of approximation

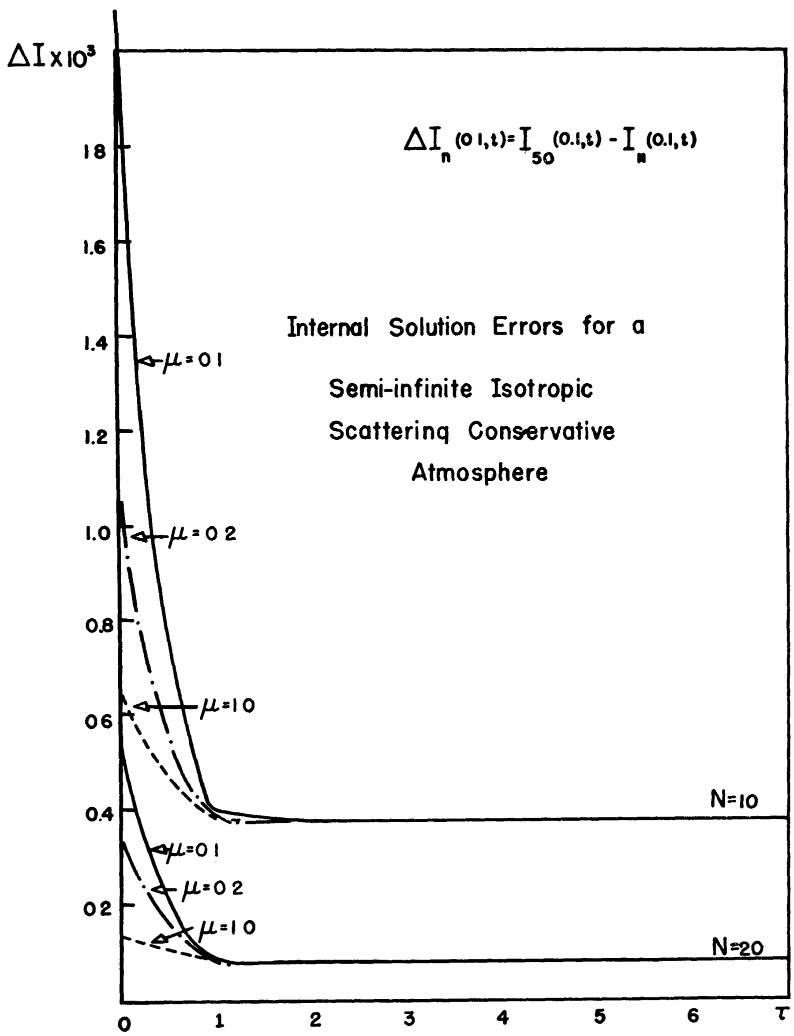

FIG. 2.—Sample errors of the internal radiation field as compared to the n = 50 solutions

solution will be finite, it can be shown that Q will remain finite in any order of approximation. Indeed, Kourganoff (1963) demonstrates this proof and gives a limiting value for Q of 0.71044609. Figure 3 describes the values of Q as n increases. From this one can see that choosing an order of quadrature greater than or equal to 10 will result in an error of Q of less than 0.1 per cent of the limiting value.

These numerical calculations were initially carried out in order to investigate the transfer problem for an arbitrary angular distribution of incident intensity. Consider, for example, the extinction of radiation from an extended source such as a gaseous nebula or the central region of a spiral galaxy by intervening interstellar matter. If the source subtends a sufficiently large solid angle as viewed from the absorbing or scattering cloud then the intensity is no longer simply reduced exponentially with τ as in the case of a point source.

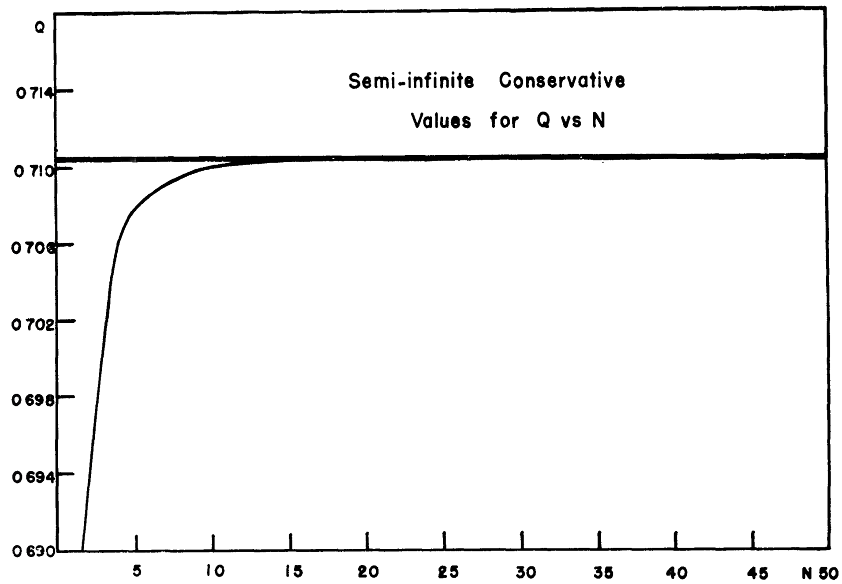

FIG. 3.—Rate of convergence of Q_N (i e., $q(\infty)$) as N becomes large. For practical purposes one may assume that Q has converged when $N = 10$.

The limiting case of an extended source is represented by a uniform angular distribution of incident intensity. It is of interest to compare the results obtained for a finite isotropic scattering medium for a point source and a uniform surface, characterized by isotropic incident radiation. The fraction of transmitted radiation from a point source is of course $e^{-\tau}$. The results for the diffuse source are given in Figure 4 for the emergent intensity normal to the surface.

These data have been used to plot the interstellar reddening-curve in Figure 5 for a uniform source and compared with the corresponding reddening for a stellar source. The point-source reddening-curve was taken from Whitford (1948) and normalized to 1 mag. extinction at λ 5000 Å. It is likely that the interstellar reddening of an actual extended source will be intermediate between these two limiting cases.

One further example is illustrated in Figure 6 where Doppler-broadened line profiles are compared for these two limiting cases. In this example, the optical depth is assumed to be given by

$$\tau_\nu = \tau_0 e^{-(\Delta\lambda/\Delta\lambda_0)^2} \tag{9}$$

where $\Delta\lambda_0$ is the Doppler width and the optical depth in the center of the line τ_0 is taken to be 2. The ratio of equivalent widths for the profiles illustrated is 1.80.

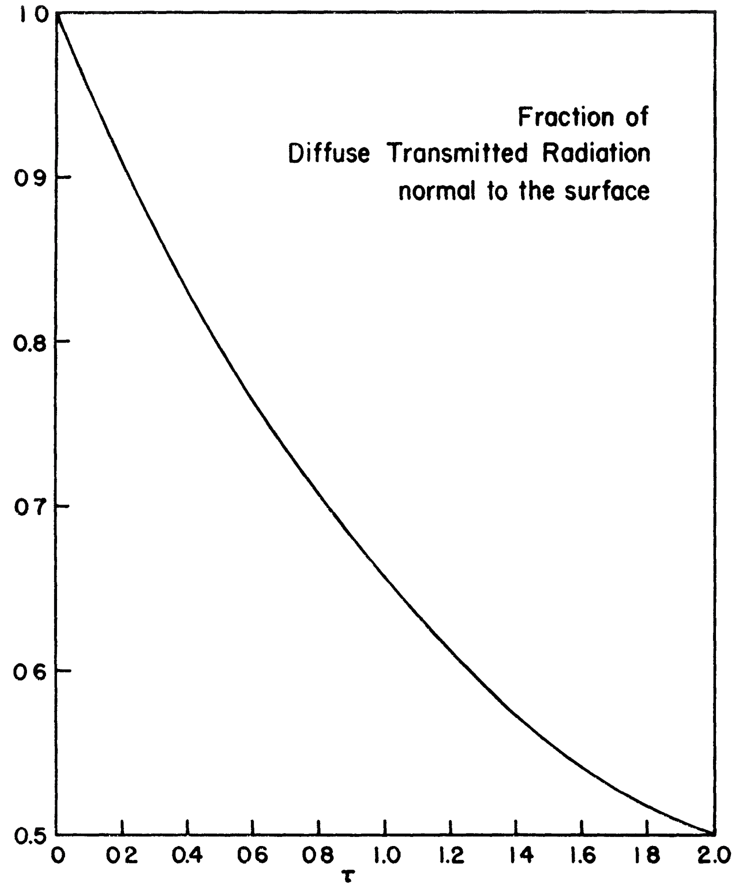

FIG. 4.—Rate of decline of the transmitted intensity of an extended source as a function of optical depth.

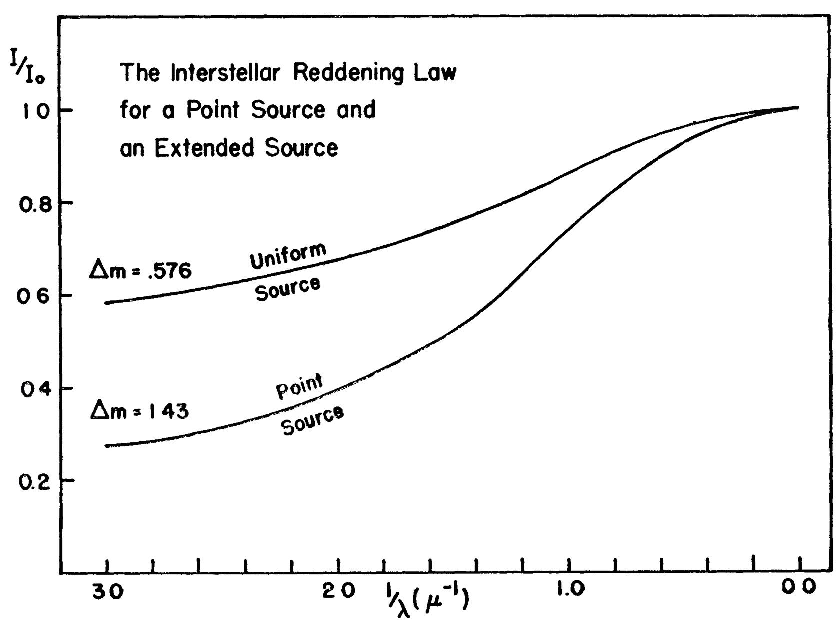

FIG. 5.—Comparison of the reddening law for an extended uniform source subtending a solid angle of 2π at the reddening material with that for a point source. The extinction has been normalized to 1 mag. at λ 5000 Å.

These numerical techniques are capable, however, of being extended to a much wider class of transfer problems.

Having obtained a set of solutions against which we may test more general techniques, we shall proceed to the description of these techniques.

III. THE INTEGRATING FACTOR METHOD

We may write the defining differential equations (2) in a vector form as follows:

$$I' = \mathfrak{A} I \tag{10}$$

where I is a $2n$-dimensional vector representing the solution and $\mathfrak{A}$ is a $2n \times 2n$ matrix whose elements are

$$a_{ij} = [\delta_{ij} - P_{ij}(\tau) a_j/2]/\mu_i \, . \tag{11}$$

If we restrict ourselves to atmospheres which are of finite extent τ_0, equation (10) is subject to the restrictions that $I_k(0)$ and $I_{k+n}(\tau_0)$ are known boundary conditions. When

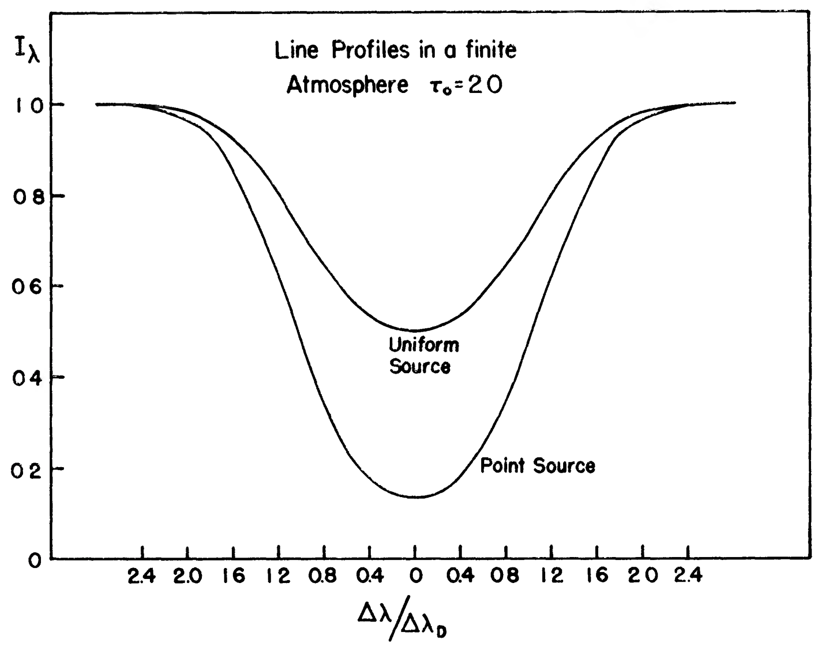

FIG. 6.—The effect of scattering of light from an external source upon a line profile

the albedo is not a function of the optical depth, then equation (10) has the following solution:

$$I(\tau) = e^{\tau \mathfrak{A}} C \tag{12}$$

where $e^{\tau\mathfrak{A}}$ is defined by

$$e^{\tau \mathfrak{A}} = \sum_{k=0}^{\infty} \frac{\tau^k \mathfrak{A}^k}{k!} \equiv \mathfrak{D}(\tau) \tag{13}$$

and the constant vector C may be determined by the boundary conditions. In practice, the matrix $\mathfrak{D}(\tau)$ was computed by summing the series given in equation (13) until the addition to every element in the matrix by the next term was less than 1 part in 10^8 of the present matrix element value. Solutions to problems determined in this manner agreed with solutions obtained by the method outlined in § II to better than 1 part in 10^6. The method has the advantage over the method of Chandrasekhar in that a new characteristic equation need not be solved for each new scattering function P_{ij} that is considered. However, it has the significant disadvantage that the intensity may only be determined at the points of the Gaussian division. Also, though it is much simpler to formulate than the Chandrasekhar method, it is numerically a more lengthy procedure.

It should be noted that this method of the "integrating factor" can be shown to be equivalent to a method described by Gantmacher (1959) based on the infinitesimal product calculus of Volterra.

Figures 7 and 8 illustrate solutions obtained for a finite conservative atmosphere in this manner. These integrations were carried out in the $n = 10$ approximation with uniform illumination at the boundary $\tau = 1$ and no illumination at the boundary $\tau = 0$.

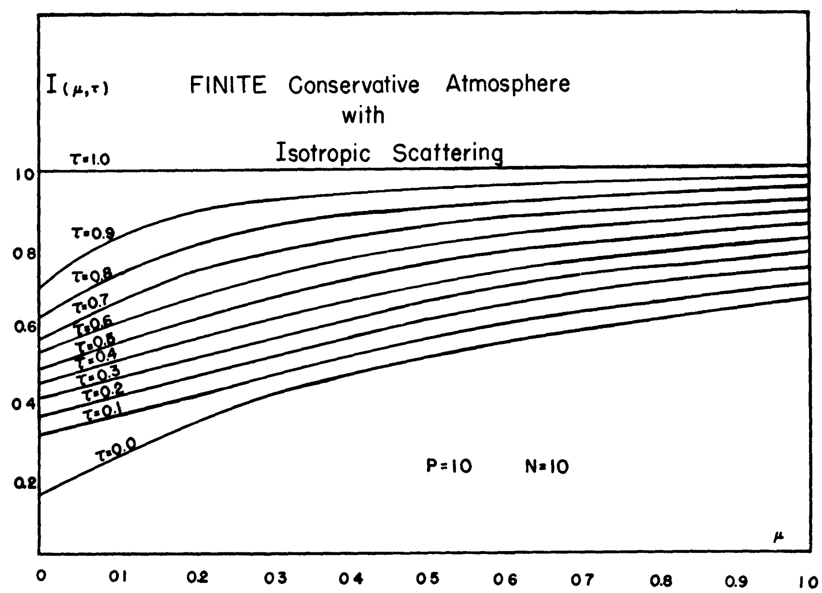

FIG. 7.—The radiation field in a finite isotropically scattering conservative atmosphere represented by lines of intensity at given optical depths.

IV. SOLUTION BY DIRECT INTEGRATION

In this section we shall consider a method for solving equation (2) even when the albedo function $P(\mu_i, \mu_j, \tau)$ is allowed to vary with τ. It is possible to show that if P is not constant with τ then no solution of the form

$$I = e^{\int \mathfrak{A}(\tau) d\tau} \cdot \mathfrak{S} \cdot C \, , \tag{14}$$

where $\mathfrak{S}$ is an arbitrary diagonal matrix, exists. Thus, we shall turn to another method for the general solution of equation (2). If one has a system of equations

$$Y' = \mathfrak{B} Y \tag{15}$$

and a one-step method of numerical integration such as that of Runga-Kutta, then it is possible to write the solution at one boundary in terms of the solution at the other boundary and a matrix $\mathfrak{R}$ which depends only on $\mathfrak{B}$ and the method of numerical integration. That is

$$Y(a) = \mathfrak{R} Y(b) . \tag{16}$$

This method has been discussed in detail by Day and Collins (1964). They have shown that equation (16) yields a system of linear equations relating the known and unknown boundary values that may be readily solved for the unknown boundary values. This reduces the problem from that of a boundary-value problem to that of an initial-value problem, which in turn may be solved by conventional methods.

This method was applied to a finite isotropic scattering atmosphere of optical depth 1 and uniformly illuminated with a specific intensity which was unity for all values of μ at $\tau = 1$. Several different variations of albedo with optical depth were considered.

Figures 6 and 7 illustrate some of the results of these calculations. Since P is a function of τ, there will be places in the atmospheres where the flux is not conserved. Thus, we would expect the flux to be a monotonically decreasing function as one moves outward in the atmosphere. This is clearly shown in Figure 6.

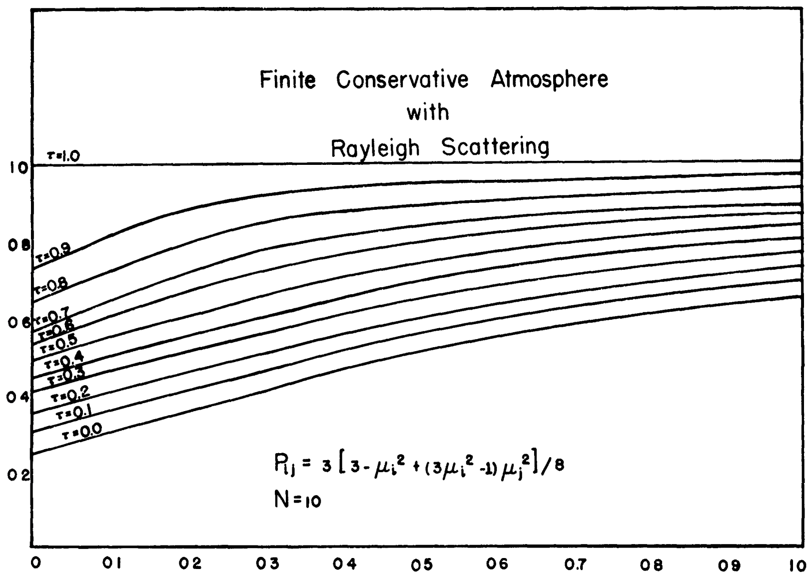

FIG 8.—The radiation field in a finite conservative atmosphere, where the scattering mechanism is Rayleigh scattering, represented by lines of intensity at given optical depths.

It can be shown (Capriotti 1964) that the albedo functions $P(\tau) = [1 - f(\tau)]$ and $P(\tau) = f(\tau)$ will yield solutions to the transfer equation for which the emergent flux will be the same providing the boundary conditions are the same. Furthermore, this will be true in any order of approximation in μ. This provides us with a check on the accuracy of the Runga-Kutta integration scheme. The numerical results for the flux of the two albedo functions described above in addition to one other function are displayed in Figure 9. Since the values of the emergent fluxes for these two problems agree to 1 part in 10^6, one might conclude that the Runga-Kutta method is quite accurate. However, the laws of darkening for these cases will be quite different as is illustrated in Figure 10.

When this method was applied to problems considered in §§ II and III, the agreement between solutions obtained in those sections and those obtained by this method was excellent. At no time was a difference between the methods of more than 1 part in 10^6 observed. Although this method is numerically more arduous than either of the previous two methods, it is also simpler to formulate than either one. Even though it introduces additional error due to the numerical integration of τ, it is felt that it is of significant value because of the larger number of problems that can be handled by this technique. It should be remembered that, since the additional error results from the integration

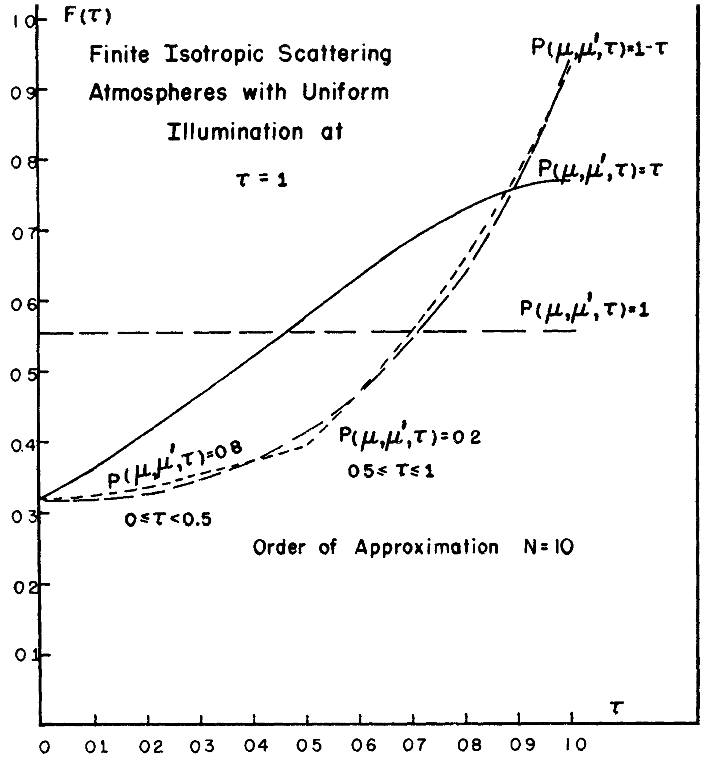

FIG. 9.—The flux transport through a non-conservative scattering atmosphere where the albedo is a function of optical depth. The finite conservative case is included for reference. The units of flux are essentially defined by the boundary conditions at $\tau = 1$. $I(1, u_i)$ is assumed to be 1.

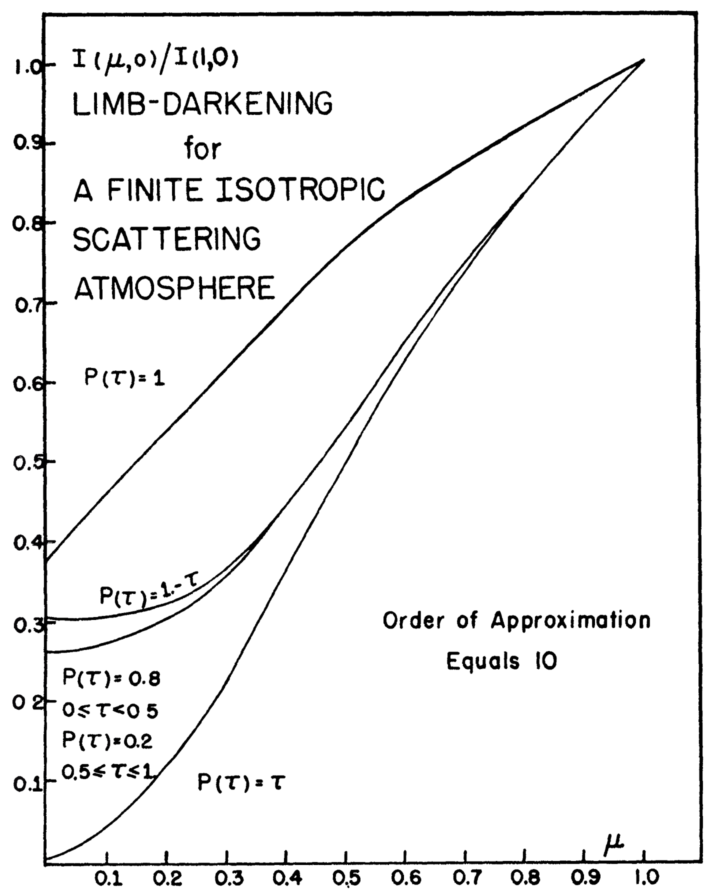

FIG. 10.—The limb-darkening laws for the atmospheres described in Fig. 9

methods, then it is possible to control the error by control of the step size and method of integration.

In an earlier work (Day and Collins 1964), it was pointed out that the method described above was also applicable to equations of the form

$$Y' = \mathfrak{B}Y + C(x) . \tag{17}$$

At present one of the authors (G. W. C. II) and E. R. Capriotti are employing this method to the problem of transfer of resonance radiation in an expanding atmosphere including redistribution in frequency.

The authors would like to acknowledge the aid of the Space Astronomy Laboratory and the Numerical Computation Laboratories of the University of Wisconsin and the Ohio State University. Additional thanks are due E. R. Capriotti for many fruitful discussions on the subject.

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