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ON THE USE OF VARIABLE EDDINGTON FACTORS IN NON-LTE STELLAR ATMOSPHERES COMPUTATIONS

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SUMMARY

It is shown that by use of variable Eddington factors, the accuracy of difference-equation solutions of transfer problems may be greatly improved with only small additional computational effort. It is found that a direct iterative calculation of the Eddington factors leads to a strongly convergent procedure. The resulting set of equations is of wide applicability to problems involving non-coherent radiative transfer. The method is illustrated by application to the classical grey problem, and to a non-LTE stellar atmospheres computation.

1. INTRODUCTION

There now exist a wide variety of possible techniques for the solution of transfer equations; among these the difference-equation approach is one of the most general and most flexible. The particular class of transfer problems where the difference-equation technique has proven to be most valuable is that where the source function involves coupling from frequency to frequency in the radiation field, that is, in any *non-coherent* transfer problem.

The primary drawback to this method is that in order to achieve accuracy in the angular distribution of the radiation field, it is, unfortunately, necessary to include explicitly a large number of angular quadrature points. This results in a technical problem, in that the computation then becomes very time-consuming, since the basic matrix operations required in the difference-equation approach scale as the cube of the number of quadrature points. In the past, it has been necessary, in practice, to employ low-order quadrature formulae using perhaps one or, at most, two angle points. This obviously restricts the accuracy of the solution.

Recently, difference-equations have been employed extensively in model atmospheres calculations. For example, in recent papers (**1**–**4**) we have developed effective methods for calculating model stellar atmospheres subject to the constraints of hydrostatic, radiative, and steady-state statistical equilibrium, including bound–bound transitions. We have shown (**2**) that by a complete linearization of all equations, including constraints, one obtains an extremely stable, efficient, and strongly-convergent scheme that allows fully for the global properties of the solution, and is capable of treating complicated non-LTE models successfully (**3**), (**4**). An essential part of the method is the use of difference-equations. For the reasons mentioned above, our exploratory work has, thus far, employed the Eddington approximation. In the present paper we wish to show that this approximation can economically be removed, and that the difference-equation approach can be significantly improved in a simple and elegant way.

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2. METHOD

Feautrier (5) has suggested that the transfer equation be written as a system of second-order equations:

$$\mu_i^2 \frac{\partial^2 P_i}{\partial \tau_i^2} = P_i - S_i, \quad (i = 1, \ldots, n_\nu n_\mu) \tag{1}$$

where n_μ is the number of angle-quadrature points and n_ν is the number of frequency-quadrature points. These equations are subject to the boundary conditions

$$\mu_i \frac{\partial P_i}{\partial \tau_i} = P_i(0) - I_i^- \tag{2}$$

at $\tau = 0$, and

$$\mu_i \frac{\partial P_i}{\partial \tau_i} = I_i^+ - P_i \tag{3}$$

at the lower boundary $\tau = \tau_{\max}$. In the above equations, the subscript i denotes a specific choice of frequency *and* angle, and

$$P_i \equiv \tfrac{1}{2}[I(\tau, \mu_i, \nu_i) + I(\tau, -\mu_i, \nu_i)]. \tag{4}$$

In equations (2) and (3), I_i^+ and I_i^- are the incident intensities at the lower and upper boundaries respectively, and in all equations the continuous variables μ and ν are discretized. In general, the physical form of the source function S will imply coupling among all $n_\mu \times n_\nu$ equations.

To solve the resulting set of differential equations, one replaces them by difference equations, and solves for P_i at a discrete set of depth-points. There are a large number of advantages to this formulation: (1) The difference equations are extremely flexible, in that they are written in terms of *local* quantities (in contrast to the integral equations). (2) The second-order form is almost ten times faster to solve than the equivalent first-order form (because the size of the system is reduced by factor of two). (3) The difference equations themselves are tridiagonal in form, diagonally dominated, extremely stable, and can be solved by a simple recursive algorithm requiring a minimum of core storage. (4) Our experience has shown that the multi-scale problem causes no difficulty and that exponentially increasing depth-steps may be chosen. (5) The computing time increases only linearly with the number of depth points while the accuracy increases quadratically.

The basic disadvantage of the method is caused by the fundamental three-dimensionality of the problem (depth, frequency, angle), which necessitates the explicit introduction of angle-quadrature points. The computing time, consequently scales as n_μ^3 for this method; in the integral equation approach, the angular integration is automatically exact, and the problem is only two-dimensional.

The model atmospheres computer code, which we have mentioned above, depends heavily on the flexibility of the difference equation approach. Indeed, we have found that it is literally the only practical way to compute complex non-LTE model atmospheres problems. Yet, faced with the fact that the physical nature of the problem requires a *large* number of frequency-points ($n_\nu \approx 100$), and given a finite computer capability, we have been constrained, in order to make a survey of non-LTE effects, to restrict ourselves to a single angle-point ($\mu = 1/\sqrt{3}$), which is equivalent to use of the Eddington approximation. That this is in fact an astute first choice will be justified below. Nevertheless, it was clear from the beginning that it would be highly desirable to have some method of improving the angular accuracy of the difference-equation scheme without paying the prohibitive price of simply increasing the number of angle-points.

In view of the above considerations, it is both fortunate and noteworthy that it is possible to derive a set of equations that: (a) retain all of the desirable features of equation (1), but (b) treat the angular quadratures as accurately as integral equations, and at the same time (c) are no more difficult to solve than equation (1) is in the case of a single angle-point.

To derive the desired system we start with the first-order moment equations

$$\frac{\partial H_i}{\partial \tau_i} = J_i - S_i \tag{5a}$$

and

$$\frac{\partial K_i}{\partial \tau_i} = H_i. \tag{5b}$$

In writing the above equations we have assumed that both absorption and emission processes are isotropic (which is the usual situation in stellar atmospheres work). We can close this system by introducing a frequency and depth-dependent *variable Eddington factor*, defined by

$$K_i(\tau) = f_K(\tau) J_i(\tau). \tag{6}$$

At the boundaries we may also introduce

$$H_i = f_H J_i \tag{7}$$

With these definitions we are led to the second-order system

$$\frac{\partial^2 (f_K J_i)}{\partial {\tau_i}^2} = J_i - S_i \tag{8}$$

with boundary conditions

$$\frac{\partial (f_K J_i)}{\partial \tau_i} = f_H J_i. \tag{9}$$

At depth, an alternative boundary condition is to assume the asymptotic validity of the Eddington approximation ($f_K \equiv \frac{1}{3}$). Note that equation (8) is of *precisely the same form as equation* (1) and correspondingly may be replaced, in exactly the same manner, by a set of difference equations. The resulting system is no more difficult to solve than equation (1), yet if correct values of f_K and f_H are used, the equations are *exact* (aside from errors introduced by the depth- and frequency-discretizations). In fact, anywhere that equations (1) may be used, equation (8) may be substituted with a corresponding increase in accuracy and efficiency.

The main thrust of this paper is to show that the Eddington factors f_K and f_H may be evaluated by a straightforward iteration scheme, even in the most complex situations involving non-coherent scattering or non-LTE effects. It has been pointed out to us that Feautrier actually suggested such an approach (9), but he has not, to our knowledge, carried out detailed calculations. The procedure is as follows: (1) Using an estimate for f_K and f_H (a good initial guess is the Eddington approximation $f_H = \frac{1}{3}$, $f_H = 1/\sqrt{3}$) solve equation (8). (2) With the values of J_i so derived, re-evaluate the (in general) frequency-dependent source-function S_i. (3) Given the source function S_i, solve for the angular distribution of the radiation field *frequency by frequency* with a high-order angle-quadrature. The time required for such a solution is negligible compared to the solution of the coupled set of equations (8), and (4) With this solution, re-evaluate the Eddington factors f_K and f_H directly from their definitions in terms of the radiation field. The important point to realize here is that even if J and K are themselves only moderately well determined, the Eddington factors can have a much higher order of accuracy because they are *ratios* of these quantities. While this in itself does not *guarantee* higher-order accuracy, calculations for test problems with known exact solutions have verified that the expected high accuracy is in fact obtained. The above procedure is then iterated.

Experience has shown that in two or three iterations f_K is already determined to roughly four decimal places. This is usually as accurate as allowed by the discretizations and is probably more accurate than the physical theory in many cases. Of course, a solution of the same accuracy could have been obtained by using equation (1) with an equivalent number of angle points as employed in step three above. But such a solution would have required a factor of roughly n_μ^3 times as much computation and n_μ^2 times as much storage as the variable Eddington factor method. Before passing on to a discussion of specific examples, we should mentioned that somewhat similar ideas have been used in neutron transport and radiation-hydrodynamics calculations (6), (7). However, those applications use first-order equations and an *approximate a priori definition* of f_K in terms of an interpolation formula. In contrast, the present work uses second-order equations and actually evaluates f_K consistently with the radiation field.

3. TEST WITH A GREY ATMOSPHERE

One of the key points we must prove is that the method described above is in no sense a Λ-iteration. A simple and convincing demonstration is to consider the classical grey atmosphere problem. In this case the equations become

$$\frac{d^2(f_K J)}{d\tau^2} = 0 \tag{10}$$

with

$$\frac{d(f_K J)}{d\tau} = f_H J \tag{11}$$

and $\tau = 0$ and

$$\frac{d(f_K J)}{d\tau} = H \tag{12}$$

at $\tau = \tau_{\max}$. Table Ia lists the solutions obtained for $q(\tau) \equiv [(J/3H) - \tau]$ and Table Ib lists f_K, for six iterations, using 2- and 3-angle quadratures, starting from: $f_K = \frac{1}{3}$, $f_H = 1/\sqrt{3}$, and $q(\tau) \equiv 1/\sqrt{3}$. We note that *rapid*, *global* convergence is obtained. In particular, the convergence of q at $\tau = 10$, shows that the solution is

TABLE Ia

Values of $q(\tau)$ and maximum flux errors obtained using variable Eddington factors

	Exact Solution	2-point quadrature 1	2	3	4	5	6	3-point quadrature 1	2	3	4	5	6
0	0·57735	0·57756	0·57756	0·57756	0·57756	0·57756	0·57756	0·57756	0·57756	0·57756	0·57756	0·57756	0·57756
0·01	0·58824	0·58212	0·58213	0·58214	0·58214	0·58214	0·58214	0·58403	0·58401	0·58401	0·58401	0·58402	0·58402
0·10	0·62792	0·61550	0·61678	0·61690	0·61692	0·61692	0·61692	0·62434	0·62614	0·62628	0·62630	0·62630	0·62630
1·0	0·69854	0·69696	0·70570	0·70690	0·70711	0·70715	0·70716	0·69066	0·69732	0·69805	0·69815	0·69817	0·69817
10·0	0·71045	0·71122	0·71122	0·71122	0·71122	0·71122	0·71122	0·71122	0·71056	0·71047	0·71046	0·71046	0·71046
$\|\Delta H/H\|$	0	$5·61\times10^{-3}$	$7·41\times10^{-4}$	$1·20\times10^{-4}$	$3·09\times10^{-5}$	$6·7\times10^{-6}$	$1·4\times10^{-6}$	$4·81\times10^{-3}$	$5·76\times10^{-4}$	$9·49\times10^{-5}$	$1·94\times10^{-5}$	$4·0\times10^{-6}$	8×10^{-7}

TABLE Ib

Eddington factors f_K

τ	Exact solution	2-point quadrature 1	2	3	4	5	6	3-point quadrature 1	2	3	4	5	6
0	0·41018	0·41047	0·41047	0·41047	0·41047	0·41047	0·41047	0·41047	0·41009	0·41004	0·41003	0·41003	0·41003
0·01	0·40143	0·40601	0·40600	0·40600	0·40600	0·40600	0·40600	0·40471	0·40434	0·40430	0·40429	0·40429	0·40429
0·10	0·37113	0·37793	0·37725	0·37719	0·37718	0·37718	0·37718	0·37332	0·37208	0·37197	0·37196	0·37196	0·37196
1·0	0·33567	0·33613	0·33441	0·33418	0·33413	0·33413	0·33412	0·33738	0·33593	0·33577	0·33575	0·33575	0·33575
10·0	0·33333	0·33333	0·33333	0·33333	0·33333	0·33333	0·33333	0·33333	0·33333	0·33333	0·33333	0·33333	0·33333

not a Λ-iteration. We see that little improvement is obtained after two iterations, and, in fact, the remaining small changes are really only formal because the accuracy of the solution is already as good as the discretization in depth allows (1). A more accurate solution can, of course, be obtained by using a finer depth-discretization. Ignoring this question, the *mathematical* consistency of the system is shown by the maximum flux errors listed in the last row of Table Ia; after nine iterations the computed and nominal fluxes agreed to *at least* nine places. Inspection of Table I shows that the three-point formula clearly gives superior results, but higher-order formulae will give improved results only up to a certain point, where errors in depth-discretization again dominate (1). In any case, it is important to realize that the iterated variable-Eddington-factor equations converge to *exactly* the same values as obtained from a direct solution of equation (1) using the angle-quadratures and depth steps.

4. TEST WITH NON-GREY AND NON-LTE ATMOSPHERES

From the standpoint of stellar atmospheres computations, the importance of the above development is that the form of equation (8) is identical to that used in our linearization procedure, (2), and hence can be linearized in precisely the same way as before. Unfortunately the linearization of f_K and f_H is extremely difficult; in fact it is equivalent to linearizing the integral equations. The model atmospheres code (2) has therefore been modified to use variable Eddington factors, *ignoring* linearization of f_K and f_H which are computed *iteratively*. This of course is not a disadvantage since iteration is required in any case to satisfy the constraints of radiative, hydrostatic, and statistical equilibrium. The price that must be paid in this approach is that the solution is no longer *strictly* first-order consistent at each stage of the calculation, and rigorous quadratic convergence is, therefore, sacrificed. As we shall see below, however, one still obtains at least order-of-magnitude convergence on each iteration, and, in fact, convergence often approaches quadratic.

Given this new method, it is natural to examine the accuracy of the Eddington approximation employed in our previous work. To this end we have recomputed the 35 000 °K model described in an earlier paper (4) now using variable Eddington factors. Because we may now expect to obtain mathematically accurate models, it was deemed worthwhile to upgrade our previously schematic opacity calculations. In particular, we now include the full temperature and frequency variation of the free–free Gaunt factors, have allowed for Gaunt factors in the He II cross-sections, and have allowed six discrete levels of He II instead of four in order to improve the accuracy of the computed continuum jumps.

Properties of LTE and non-LTE pure-continuum models are listed in Table II, using Eddington factors computed with 1, 2, and 3 angle-points. The solutions were started from the old models, assuming $f_K = \frac{1}{3}$, and $f_H = 1/\sqrt{3}$ in the first iteration, and then re-computing the Eddington factors after each linearization-correction. The one-point Eddington factors are exactly equivalent to the assumption $f_K \equiv \frac{1}{3}$, and these models differ from our previously reported results only because of changes in the opacities now used. In the 2- and 3-point models we see clearly changes brought about by using accurate Eddington factors. As might be expected, the effects are largest in the far ultra-violet since small temperature changes result in large changes in source terms when $h\nu/kT \gg 1$. Also, as might be expected, the Eddington factors depart most strongly from their limiting values at transparent

TABLE II

Properties of models using variable Eddington factors

$T_{eff} = 35\,000\,°K$, $\log g = 4$

Number of angles	LTE 1	LTE 2	LTE 3	NLTE 1	NLTE 2	NLTE 3
T_0	24819	25839	25821	26762	27260	27238
T_{min}				25762	26445	26453
ΔT				1000	815	785
D_L	1·922	1·610	1·613	1·569	1·426	1·433
D_B	0·103	0·083	0·083	0·164	0·150	0·148
D_P	0·020	0·017	0·017	0·030	0·031	0·030
D(He I)	2·265	2·023	2·009	0·803	0·523	0·529
D(He II)	9·542	10·514	10·523	13·543	14·026	14·033
R_{1K}(H)	$2·10 \times 10^6$	$2·87 \times 10^6$	$2·86 \times 10^6$	$2·75 \times 10^6$	$3·23 \times 10^6$	$3·22 \times 10^6$
R_{1K}(He I)	$4·93 \times 10^4$	$1·17 \times 10^5$	$1·17 \times 10^5$	$2·34 \times 10^5$	$4·75 \times 10^5$	$4·67 \times 10^5$
R_{1K}(He II)	$4·07 \times 10^{-2}$	$1·12 \times 10^{-1}$	$1·10 \times 10^{-1}$	$4·88 \times 10^{-3}$	$8·13 \times 10^{-3}$	$7·99 \times 10^{-3}$

wavelengths with large gradients; for example, at the long-wavelength side of the He II edge, f_H reaches a value of 0·805 and f_K rises to 0·681.

Fig. 1 shows a comparison of the one-point and three-point LTE models with an LTE flux-distribution interpolated from models (**8**) obtained using the exact exponential-integral functions in the solution of the transfer equation; the agreement

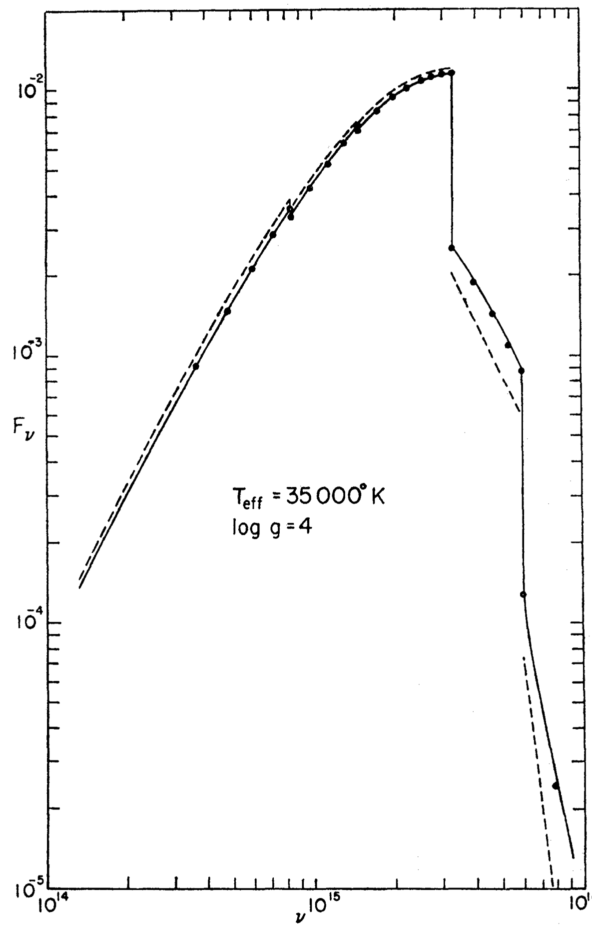

FIG. 1. *Comparison of Eddington-factor and integral-equation calculations for an LTE model atmosphere with* T_{eff} = 35 000 °K, log *g* = 4. *Solid curve: solution with variable Eddington factors evaluated with three angle-points; dotted curve: solution with one angle-point (standard non-variable Eddington approximation); heavy dots: integral-equation solution interpolated from reference* (**8**).

is excellent. The interpolated values of the Balmer jump (0·084 mag) and Paschen jump (0·017 mag) are also in remarkably good agreement with the present computation. Considering the complete independence of the computational techniques, this comparison provides a strong verification of the accuracy of the variable Eddington factor approach. It would be even more interesting to compare non-LTE models, but unfortunately an adequate grid of non-LTE models obtained using the exact integral equations does not exist. Although substantial differences exist between the absolute values of some of the properties of the one-point and three-point models (e.g. in photoionization rates), Table III shows that when a *differential* comparison is made between LTE and non-LTE models, even the one-point models yield good results. In particular, the non-LTE change in the Balmer jump found earlier (of great importance if D_B is used to estimate T_{eff} for O-stars) is verified by the present

TABLE III

Differential comparison of LTE and Non-LTE Models

Number of Angles	1	2	3
$D_L - D_L^\star$	−0·353	−0·184	−0·180
$D_B - D_B^\star$	+0·061	+0·067	+0·065
$D_P - D_P^\star$	+0·010	+0·014	+0·013
D(He I) − $D^\star$(He I)	−1·462	−1·500	−1·480
D(He II) − $D^\star$(He II)	+4·001	+3·512	+3·510
R_{1K}(H)/$R_{1K}^\star$(H)	1·309	1·128	1·125
R_{1K}(He I)/$R_{1K}^\star$(He I)	4·746	4·059	3·991
R_{1K}(He II)/$R_{1K}^\star$(He II)	0·120	0·073	0·073

Note: Starred quantities denote LTE values, unstarred denote non-LTE values.

more accurate results. Thus the procedure suggested in our earlier work (3), (4) of applying differential corrections derived from approximate LTE and non-LTE models to the best available LTE models is actually found to be better than adopting absolute rates as computed from the approximate models themselves. In the future, however, this will no longer be necessary since it is now possible to obtain very accurate results using variable Eddington factors.

Analysis of the convergence properties of these computations shows that in general the quadratic nature of the convergence has been sacrificed, as anticipated. However, one still obtains a factor of 5 to 10 improvement in each iteration step; thus instead of 5 or 6 iterations per model, one must now perform perhaps 6 to 8 iterations to attain fractional errors or, say, 10^{-6} to 10^{-7} in all quantities throughout the atmosphere. Thus at an increase of about 30 per cent in the computing time one may obtain models that would have required 27 times as much computation by use of the direct method! This enormous saving implies that the difference-equation solution of the transfer equation becomes competitive with integral-equation methods both in speed *and* in accuracy. With the additional *large* benefits offered by complete linearization, the difference-equation method appears to have substantial advantages. Linearization of the integral equations is, to be sure, possible in principle, but extremely complex because one must allow for the effects of non-local changes of the optical depth scale upon the kernel functions of the integral operators.

4. CONCLUSIONS

By use of variable Eddington factors, the accuracy of difference-equation solutions may be greatly improved with only small additional expense and effort. We have shown that direct iterative evaluation of the Eddington factors is a strongly convergent procedure. A particularly important application of this method is the incorporation of variable Eddington factors into the linearization scheme previously developed, which results in an accurate, stable, and strongly convergent method of computing stellar atmospheres. This method offers very substantial advantages in non-LTE computations. The quadratic convergence characteristic of the complete linearizaton method itself is partially sacrificed, but tests show that at least order-of-magnitude improvement is still obtained from iteration to iteration. It is thus now possible to obtain models of hitherto unachievably high quality both in physical consistency and in mathematical accuracy, at a reasonable cost. Future work will be directed towards producing models that apply to individual stars for which there exist high-quality observational data, with the goal of performing a complete non-LTE spectroscopic analysis of these objects.

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