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An iterative solution to Chandrasekhar X and Y equations for isotropic scattering

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The X and Y functions of Chandrasekhar are defined in terms of two coupled integral equations whose solution for certain values of optical depth and albedo have already been found by means of iterative methods. This paper discusses the numerical difficulties of past iterative methods and describes an iterative approach which attempts to overcome some of these difficulties. This technique uses improved trial functions and is applied to the isotropic scattering case. Reasonable accuracy is achieved for certain cases at the expense of little computing time.

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I. INTRODUCTION

In the theory of radiative transfer in plane-parallel atmospheres we can express exact solutions for many of the standard problems in terms of certain H or X and Y functions. The H functions occur in the solution of problems in semi-infinite atmospheres while the X and Y functions occur in the corresponding problems in atmospheres of finite optical thicknesses. These X and Y functions were first introduced by Chandrasekhar,[1] and are of great importance in the study of finite plane-parallel atmospheres.

In some ways, the most fundamental problem in the theory of radiative transfer in plane-parallel atmospheres is the diffuse reflection and transmission of a parallel beam of radiation—the solution of many other problems can be reduced to this one. Chandrasekhar[1] has shown how exact solutions for this problem can be found under a variety of scattering conditions. The solutions can be expressed in terms of the functions which satisfy the pair of integral equations of the standard form

$$X(\mu) = 1 + \mu \int_0^1 \frac{\Psi(\mu')}{(\mu + \mu')} \{ X(\mu) X(\mu') - Y(\mu) Y(\mu') \} d\mu', \quad (1)$$

and

$$Y(\mu) = e^{-\tau/\mu} + \mu \int_0^1 \frac{\Psi(\mu')}{(\mu - \mu')} \{ Y(\mu) X(\mu') - X(\mu) Y(\mu') \} d\mu', \quad (2)$$

where τ denotes the optical thickness of the atmosphere and the characteristic function $\Psi(\mu)$ is, generally, an even polynomial in μ, satisfying the condition

$$\int_0^1 \Psi(\mu) d\mu \leqslant \tfrac{1}{2}. \quad (3)$$

These X and Y functions have been rigorously discussed by Busbridge.[2]

Numerical solutions of these equations were first obtained by Chandrasekhar and Elbert[3] for

$$\Psi(\mu) = \tfrac{1}{2}\omega_0, \quad (4)$$

which applies to isotropic scattering problems, ω_0 being the albedo for single scattering. Tables of $X(\mu)$ and $Y(\mu)$ were presented for $\omega_0 = 0.5$, 0.8, 0.9, 0.95, and 1.0 and $\tau = 0.05$, 0.1, 0.15, 0.20, 0.25, 0.5, and 1.0. The method of solution was an iterative one. From an nth approximation to the solution of Eqs. (1) and (2) an $(n+1)$th approximation was obtained by substituting the nth approximation into the integrals in Eqs. (1) and (2), which were then evaluated using numerical quadrature. However, as discussed in Sec. II, numerical problems arise in connection with the singularity in Eq. (2) when $\mu = \mu'$ (particularly, at $\mu = 1$) and for values of ω_0 close to unity, when the solution is no longer unique.

The numerical difficulties arising in the work of Chandrasekhar and Elbert[3] have been investigated in detail by Mayers[4] and many others. Also a noniterative method of solution for all values of optical depth has been developed by Caldwell.[5]

The purpose of this paper is to outline the numerical difficulties of past iterative methods and to describe a method which attempts to overcome some of these difficulties in obtaining accurate solutions $X(\mu)$ and $Y(\mu)$ for values of μ close to one.

II. NUMERICAL DIFFICULTIES

Chandrasekhar and Elbert[3] found the solutions of the pair of integral Eqs. (1) and (2) by a direct process of iteration for the case in Eq. (4). The iterative scheme used was

$$X_{n+1}(\mu) = 1 + \mu \Psi(\mu) \int_0^1 \{ X_n(\mu) X_n(\mu') - Y_n(\mu) Y_n(\mu') \} \frac{d\mu'}{(\mu + \mu')}, \quad (5)$$

and

$$Y_{n+1}(\mu) = e^{-\tau/\mu} + \mu \Psi(\mu) \int_0^1 \{ Y_n(\mu) X_n(\mu') - X_n(\mu) Y_n(\mu') \} \frac{d\mu'}{(\mu - \mu')} \quad (n = 0,1,2,\ldots). \quad (6)$$

The first 'trial' functions $X_0(\mu)$ and $Y_0(\mu)$ must be well chosen for this iterative scheme to be successful. For small values of τ, the iteration was started with the functions

$$X_0(\mu) = 1 \text{ and } Y_0(\mu) = e^{-\tau/\mu}. \quad (7)$$

One of the main drawbacks of this approach was that numerical problems arose in connection with the singularity in Eq. (6) when $\mu = \mu'$, particularly at $\mu = 1$.

For $\tau < 0.25$ it was found that no more than three iterations were required for satisfactory convergence. However,

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for $\tau = 0.5$ and 1 as many as six or seven iterations were necessary. Also, the iterated functions showed a certain 'raggedness' for some values partly due to the fact that the integrands in Eqs. (1) and (2) are sensitive to rounding errors. Chandrasekhar and Elbert 'smoothed' the solutions by plotting the deviations from the corrected second approximations.

An idea of the overall accuracy reached in the final solutions can be obtained by seeing how well the relation

$$\alpha_0 = 1 - \{1 - 2\int_0^1 \Psi(\mu')d\mu' + \beta_0^2\}^{1/2}, \tag{8}$$

between the moments

$$\alpha_0 = \int_0^1 X(\mu')\Psi(\mu')d\mu' \text{ and } \beta_0 = \int_0^1 Y(\mu')\Psi(\mu')d\mu', \tag{9}$$

is satisfied. For $\tau \leqslant 0.25$ the solutions are probably trustworthy to one part in 10 000, while for $\tau = 0.5$ and 1 the solutions for the larger values of the albedo are probably to be trusted to only one part in 1000.

Mayers[4] has investigated these numerical difficulties in detail. The weakness in the method lies in the fact that the integrand in the definition of $Y_{n+1}(\mu)$ becomes indeterminate at the point $\mu = \mu'$. The functions $X_n(\mu)$, $Y_n(\mu)$ will appear to converge with increasing n until we get near to $\mu = 1$; large variations will then appear near $\mu = 1$ and spread throughout the range until, if the process is continued, the approximations are smooth again and the cycle of events is repeated. This is the explanation of the fact noted by Chandrasekhar and Elbert[3] that near $\mu = 1$ the differences of $X(\mu)$ and $Y(\mu)$ become erratic. They do state that improved values were obtained by smoothing but give no further details.

Mayers[4] was able to obtain accurate solutions to Eqs. (1) and (2) using a combination of the Chandrasekhar method and a method based on an iterative solution of the Schwarzschild-Milne integral equations

$$J(t,\mu) = e^{-t/\mu} + \Psi(\mu)\int_0^t J(x,\mu)E_1(|x-t|)dx, \tag{10}$$

where

$$E_1(x) = \int_0^1 e^{-x/t}\frac{dt}{t}, \tag{11}$$

the X and Y functions being obtained from

$$X(\mu) = J(0,\mu) \text{ and } Y(\mu) = J(\tau,\mu). \tag{12}$$

The procedure was to correct the X and Y functions obtained from solutions to Eq. (10) at small values of μ only, where they are least accurate, using the Chandrasekhar method which is accurate in this region. The equations were also linearized by solving for the corrections to the approximations rather than the approximations themselves. Mayers has presented tables of the X and Y functions for the characteristic function Eq. (4) with $\omega_0 = 0.8$ and $\tau = 2.5$, $\omega_0 = 0.9$ and $\tau = 2$ and 4, and $\omega_0 = 0.95$ and $\tau = 2,4$, and 10. The technique used is considerably complicated and becomes more so when extended to take account of characteristic functions other than that pertaining to isotropic scattering.

In order to avoid the singularities, a noniterative method of solution was devised by Caldwell.[5] In this method values of the X and Y functions were obtained by solving a set of coupled integrodifferential equations and using Lobatto quadrature. The singularity was removed by using the properties of the X and Y functions. This method was used to obtain solutions for the X and Y functions for albedo $\omega_0 = 1$ and values of the optical thickness $\tau = 0.5(0.5)4.5$. The solutions obtained satisfied, to four significant figures, the analytical criterion given by Eqs. (8) and (9).

The accuracy of this method is limited due to the fact that in the region of $\tau = 0$, Y changes extremely rapidly since $Y(\mu,0)$ is discontinuous at $\tau = 0$, jumping from 0 to 1 as μ increases from 0. In practice, this can be partly overcome by using a very small interval ($\Delta\tau \sim 0.0001$) in the numerical integration procedure in the region of $\tau = 0$. The use of this small $\Delta\tau$ leads to one of the disadvantages of this noniterative method. A comparison of the speed of calculation obtained by counting the number of arithmetic operations involved in obtaining a given τ shows that this noniterative method is slower than the iterative methods.

III. ITERATIVE APPROACH USING IMPROVED TRIAL FUNCTIONS

In an attempt to overcome the difficulty in obtaining accurate solutions for $X(\mu)$ and $Y(\mu)$ for values of μ close to 1, a small parameter ϵ is introduced into Eq. (2). This means that we consider the equation

$$Y(\mu) = \lim_{\epsilon \to 0}\{e^{-\tau/\mu} + \mu\Psi(\mu)\int_0^{1-\epsilon}\{X(\mu')Y(\mu) - Y(\mu')X(\mu)\}\frac{d\mu'}{(\mu-\mu')}\}, \tag{13}$$

and solve for different small values of ϵ and then extrapolate to the limit $\epsilon = 0$. This work is carried out by taking better 'trial' functions $X_0(\mu)$ and $Y_0(\mu)$ in the iterative scheme defined by Eqs. (5) and (6). In this way reasonably accurate values of $X(\mu)$ and $Y(\mu)$ are obtained after only two iterations even for the most difficult case $\mu = 1$.

Since $X(\mu) \to 1$ and $Y(\mu) \to e^{-\tau/\mu}$ as $\tau \to 0$, we perform one step of the iteration given by Eqs. (5) and (6) by taking the initial approximation Eq. (7).

For the $\Psi(\mu) = \frac{1}{2}\omega_0$ case, this gives

$$X_1(\mu) = 1 + \frac{\mu\omega_0}{2}\int_0^1 \times\left[1 - \exp\left\{-\tau\left(\frac{1}{\mu} + \frac{1}{\mu'}\right)\right\}\right]\frac{d\mu'}{(\mu+\mu')}, \tag{14}$$

$$Y_1(\mu) = e^{-\tau/\mu} + \frac{\mu\omega_0}{2}\int_0^1 (e^{-\tau/\mu} - e^{-\tau/\mu'})\frac{d\mu'}{(\mu-\mu')}. \tag{15}$$

The analytical solution is

$$X_1(\mu) = 1 + \frac{\mu\omega_0}{2}\left[\ln\left(\frac{\mu+1}{\mu}\right) - Ei\left\{-\frac{\tau(\mu+1)}{\mu}\right\} + e^{-\tau/\mu}Ei(-\tau)\right] \quad (0 \leqslant \mu \leqslant 1), \tag{16}$$

$$Y_1(\mu) = e^{-\tau/\mu} + \frac{\mu\omega_0}{2}\left[e^{-\tau/\mu}\ln\left(\frac{\mu}{1-\mu}\right) + e^{-\tau/\mu}Ei\left\{-\frac{\tau(\mu-1)}{\mu}\right\} - Ei(-\tau)\right](0\leqslant\mu<1), \quad (17)$$

and

$$Y_1(1) = e^{-\tau} + \frac{\omega_0}{2}\{e^{-\tau}(\gamma + \ln\tau) - Ei(-\tau)\}, \quad (18)$$

where $\gamma = 0.57721...$is Euler's constant and

$$Ei(x) = \int_{-\infty}^{x} \frac{e^t dt}{t}, \quad -\infty < x < +\infty. \quad (19)$$

From Eqs. (16)–(18) the values of $X_2(\mu)$ and $Y_2(\mu)$ can be calculated.

A computer program has been written to calculate $X_1(\mu)$ and $Y_1(\mu)$ using Eqs. (16)–(18) and then used to compute $X_2(1)$ and $Y_2(1)$ using Eq. (5) and

$$Y_2(1) = e^{-\tau} + \frac{\omega_0}{2}\lim_{\epsilon\to 0}\int_0^{1-\epsilon}\{Y_1(1)X_1(\mu') - X_1(1)Y_1(\mu')\}\frac{d\mu'}{(1-\mu')}. \quad (20)$$

The integral in Eq. (20) was evaluated using Simpson's rule (with a smaller interval near $\mu = 1$) for various small values of ϵ and then extrapolated to the limit $\epsilon = 0$. The extrapolation was carried out by taking $\epsilon_1 = 0.001$, 0.002, and 0.003 for $i = 1$, 2, and 3 respectively, and then extrapolating to the limit $\epsilon = 0$ by using

$$Y_i = Y + a\epsilon_i + b\epsilon_i^2, \quad (21)$$

where $Y_i = Y(\epsilon_i)$. This removes the difficulty of having to evaluate the integrand in Eq. (20) for $\mu' = 1$.

In an effort to improve the accuracy of the results improved trial functions for the X and Y functions are now used. This seems particularly necessary for large values of τ and ω_0, and hence a curve fitting procedure based on the previous results was used.

First of all, a linear fit of $X(\mu)$ of the form

$$X_2(\mu) = a_0 + a_1\mu, \quad (22)$$

and an exponential fit of $Y(\mu)$ of the form

$$Y_2(\mu) = Ae^{-\tau/\mu}, \quad (23)$$

were tried, where a_0, a_1, and A are unknown constants. The constant A was calculated using

$$A = e^{\tau}Y_2(1), \quad (24)$$

and a_0,a_1 were determined by using a least squares fit to $X_2(\mu)$ obtained by substituting Eqs. (12) and (13) into Eq. (5).

Secondly, we choose a quadratic fit of $X(\mu)$ of the form

$$X_2(\mu) = a_0 + a_1\mu + a_2\mu^2, \quad (25)$$

with the same exponential fit of $Y(\mu)$ given by Eq. (23). As before the constants a_0, a_1, and a_2 were determined by using a least squares fit to $X_2(\mu)$. The approximations in Eqs. (22), (23), and (25) are superior to those in Eq. (7), and are chosen with the intention of accelerating the convergence of the iterative process. Also this technique is preferable to the direct substitution of the numerical values of X_2 and Y_2 as it produces analytical expressions for X_3 and Y_3.

On substituting Eqs. (23) and (25) into Eqs. (5) and (6) and solving analytically, we have

$$X_3(\mu) = 1 + \frac{\mu\omega_0}{2}\left\{a_1 + \frac{a_2}{2} - a_2\mu + (a_0 - a_1\mu + a_2\mu^2)\ln\left(\frac{\mu+1}{\mu}\right)\right\}X_2(\mu) + \frac{\mu\omega_0 A^2}{2}\left\{e^{-\tau/\mu}Ei(-\tau) - Ei\left[\frac{-\tau(\mu+1)}{\mu}\right]\right\} \quad (0\leqslant\mu\leqslant 1), \quad (26)$$

$$Y_3(\mu) = e^{-\tau/\mu} + \frac{\mu\omega_0}{2}\left\{X_2(\mu)\ln\left(\frac{\mu}{1-\mu}\right) - a_1 - (\mu + \tfrac{1}{2})a_2\right\} \times Y_2(\mu) - \frac{\mu\omega_0 A}{2}\left\{Ei(-\tau) - e^{-\tau/\mu}Ei \times\left[\frac{-\tau(\mu-1)}{\mu}\right]\right\}X_2(\mu) \quad (0\leqslant\mu<1), \quad (27)$$

and

$$Y_3(1) = e^{-\tau} + \frac{\omega_0 A}{2}\left\{[e^{-\tau}(\gamma + \ln\tau) - Ei(-\tau)] \times X_2(1) - e^{-\tau}\left(a_1 + \frac{3a_2}{2}\right)\right\}. \quad (28)$$

The corresponding equations for the linear fit case can be obtained by putting $a_2 = 0$ in Eqs. (26) – (28). Also Eqs. (16) – (18) for the simple trial function case given by Eq. (7) are easily obtained by putting $a_0 = 1$, $a_1 = a_2 = 0$ and $A = 1$ in Eqs. (26)–(28). As explained earlier, $X_3(\mu)$ and $Y_3(\mu)$ are computed from Eqs. (26)–(28) and hence $X_4(1)$ and $Y_4(1)$ are obtained from Eqs. (5) and (20).

IV. RESULTS AND DISCUSSION

The iterative scheme described in the previous section has been used to obtain approximations to the X and Y func-

TABLE I. Values of X(1) for $\omega_0 = 0.1$ and $\tau = 0.05$, 0.1, 0.5, 1.0, 2.0.

		$X_0 = 1$, $Y = e^{-\tau/\mu}$		Straight line fit		Quadratic fit	
τ	Direct method	Anal.	Simp.	Anal.	Simp.	Anal.	Simp.
0.05	1.0085	1.0084	1.0093	1.0085	1.0093	1.0085	1.0093
0.1	1.0135	1.0133	1.0142	1.0135	1.0142	1.0135	1.0142
0.5	1.0298	1.0287	1.0301	1.0298	1.0301	1.0299	1.0301
1.0	1.0348	1.0331	1.0349	1.0347	1.0349	1.0348	1.0350
2.0	1.0366	1.0345	1.0365	1.0364	1.0366	1.0365	1.0366

TABLE II. Values of Y(1) for $\omega_0 = 0.1$ and $\tau = 0.05, 0.1, 0.5, 1.0, 2.0$.

τ	Direct method	$X_0 = 1$, $Y_0 = e^{-\tau/\mu}$		Straight line fit		Quadratic fit	
		Anal.	Simp.	Anal.	Simp.	Anal.	Simp.
0.05	0.9596	0.9596	0.9597	0.9595	0.9597	0.9599	0.9605
0.1	0.9181	0.9179	0.9181	0.9178	0.9181	0.9184	0.9192
0.5	0.6321	0.6310	0.6321	0.6320	0.6321	0.6326	0.6328
1.0	0.3909	0.3895	0.3909	0.3909	0.3910	0.3913	0.3911
2.0	0.1474	0.1464	0.1474	0.1475	0.1475	0.1476	0.1474

tions of Chandrasekhar. As only two iterations are involved, one of which is carried out analytically, the amount of computer time required is minimal. The results are presented for $\tau = 0.05, 0.1, 0.5, 1.0$, and 2.0 and $\omega_0 = 0.1$ in Tables I and II for the problem case $\mu = 1$ already mentioned.

In each table column 3 gives the results obtained by setting $X_0(\mu) = 1$, $Y_0(\mu) = e^{-\tau/\mu} (0 \leqslant \mu \leqslant 1)$ and X_1, Y_1 are calculated by using Eqs. (16) – (18), the case $\mu = \mu'$ being dealt with by using a limiting argument. Column 4 contains the results $X_2(1), Y_2(1)$ obtained by using these values $X_1(\mu), Y_1(\mu)$ in the iterative process. The integrals are evaluated by using Simpson's rule with interval $h = 0.02$ up to $\mu' = 0.98$ and smaller interval $h = 0.001$ for $0.98 < \mu' < 1$. Column 5 is obtained by, firstly, fitting a linear curve to $X_1(\mu)$ and a curve of the form $A e^{-\tau/\mu}$ to $Y_1(\mu)$ and, secondly, using these curves in the iterative process to give $X_3(\mu)$ and $Y_3(\mu)$ as analytical expressions in μ. Column 7 is obtained in the same way by using a quadratic curve to fit $X_1(\mu)$. Columns 6 and 8 are then obtained by using $X_3(\mu)$ and $Y_3(\mu)$ in the iterative process to yield $X_4(1)$ and $Y_4(1)$. Again the integrals are evaluated by using Simpson's rule with the awkward point $\mu' = \mu = 1$ being dealt with by using the extrapolation procedure.

As a check on the accuracy the results are compared with the accurate ones in column 2 obtained by Caldwell[5] by using a direct method as opposed to an iterative approach. We must also bear in mind that the results are tabulated for the worst possible case $\mu = 1$. They will be more accurate for other values of μ.

Clearly agreement is good particularly in columns 5 and 7. The accuracy decreases for higher values of ω_0 but is greatly improved for $X(\mu)$ values (i.e., columns 6 and 8) by using Simpson's rule in the additional iteration step. Numerical problems will still arise in connection with the singularity in Eq. (2) when $\mu = \mu' = 1$ and numerical instabilities increase for values of ω_0 close to unity. However, this method is useful in that it quickly provides good results in certain cases with minimal computing time. For these cases calculation up to X_4 and Y_4 is quite sufficient. Also the present method is equally valid for obtaining $X(\mu)$ and $Y(\mu)$ for larger values of τ. Questions still remain concerning the convergence of the solution if the iteration is continued beyond X_4 and Y_4.

Further difficulties might be expected in the solution of Eqs. (1) and (2) as there is no unique solution for the case $\Psi(\mu) = \frac{1}{2}\omega_0$. For a discussion of nonuniqueness and of the additional equations needed to specify the physical solution refer to Mullikin.[6,7] Also one possible approach to numerical computations, asymptotic formula (for large τ) and extensive numerical tables are all provided by Carlstedt and Mullikin.[8]

It has been observed many times since the initial work of Chandrasekhar and Elbert that iterative methods give good results even though the equations have a continuous family of solutions. Although this particular aspect has not been extensively dealt with in the literature one possible explanation is given by Mullikin.[9]

Mullikin points out that iterative methods, if computed with absolute precision, lead to the desired solution of Eqs. (1) and (2) for the case of isotropic scattering by reason of the analyticity. There are other solutions which are not analytic in ω_0 and in theory will not be reached by iterative methods as long as the initial functions in the iteration are not chosen to be one of these extraneous solutions. There are, however, extraneous solutions which are arbitrarily close to the desired solution. In these cases, when the iterations appear to converge, numerical errors introduce the influence of the extraneous solutions and cause oscillations. This means that, in theory, the iterative methods will converge to a unique solution but, in practice, the presence of extraneous solutions arbitrarily near the limit will introduce instability into the calculations. This instability can be avoided in treating the X and Y equations by using extreme accuracy. Clearly there will be a limit to the accuracy which can be achieved for large values of τ, at least in the conservative and near-conservative cases.

It should be pointed out that further improvement in the accuracy of this method could be expected by using

$$X_{n+1}(\mu) = 1 + \frac{\mu\omega_0}{2} \int_0^1 \{X_n(\mu)X_n(\mu') - Y_n(\mu)Y_n(\mu')\} \frac{d\mu'}{(\mu + \mu')}, \tag{29}$$

$$Y_{n+1}(\mu) = e^{-\tau/\mu} + \frac{\mu\omega_0}{2} \int_0^1 \{X_{n+1}(\mu')Y_n(\mu) - X_{n+1}(\mu)Y_n(\mu')\} \frac{d\mu'}{(\mu - \mu')}, \tag{30}$$

since the latter should accelerate convergence in the awkward cases $\tau = 0.5$ and 1 ($\omega_0 \sim 1$). Also when calculating $X_{n+1}(\mu_r)$, say, from Eq. (29) it would be advantageous not to use $X_n(\mu)$ over the complete range $0 \leqslant \mu \leqslant 1$, but instead to use $X_{n+1}(\mu_i)$ for $i = 0,1,2,\ldots,r-1$ and $X_n(\mu_i)$ for $i = r, r+1,\ldots,m$. The same thing applies in the calculation of $Y_{n+1}(\mu_r)$.

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