

On the Fundamental Solution of the Radiative Transfer Equation

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This paper outlines the general solution of the one-dimensional, azimuthally averaged radiative transfer equation in terms of a matrix exponential. The link between this fundamental solution and those more commonly used in radiative transfer is established. The formulation is developed for a general vertically inhomogeneous atmosphere with sources. Several new concepts, based on properties of the matrix exponentials, are described in the context of radiative transfer, including the use of the commutator and product integrals. It is also demonstrated how the matrix exponential formulation provides for new insights, not only into improvements of the numerical efficiency and stability of the solution, but also into the understanding of radiative transfer through a layered atmosphere. The various concepts introduced in this paper are illustrated throughout by the two-stream simplification of the general radiative transfer equation.

1. INTRODUCTION

The transfer of solar and infrared radiation through the terrestrial atmosphere is one of a class of transport phenomena that are important to many studies in the engineering and physical sciences (e.g., see *Duderstadt and Martin* [1979] for a general review). Radiative transport theory, which began in its present form with the work of Schuster in 1905, has been widely used in many diverse problems, such as in the calculation of the radiative energy budgets of stars, planetary atmospheres, crops, cattle, and sheep; in atmospheric and underwater visibility studies; in the determination of the reflecting properties of snow, ice sheets, paint surfaces, photo emulsions, and of blood tissues and viruses; in the estimation of the insulating properties of fiberglass materials; and in the research on the thermal structures of blast furnaces and other high-temperature machinery, among several others. The interested reader is referred to the *Journal of Quantitative Spectroscopy and Radiative Transfer*, 36 (1), 1986, for examples of many different applications of radiative transfer.

Because of the diversity of topics that use radiative transfer theory, a wide range of solution methodologies of the radiative transfer equation (RTE) can be found in the literature (as exemplified in the monograph of *Lenoble* [1985] and in the review article of *Stamnes* [1986]). While there seems to be an abundance of different methods of solution, most start by replacing the continuous dependence of radiation intensity on direction by a discrete set of directions. The discretized transfer equations then take the form of a coupled system of first-order differential equations. An analogous set of coupled equations also results when the spatial Fourier transform method is employed on the full three-dimensional transfer equation [e.g., *Stephens*, 1986, 1988]. As it turns out, such systems can be represented in a classical mathematical way in terms of a matrix-exponential operation, in which the array of coupling coefficients appears in the exponent. This procedure has been applied to various problems in a limited way; notably in studies involving electromagnetic wave propagation [*Keller*, 1960], in seismology [*Fryer and Frazer*, 1984], and in radiative transfer [*Water-*

man, 1981]. Even though many methods exist for solving the radiative transfer equation, there is still a need to develop more efficient numerical techniques. This need is particularly apparent in those studies of radiative transfer set on two- and three-dimensional geometries [e.g., *Stephens*, 1988]. The object of this paper is to formulate the solution of the radiative transfer equation in terms of the matrix exponential and to demonstrate the link between this fundamental solution and those more commonly encountered in radiative transfer literature. This formulation is developed for a general vertically inhomogeneous atmosphere with sources. Several concepts, such as the commutator and commutator identities, product integral, extinction transformation, and two-point boundary value problems, are introduced in this paper and are relatively new to the context of radiative transfer but are actively used in other physical disciplines.

The formulation described in this paper presents the framework for the unification of the many different existing methods of solution and not only provides new insights into the possible improvements in numerical efficiency and stability, but also provides important new insight into radiative transfer through a vertically inhomogeneous atmosphere. Examples can be found in the discussion of small τ solutions, the discussion of stability, and the discussion of the commutator. These aspects, to our knowledge, are new to radiative transfer and warrant even further consideration than is given here. The formulations described in this paper use the two-stream representation of the RTE throughout to illustrate the different concepts introduced. As such, the examples provide new and meaningful insight on the mathematical structure of the two-stream model.

The outline of the paper is as follows. Section 2 briefly introduces the radiative transfer equation in its matrix form. The fundamental solution of this matrix equation is then represented in terms of the propagator function and the boundary conditions. Section 3 describes methods for evaluating the matrix exponential $\exp(A\tau)$ particularly for small τ . The interaction principle and the extinction operator are introduced in section 4, and the connection between the extinction operator and the Riccati equations is demonstrated. Section 5 describes the eigenvector method for evaluating $\exp(A\tau)$ in terms of similarity transformations and demonstrates that the use of a Riccati transform is, in fact, a similarity transformation. The solution for a vertically inhomogeneous atmosphere is presented in section 6, in which

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adding, doubling, initialization, stability, and the commutator are discussed. Examples of the latter two concepts are presented in the context of a two-stream model.

2. BASIC CONCEPTS

It will be supposed throughout this paper that the absorbing-scattering medium is horizontally homogeneous. The radiative transfer equation describing the transfer of monochromatic radiation through such a medium is then

$$\mu \frac{dI(\tau, \mu, \phi)}{d\tau} = I(\tau, \mu, \phi) - \frac{\tilde{\omega}_0}{4\pi} \int_0^{2\pi} \int_{-1}^1 p(\tau, \mu, \phi; \mu', \phi') \cdot I(\tau, \mu', \phi') d\mu' d\phi' + S(\tau, \mu, \phi) \quad (1)$$

where $I(\tau, \mu, \phi)$ is the specific intensity at level τ along the direction represented by the angle pair μ, ϕ , and where τ is the optical depth, ϕ the azimuth angle, and μ the cosine of the polar angle, and the wavelength dependence on all variables is taken to be understood.

We consider, for convenience, that the intensity is azimuthally independent, in which case (1) simplifies to

$$\mu \frac{dI(\tau, \mu)}{d\tau} = I(\tau, \mu) - \frac{\tilde{\omega}_0}{2} \int_{-1}^{+1} p(\tau, \mu, \mu') \cdot I(\tau, \mu') d\mu' + S(\tau, \mu) \quad (2)$$

where I , p , and S are now taken to be azimuthally averaged quantities.

Discretization of RTE

Consider the medium as shown in Figure 1 and represent the continuous intensity field as a set of $2n$ discrete directions (as shown). If we choose these directions according to some quadrature scheme, then the integral (i.e., path radiance term of equation (2)) becomes

$$\int_{-1}^{+1} p(\tau, \mu, \mu') I(\tau, \mu') d\mu' \approx \sum_{i=1}^n w_i p(\tau, \mu, \mu_i) I(\tau, \mu_i) + \sum_{i=1}^n w_i p(\tau, \mu, -\mu_i) I(\tau, -\mu_i) \quad (3)$$

With the definition of the n -dimensional specific intensity vector $\mathbf{I}$ as (a similar definition applies for source vector $\mathbf{S}$)

$$\mathbf{I}_d = \begin{bmatrix} I(\tau, -\mu_1) \\ I(\tau, -\mu_2) \\ \vdots \\ I(\tau, -\mu_n) \end{bmatrix} \quad \mathbf{I}_u = \begin{bmatrix} I(\tau, +\mu_1) \\ I(\tau, +\mu_2) \\ \vdots \\ I(\tau, +\mu_n) \end{bmatrix} \quad (4)$$

and with the definition of the following matrices

$$\mathbf{m} = \mu_i \delta_{ij}, \quad \mathbf{w} = w_i \delta_{ij}, \quad \mathbf{p}_b = \frac{\tilde{\omega}_0}{2} p(-\mu_i, \mu_j) \\ \mathbf{p}_f = \frac{\tilde{\omega}_0}{2} p(\mu_i, \mu_j) \quad i, j, = 1, \dots, n \quad (5)$$

the discretized, matrix form of (2) becomes

$$-\mathbf{m} \frac{d\mathbf{I}_d}{d\tau} = \mathbf{I}_d - \mathbf{p}_f \mathbf{w} \mathbf{I}_d - \mathbf{p}_b \mathbf{w} \mathbf{I}_u + \mathbf{S}_d \quad (6)$$

$$\mathbf{m} \frac{d\mathbf{I}_u}{d\tau} = \mathbf{I}_u - \mathbf{p}_b \mathbf{w} \mathbf{I}_d - \mathbf{p}_f \mathbf{w} \mathbf{I}_u + \mathbf{S}_u \quad (7)$$

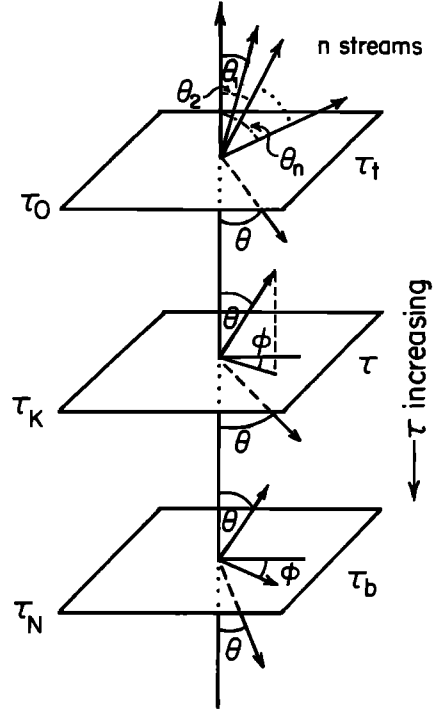


Fig. 1. Schematic representation of the radiation flow and discretization of the medium. The convention used for the optical depth scale to the left is for the layered medium, while the τ convention to the right applies to the continuous case.

where we use the convection $\mathbf{p}_b$ and $\mathbf{p}_f$ for the symmetric phase matrices associated with back and forward scattering, respectively. Subscripts d and u refer to the sense of the flow in the downward and upward directions, respectively. Equations (6) and (7) can be more succinctly written as

$$\frac{d\mathbf{I}}{d\tau} = \mathbf{A} \mathbf{I} + \mathbf{S} \quad (8)$$

where now the $2n \times 2n$ matrix $\mathbf{A}$ is composed of the $n \times n$ matrices $\mathbf{a}_1$ and $\mathbf{a}_2$

$$\mathbf{A} = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 \\ -\mathbf{a}_2 & -\mathbf{a}_1 \end{bmatrix} \quad (9)$$

which are defined by

$$\mathbf{a}_1 = \mathbf{m}^{-1} \mathbf{p}_u \mathbf{w} - \mathbf{m}^{-1} \quad (10)$$

$$\mathbf{a}_2 = \mathbf{m}^{-1} \mathbf{p}_d \mathbf{w} \quad (11)$$

and

$$\mathbf{I} = \begin{bmatrix} \mathbf{I}_d \\ \mathbf{I}_u \end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix} \mathbf{S}_d \\ \mathbf{S}_u \end{bmatrix} \quad (12)$$

The matrices $\mathbf{a}_1$ and $\mathbf{a}_2$ depend on local optical properties of the atmosphere (such as the single scattering albedo $\tilde{\omega}_0$ and the asymmetry parameter g). Since we use two-stream models as a means of illustrating various of the concepts introduced throughout this paper, we now present the appropriate form of these coefficients for the Eddington approximation. From Meador and Weaver [1980], for example, it readily follows

$$\mathbf{a}_1 = -\frac{1}{4} [7 - \tilde{\omega}_0 (4 + 3g)] \quad (13)$$

$$a_2 = -\frac{1}{4}[1 - \tilde{\omega}_0(4 - 3g)] \quad (14)$$

where a_1 and a_2 are now scalar quantities (note also that the two-stream version of equation (6) follows with $n = 1$). Slightly different definitions of these coefficients which correspond to different types of two-stream models, as discussed by Meador and Weaver [1980], could also have been used. The Eddington approximation is used only as a matter of convenience. The generality of the results that follows will not be altered with different forms of a_1 and a_2 .

Fundamental Solution of the Matrix RTE

It can be shown (e.g., refer to mathematical texts on ordinary differential equations (ODE), such as that of Cole [1968], and Gantmacher [1959]) that for $\mathbf{A}(\tau)$ continuous on $\tau_i \leq \tau \leq \tau_b$, there exists a unique solution to the vector differential equation

$$\frac{d\mathbf{I}}{d\tau} = \mathbf{A}(\tau)\mathbf{I} \quad (15)$$

with (one-point) boundary conditions $\mathbf{I}(\tau_i)$. This solution may be written in the form

$$\mathbf{I}(\tau) = \mathbf{P}_d(\tau, \tau_i) \mathbf{I}(\tau_i) \quad (16)$$

where $\mathbf{P}_d$ is a $2n \times 2n$ fundamental solution matrix which is the unique matrix satisfying the matrix differential equation

$$\frac{d\mathbf{P}_d}{d\tau} = \mathbf{A}(\tau)\mathbf{P}_d \quad (17)$$

with $\mathbf{P}_d(\tau_i) = \mathbf{I}$. (Here the subscript d reminds us that "propagation" occurs from the top of the medium downward to level τ .)

The propagator for a homogeneous atmosphere. Consider the solution of the homogeneous part of (8) for constant $\mathbf{A}$; then (16) may be written as

$$\mathbf{I}(\tau) = e^{\mathbf{A}(\tau - \tau_i)} \mathbf{I}(\tau_i) \quad (18)$$

for a layer of thickness $\tau - \tau_i$. As discussed later, the matrix exponential

$$\mathbf{P}(\tau, \tau_i) = e^{\mathbf{A}(\tau - \tau_i)} \quad (19)$$

contains most of the information about the solution of the RTE. It is called the fundamental solution or the matrixer in the theory of ordinary differential equations [Cole, 1968; Coddington and Levinson, 1955; Gantmacher, 1959], the transfer matrix solution [Aronson and Yarmush, 1966] in neutron physics, and the propagator [Kennett and Kerry, 1979; Gilbert and Backus, 1966; Fryer and Frazer, 1984] in seismology. In oceanography, Preisendorfer [1988] uses the term fundamental matrix, and in optimal control, Denman [1986] calls $\mathbf{P}$ the transition matrix. We have chosen to call this factor the propagator, in keeping with its interpretative meaning. For example, given the boundary conditions at one point, say $\mathbf{I}(\tau_i)$ in (16), then the solution deeper in the medium can be recovered (propagated) down from this boundary by applying this propagator. However, it has to be stressed in this context that the radiative transfer equation can not be treated as an initial value problem. The propagator matrix as such is not a solution to the RTE. Only after the boundary conditions are applied are the solutions recovered. The above-mentioned "boundary conditions at one point" mean both sets of upward and downward intensities,

and only one set is known in advance. This by no means reduces the usefulness of propagator, as demonstrated more fully later.

Inhomogeneous atmosphere: Definition of the product integral. It can be shown that the propagator $\mathbf{P}_d(\tau, \tau_i)$ between the top of the atmosphere τ_i and the internal point τ can be written as a product of individual fundamental solutions of the sublayers [Gilbert and Backus, 1966; Gantmacher, 1959; Karp et al., 1980] in the form

$$\begin{aligned} \mathbf{P}_d(\tau, \tau_i) &= \mathbf{P}_d(\tau, \tau_{k-1}) \mathbf{P}_d(\tau_{k-1}, \tau_{k-2}) \times \cdots \times \mathbf{P}_d(\tau_1, \tau_i) \\ &= \prod_{i=1}^k \mathbf{P}_d(\tau_i, \tau_{i-1}) \end{aligned} \quad (20)$$

Notice that the continuous interval (τ, τ_i) has been divided here into k layers and that $\tau_i = \tau_0$ and $\tau = \tau_k$ (see Figure 1). Equation (20) has simple intuitive appeal: starting with the intensities at the top of the medium (which are assumed to be known) we get intensities at the internal point τ_1 by applying the downward propagator $\mathbf{P}_d(\tau_1, \tau_i)$. Operator $\mathbf{P}_d(\tau_2, \tau_1)$ is then applied to these intensities to get the intensities even further down into the layer, this time at point τ_2 . Continuing this procedure, solutions at each internal point are obtained, and $\mathbf{P}_d(\tau, \tau_i)$ is constructed. For a vertically contiguous medium composed of k homogeneous layers, (20) can be expressed, with the aid of (19), as

$$\begin{aligned} \mathbf{P}_d(\tau, \tau_i) &= e^{\mathbf{A}(\tau, \tau_{k-1})\Delta\tau_k} e^{\mathbf{A}(\tau_{k-1}, \tau_{k-2})\Delta\tau_{k-1}} \\ &\times \cdots \times e^{\mathbf{A}(\tau_2, \tau_1)\Delta\tau_1} = \prod_{i=1}^k e^{\mathbf{A}(\tau_i, \tau_{i-1})\Delta\tau_i} \end{aligned} \quad (21)$$

In the limiting case of infinitesimally small sublayers for which assumption about homogeneity is satisfied, we can define the product integral

$$\mathbf{P}_d(\tau, \tau_i) = \prod_{\tau_i}^{\tau} e^{\mathbf{A}(\tau) d\tau} \quad (22)$$

Because we use the subscript d in definitions (20), (21), and (22), it is logical to assume that the operator $\mathbf{P}_d$ does not depend on the order of its arguments. Propagation of the solution from the bottom to the top of the atmosphere will be indicated by subscript u . The appendix contains more details on properties of product integrals, which will prove to be useful in further analysis of (21).

Boundary Conditions

In atmospheric radiative transfer problems one usually encounters a two-point (TP) boundary value problem (BVP) where for solar radiation, say, the downward intensities at cloud top and the upward intensities at cloud base reflected from an underlying surface, are specified. The emerging intensities from cloud top and base are then the required quantities. Thus the set of $2n$ linear ordinary differential equations given by (8) with $\mathbf{A}$ defined by (9) is then supplemented by $2n$ two-point boundary conditions at the top, $\tau = \tau_i = 0$, and bottom, $\tau = \tau_b$, of the atmosphere. These boundary conditions can be expressed as

$$\mathbf{b} = \mathbf{B}_t \mathbf{I}(\tau_i) + \mathbf{B}_b \mathbf{I}(\tau_b) \quad (23)$$

where $\mathbf{B}_t$ and $\mathbf{B}_b$ are $2n \times 2n$ matrices and $\mathbf{b}$ and $\mathbf{I}$ are $2n$ column vectors. Usually, boundary conditions are separable,

which leads to $\mathbf{B}_t$ and $\mathbf{B}_b$ of the form

$$\mathbf{B}_t = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad (24)$$

and

$$\mathbf{B}_b = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \quad (25)$$

Here $\mathbf{1}$ is an $n \times n$ unit matrix and $\mathbf{0}$ is an $n \times n$ matrix whose entries are all zeros. Notice that vector $\mathbf{b}$ contains information on boundary conditions at both points.

Using (16), we can write (23) as

$$\mathbf{D}\mathbf{I}(\tau_i) = \mathbf{b} \quad (26)$$

where the characteristic matrix for the boundary problem $\mathbf{D}$ is defined as

$$\mathbf{D} = \mathbf{B}_t \mathbf{P}_d(\tau_i, \tau_i) + \mathbf{B}_b \mathbf{P}_d(\tau_b, \tau_i) \quad (27)$$

and where (26) gives upward and downward intensities $\mathbf{I}(\tau)$ at one point, in this case the top of the atmosphere, in terms of boundary conditions $\mathbf{b}$ specified at two points. Note also that $\mathbf{P}_d(\tau_i, \tau_i) = \mathbf{1}$. More explicitly, inverting (26) yields

$$\mathbf{I}(\tau_i) = \mathbf{D}^{-1} \mathbf{b} \quad (28)$$

which provides the full solution to the external response problem (without sources $\mathbf{S}$). Combining (16) and (28) we also get intensities at every internal point of the atmospheric layer between $\tau_i \leq \tau \leq \tau_b$ (again for a sourceless problem). The analogy between the present formulation of the internal and external response problems in terms of the propagator and the response problems discussed in terms of doubling and adding methods will be made more evident later.

Example of boundary conditions for the two-stream model. Consider the sourceless two-stream model equations, which are

$$\frac{d}{d\tau} \begin{bmatrix} I_d \\ I_u \end{bmatrix} = \begin{bmatrix} a_1 & a_2 \\ -a_2 & -a_1 \end{bmatrix} \begin{bmatrix} I_d \\ I_u \end{bmatrix} \quad (29)$$

The boundary conditions for $I_d(\tau_i)$ and $I_u(\tau_b)$ can be written in the notation employed so far as

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} I_d(\tau_i) \\ I_u(\tau_i) \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} I_d(\tau_b) \\ I_u(\tau_b) \end{bmatrix} = \begin{bmatrix} I_d(\tau_i) \\ I_u(\tau_b) \end{bmatrix} \quad (30)$$

The characteristic matrix for this boundary value problem is given by (27), with $\mathbf{B}_t$ and $\mathbf{B}_b$ defined by the 2×2 analog of (24) and (25), respectively. Using the propagator defined later by (100), we get

$$\mathbf{D} = \mathbf{B}_t + \frac{e^{k\Delta\tau}}{2} \mathbf{B}_b \left(1 + \frac{\mathbf{A}}{k}\right) + \frac{e^{-k\Delta\tau}}{2} \mathbf{B}_b \left(1 - \frac{\mathbf{A}}{k}\right) \quad (31)$$

and obtain the solution to the internal problem as

$$\begin{bmatrix} I_d(\tau) \\ I_u(\tau) \end{bmatrix} = \mathbf{P}\mathbf{D}^{-1} \begin{bmatrix} I_d(\tau_i) \\ I_u(\tau_b) \end{bmatrix}$$

Sources

Knowing the fundamental matrix of the homogeneous part of RTE (8), one can construct a particular solution for the given source function $\mathbf{S}$ [e.g., Cole, 1968; Bellman, 1970; Gantmacher, 1959] as

$$\mathbf{F}(\tau) = \mathbf{P}_d(\tau) \int_{\tau_i}^{\tau} \mathbf{P}_d^{-1}(s) \mathbf{S}(s) ds \quad (32)$$

Thus the intensities in an inhomogeneous atmosphere with arbitrary sources are obtained as

$$\mathbf{I}(\tau) = \mathbf{P}_d(\tau) \mathbf{D}^{-1} \mathbf{b} + \mathbf{P}_d(\tau) \int_{\tau_i}^{\tau} \mathbf{P}_d^{-1}(s) \mathbf{S}(s) ds \quad (33)$$

or more simply as

$$\mathbf{I}(\tau) = \mathbf{P}_d(\tau) \mathbf{I}(\tau_i) + \mathbf{F}(\tau) \quad (34)$$

Using the Green's function notation, we define the following matrix function as [Russell, 1985]

$$\begin{aligned} \mathbf{G}(\tau, s) &= \mathbf{P}_d(\tau) \mathbf{D}^{-1} \mathbf{B}(\tau_i) \mathbf{P}_d^{-1}(s) & \tau > s \\ \mathbf{G}(\tau, s) &= -\mathbf{P}_d(\tau) [\mathbf{1} - \mathbf{D}^{-1} \mathbf{B}(\tau_i)] \mathbf{P}_d(s)^{-1} & \tau < s \end{aligned} \quad (35)$$

and write (33) as

$$\mathbf{I}(\tau) = \mathbf{P}_d(\tau) \mathbf{D}^{-1} \mathbf{b} + \int_{\tau_i}^{\tau} \mathbf{G}(\tau, s) \mathbf{S}(s) ds \quad (36)$$

Two examples of source functions in the two-stream model. Radiative transfer problems often encounter two different types of source functions; one that represents the source of diffuse intensity as a result of the single scatter of a collimated beam of radiation and a second that represents the source of intensity that arises from thermal emission within the atmosphere. The latter is encountered in infrared transfer studies and is often approximated by

$$\mathbf{S}_{IR} = (1 - \tilde{\omega}_0) (\mathbf{B}_0 + \mathbf{B}_1 \tau) \mathbf{S}_0 \quad (37)$$

which assumes the emission to be a linear function of τ . The former type of source function is usually encountered in problems dealing with solar radiative transfer and is expressed as

$$\mathbf{S}_{solar} = a_3 e^{-\tau/\mu_0} \mathbf{S}_0 \quad (38)$$

where the constant vector $\mathbf{S}_0$ is defined as

$$\mathbf{S}_0 = \begin{bmatrix} -1 \\ 1 \end{bmatrix} \quad (39)$$

For a homogeneous atmosphere there is, at least conceptually, no difficulty in evaluating (32). The propagator is exponential in τ and source terms such as (37) or (38) are relatively simple functions of τ . Thus in some instances the integral of (32) can be evaluated analytically. Let us again provide the following example, based on two-stream theory, for an illustration. Consider a homogeneous atmosphere with constant $\mathbf{A}$, for which we have from (32) and (19)

$$\mathbf{F} = \int_{\tau_i}^{\tau} e^{\mathbf{A}(\tau-s)} \mathbf{S}(s) ds \quad (40)$$

Substitution of (100) into (40) yields

$$\mathbf{F} = \frac{1}{2} \left(1 + \frac{\mathbf{A}}{k}\right) \mathbf{S}_0 h(k, \tau, \tau_i) + \frac{1}{2} \left(1 - \frac{\mathbf{A}}{k}\right) \mathbf{S}_0 h(-k, \tau, \tau_i) \quad (41)$$

where the function $h(k, \tau, \tau_i)$ in (41) is

$$h(k, \tau, \tau_i) = \int_{\tau_i}^{\tau} e^{k(\tau-s)} f(s) ds \quad (42)$$

and where $f(\tau)$ is given by (37) or (38) without the $\mathbf{S}_0$ factor. In both cases, $\mathbf{S}_0$ is defined by (39).

The integral in (42) can be evaluated for a homogeneous atmosphere, and the two-stream approximation to

the RTE's particular solution is given analytically for two important cases of source functions:

$$h_{IR}(k, \tau, 0) = -\frac{\tau B_1}{k} + \frac{(B_1 + kB_0)}{k^2} (e^{k\tau} - 1) \quad (43)$$

$$h_{solar}(k, \tau, 0) = \frac{\mu_0}{1 + k\mu_0} \left(e^{k\tau} - e^{-\frac{\tau}{\mu_0}} \right) \quad (44)$$

For the more complex case of the n -stream problem and for a more general form of source function, F can be obtained numerically by techniques to be described later.

3. EVALUATION OF THE MATRIX EXPONENTIAL

We now describe some methods used to evaluate the propagator. The review article by *Moler and van Loan* [1978] provides a much more extensive discussion of the subject of calculating $\exp(A\tau)$ and is recommended to the interested reader. We will first consider those methods that provide an approximation to $\exp(A\tau)$ for small τ , as these will be utilized in later discussions. We also describe the similarity transformation, which provides the basis for the eigenvector approach often used in radiative transfer literature.

Taylor Series Decomposition of Matrix Exponent

The formal Taylor series definition of (19) is

$$e^{A\tau} = 1 + A\tau + \cdots + \frac{A^n \tau^n}{n!} + \cdots \quad (45)$$

where 1 is a $2n \times 2n$ unit matrix. This series exists for all A and τ and is convergent [Cole, 1968; Gantmacher, 1959; Campbell, 1980]. Suppose now that τ is small and consider only second-order terms in τ , then, using (45) and (9), we obtain

$$e^{A\tau} = 1 + A\tau + \frac{A^2 \tau^2}{2} + \cdots \approx \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \tau \begin{bmatrix} a_1 & a_2 \\ -a_2 & -a_1 \end{bmatrix} + \frac{\tau^2}{2} \begin{bmatrix} a_1 & a_2 \\ -a_2 & -a_1 \end{bmatrix}^2 \quad (46)$$

It is shown later that (46) constitutes the existing methods of initialization for the doubling and adding schemes.

The assumption behind (46) is that $A\tau$ is somehow small. A more quantitative representation of this criterion can be stated as $\|A\| \tau < 1$ where we denote the matrix norm of A by $\|A\|$ (see Cole [1968] and Moler and van Loan [1978] for definitions of various matrix norms and their properties).

Rational Approximation and Ward's Algorithm

Here we describe a method based on the work of Ward [1977], which uses the diagonal Padé table rational approximation to compute the exponential matrix. Following Ward [1977], the p th diagonal Padé approximation to the exponential of the matrix A is given by

$$Q_p^{-1}(-A)Q_p(A) \quad (47)$$

where $Q_p(X)$ is a polynomial in X of degree p defined by

$$Q_p(X) = \sum_{k=0}^p c_k X^k \quad (48)$$

where

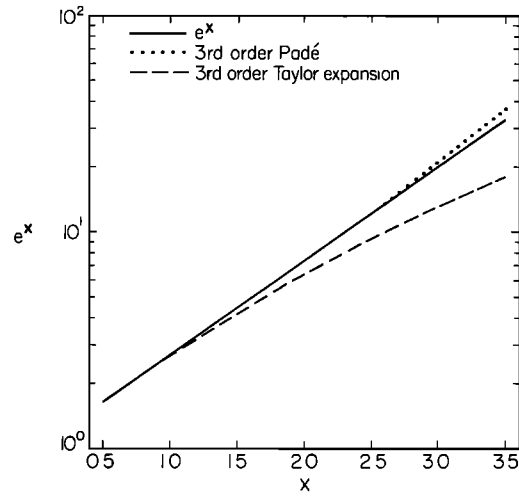


Fig. 2. Comparisons of various approximations to the exponent for small x .

$$c_k = \frac{(2p-k)!p!}{(2p)!k!(p-k)!} \quad (49)$$

The error in approximating the matrix exponent by diagonal Padé entries increases as the norm of the matrix increases. Therefore one of the objectives of Ward's [1977] algorithm is to decrease the matrix norm to some desirable prescribed level. The algorithm uses three techniques to achieve such a decrease in matrix norm. The first technique uses transformations based on the estimated value of the eigenvalues. The second technique attempts to minimize the norm of A over all possible diagonal similarity transformations. The third technique exploits the identity $\exp(A) = (\exp(A/m))^m$ (property 2, equation (153)). The general idea of this technique is to choose m as a power of 2 starting with $\exp(A/m)$ which has been determined reliably and efficiently, say, using (46) and then to form the matrix $[\exp(A/m)]^m$ by repeated squaring. Thus it is required to choose m as the smallest power of 2 for which $\|A\|/m \leq 1$. This method of squaring (doubling) has been used in mathematical literature to evaluate other functions which involve matrix exponentials (as, for example, in the work of van Loan [1978]). This same technique is also equivalent to the doubling scheme which is a method frequently used in radiative transfer literature.

We now provide an example of the diagonal Padé approximation to e^x . With some manipulation, it is straightforward to show that

$$e^x \approx P_{33} = \frac{1 + x/2 + x^2/10 + x^3/120}{1 - x/2 + x^2/10 - x^3/120} \quad (50)$$

Figure 2 presents a comparison of e^x , third-order power series of $\exp(x)$ and P_{33} . It can be seen that the rational function gives considerably better approximation to $\exp(x)$ than the Taylor series, and it is to be anticipated that (50) will provide a better and more efficient approximation to $\exp(A\tau)$ than that given by (46).

Similarity Transformations

We now pursue the matrix decomposition technique which is closely related to the discrete ordinate method, but the description offered here is more general.

All of the matrix decompositions are based on similarity transformations of the form [e.g., Moler and van Loan, 1978]

$$\mathbf{A} = \mathbf{TCT}^{-1} \quad (51)$$

and after some algebra involving the Taylor series definition (45), can be shown that (51) implies

$$e^{\mathbf{A}\tau} = \mathbf{T}e^{\mathbf{C}\tau}\mathbf{T}^{-1} \quad (52)$$

The idea now is to find the similarity transformation $\mathbf{T}$ for which $e^{\mathbf{C}\tau}$ is easy to compute. In particular, if $\mathbf{C}$ is diagonal of the form

$$\mathbf{C} = \text{diag}(k_1, \dots, k_{2n}) \quad (53)$$

where k_i are eigenvalues associated with $\mathbf{A}$, then the exponent of $\mathbf{C}$ is trivial to calculate, namely,

$$e^{\mathbf{C}\tau} = \text{diag}(e^{k_1\tau}, \dots, e^{k_{2n}\tau}) \quad (54)$$

In the degenerate case of repetitive eigenvalues the Jordan canonical form could be used [see Karp *et al.*, 1980], and there is no difficulty in finding exponent of this Jordan form [Moler and van Loan, 1978].

Splitting

The familiar additive law for scalar exponentials

$$\exp(a)\exp(b) = \exp(a+b) \quad (55)$$

doesn't hold when one deals with matrices, as the following short calculation shows. Using the Taylor series expansion, we get

$$\begin{aligned} e^{-\mathbf{A}_2}e^{-\mathbf{A}_1}e^{\mathbf{A}_1+\mathbf{A}_2} &= (\mathbf{I} - \mathbf{A}_2 + \frac{\mathbf{A}_2^2}{2} - \dots) \\ &\cdot (\mathbf{I} - \mathbf{A}_1 + \frac{\mathbf{A}_1^2}{2} - \dots)(\mathbf{I} + \mathbf{A}_1 + \mathbf{A}_2 \frac{(\mathbf{A}_1 + \mathbf{A}_2)^2}{2} + \dots) \end{aligned} \quad (56)$$

Multiplying terms on the right-hand side, we obtain

$$e^{-\mathbf{A}_2}e^{-\mathbf{A}_1}e^{\mathbf{A}_1+\mathbf{A}_2} = \mathbf{I} - \frac{[\mathbf{A}_1, \mathbf{A}_2]}{2} + \dots \quad (57)$$

where we defined the commutator as

$$[\mathbf{A}_1, \mathbf{A}_2] = \mathbf{A}_1\mathbf{A}_2 - \mathbf{A}_2\mathbf{A}_1 \quad (58)$$

Only if $\mathbf{A}_1$ and $\mathbf{A}_2$ commute, i.e., $[\mathbf{A}_1, \mathbf{A}_2] = 0$, does the additive law hold.

Using (157), we can finally write the following formula, which is valid through quadratic terms in $\mathbf{A}_1$ and $\mathbf{A}_2$

$$e^{\mathbf{A}_1+\mathbf{A}_2} = e^{\mathbf{A}_1}e^{\mathbf{A}_2}e^{-[\mathbf{A}_1, \mathbf{A}_2]/2} \dots \quad (59)$$

The exponential identity (59) can serve as a method to find matrix exponent when the matrix $\mathbf{A}$ can be split into matrices $\mathbf{A}_1, \mathbf{A}_2$, for which their exponents and the exponents of their commutators can be calculated efficiently. It is also sometimes possible to express (59) by a finite number of factors. This can be achieved if the decomposition of $\mathbf{A}$ into basis matrices $\mathbf{A}_i$ forms solvable Lie algebra [Wei and Norman, 1964; Magnus, 1954; Sauter, 1979]. In such a case it is possible to use Baker-Hausdorff-Campbell exponential identities of the type (59) to develop a closed-form solution. (For more details the see review by Stainberg [1988]).

4. THE INTERACTION PRINCIPLE AND THE EXTINCTION OPERATOR

The fundamental solution, characterized by the propagator, does not depend on boundary conditions in any way

and is determined solely by the internal properties of a layer. These are the single scattering properties and their distribution within the layer. The reflectance and transmittance matrices which are defined in the following discussion similarly depend only on internal characteristics of a layer and, once known, provide a solution for any arbitrary incident radiation field. Thus knowledge of reflectance and transmittance contains all information about the internal characteristics of a layer, as does the propagator. It is therefore reasonable to expect that these two concepts are closely related. It is the purpose of this section to illustrate the connection between these inherent properties of the layer. The significance of the interaction principle in establishing this link becomes evident through the definition of the extinction operator.

Interaction Principle, Extinction Matrix, and Extinction Transformations

Let us define, in the usual way, the reflectance and transmittance matrices as describing the amount of radiation reflected from the layer and transmitted through the layer. These matrices are composed of bidirectional reflectances and transmittances which are, in turn, characterized by incident and response directions of the flow. In general, radiation coming from above will be reflected and transmitted differently than radiation incident from below. As above we use the subscripts d and u to indicate downward and upward propagating radiation. Given the incident intensities $I_d(\tau_i)$ on the top of the layer, we get the following responses

$$I_d(\tau_b) = t_d I_d(\tau_i) \quad (60)$$

$$I_u(\tau_i) = r_d I_d(\tau_i) \quad (61)$$

and for the case of upward intensities incident on the bottom of the layer, we get a similar set of responses; namely,

$$I_d(\tau_b) = r_u I_u(\tau_b) \quad (62)$$

$$I_u(\tau_i) = t_u I_u(\tau_b) \quad (63)$$

In general, radiation comes from both directions and interacts linearly with the medium. Thus (60) - (63) can be combined and, with the additional contributions by internal sources, we obtain the matrix form of the interaction principle

$$\begin{bmatrix} I_d(\tau_i) \\ I_u(\tau_b) \end{bmatrix} = \mathbf{R} \begin{bmatrix} I_d(\tau_b) \\ I_u(\tau_i) \end{bmatrix} + \mathbf{G} \quad (64)$$

where we define the extinction matrix $\mathbf{R}$ as

$$\mathbf{R} = \begin{bmatrix} t_d & r_u \\ r_d & t_u \end{bmatrix} \quad (65)$$

and the source-related vector $\mathbf{G}$ as

$$\mathbf{G} = \begin{bmatrix} G_d \\ G_u \end{bmatrix} \quad (66)$$

Our goal now is to find a relationship between the $2n \times 2n$ extinction matrix and the $2n \times 2n$ propagator matrix. To this end, we define, after Saastamoinen [1980], the following matrix operations. Consider an arbitrary $2n \times 2n$ matrix $\mathbf{M}$ partitioned into $n \times n$ blocks according to

$$\mathbf{M} = \begin{bmatrix} \mathbf{m}_{11} & \mathbf{m}_{12} \\ \mathbf{m}_{21} & \mathbf{m}_{22} \end{bmatrix} \quad (67)$$

We define the downward operator S_d as

$$S_d(M) = \begin{bmatrix} m_{11} - m_{12}m_{22}^{-1}m_{21} & m_{12}m_{22}^{-1} \\ -m_{22}^{-1}m_{21} & m_{22}^{-1} \end{bmatrix} \quad (68)$$

and the upward operator S_u by

$$S_u(M) = \begin{bmatrix} m_{11}^{-1} & -m_{11}^{-1}m_{12} \\ m_{21}m_{11}^{-1} & m_{22} - m_{21}m_{11}^{-1}m_{12} \end{bmatrix} \quad (69)$$

It is simple to check that

$$S_d[S_d(M)] = M, \quad S_u[S_u(M)] = M \quad (70)$$

and that the inverse of the extinction operator is the same as the operator itself, i.e.,

$$S_d(M) = S_d^{-1}(M) \quad (71)$$

and

$$S_u(M) = S_u^{-1}(M) \quad (72)$$

Thus with matrix multiplication we find that

$$S_d(M)S_u(M) = S_u(M)S_d(M) = 1 \quad (73)$$

Relation Between Extinction and Fundamental Matrices

We now utilize the matrix definitions given earlier. Consider the interaction principle (64) for intensities emerging from the top and at the bottom of the layer. With some rearrangement and with regrouping of the intensities, (64) can be written as

$$\begin{bmatrix} 1 & r_u \\ 0 & t_u \end{bmatrix} \begin{bmatrix} I_d(\tau_b) \\ I_u(\tau_b) \end{bmatrix} = \begin{bmatrix} t_d & 0 \\ r_d & -1 \end{bmatrix} \begin{bmatrix} I_d(\tau_t) \\ I_u(\tau_t) \end{bmatrix} + \begin{bmatrix} G_d \\ G_u \end{bmatrix} \quad (74)$$

which is equivalent to the following form of the fundamental solution

$$I(\tau_b) = P_{d1}(\tau_b, \tau_t)P_{d2}(\tau_b, \tau_t)I(\tau_t) + P_{d1}(\tau_b, \tau_t)G \quad (75)$$

where we identify that

$$P_{d1} = \begin{bmatrix} 1 & -r_u \\ 0 & -t_u \end{bmatrix}^{-1} = \begin{bmatrix} 1 & -r_u t_u^{-1} \\ 0 & -t_u^{-1} \end{bmatrix} \quad (76)$$

and

$$P_{d2} = \begin{bmatrix} t_d & 0 \\ r_d & -1 \end{bmatrix} \quad (77)$$

Comparing (75) with (16), we see that $P_d(\tau_t, \tau_b)$ is

$$P_d(\tau_b, \tau_t) = P_{d1}(\tau_b, \tau_t)P_{d2}(\tau_b, \tau_t) \quad (78)$$

and with simple multiplication we obtain

$$P_d(\tau_b, \tau_t) = \begin{bmatrix} t_d - r_u t_u^{-1} r_d & r_u t_u^{-1} \\ -t_u^{-1} r_d & t_u^{-1} \end{bmatrix} \quad (79)$$

Thus (79) gives the relationship between the fundamental solution and the extinction matrix (65) as

$$P_d(\tau_b, \tau_t) = S_d(R) = \begin{bmatrix} t_d - r_u t_u^{-1} r_d & r_u t_u^{-1} \\ -t_u^{-1} r_d & t_u^{-1} \end{bmatrix} \quad (80)$$

$$P_u(\tau_t, \tau_b) = S_u(R) = \begin{bmatrix} t_d^{-1} & -t_d^{-1} r_u \\ r_d t_d^{-1} & t_u - r_d t_d^{-1} r_u \end{bmatrix} \quad (81)$$

Since the extinction operator is its own inverse, we get from (71) and (80)

$$R = S_d[P_d(\tau_b, \tau_t)] \quad (82)$$

and

$$R = S_u[P_u(\tau_t, \tau_b)] \quad (83)$$

Let us remark about the inhomogeneous term. Again, comparing (75) to (34), one has

$$F = P_{d1}G \quad (84)$$

which provides the transformation rule for inhomogeneous terms in the propagator and the extinction formulations of the RTE.

Riccati Equations

It is possible to derive a set of differential equations for the extinction matrix. Differentiating (80) with respect to τ using (17) and applying the S transformation to P_d , we get

$$\frac{dS(R)}{d\tau} = AS(R) \quad (85)$$

from which four Riccati-type matrix equations for r_u , r_d , t_u , and t_d are determined as

$$\frac{dr_u}{d\tau} = a_2 + a_1 r_u + r_u a_1 + r_u a_2 r_u \quad (86)$$

$$\frac{dr_d}{d\tau} = -a_2 + a_1 r_d - r_d a_1 - r_d a_2 r_d \quad (87)$$

$$\frac{dt_d}{d\tau} = -a_1 t_d - a_2 r_d t_d \quad (88)$$

$$\frac{dt_u}{d\tau} = a_1 t_u + a_2 r_u t_u \quad (89)$$

The extinction transformation of the two-stream propagator. Consider a homogeneous layer and assume that $r_u = r_d$ and $t_u = t_d$. It will be shown later that the propagator for the two-stream model is given by (100) which, in expanded form, is

$$e^{A\tau} = \begin{bmatrix} \frac{e^{k\tau}}{2} a_h^+ + \frac{e^{-k\tau}}{2} a_h^- & \frac{a_2}{2k} (e^{k\tau} - e^{-k\tau}) \\ -\frac{a_2}{2k} (e^{k\tau} - e^{-k\tau}) & \frac{e^{k\tau}}{2} a_h^- + \frac{e^{-k\tau}}{2} a_h^+ \end{bmatrix} \quad (90)$$

where $a_h^+ = (1 + a_1/k)$, $a_h^- = (1 - a_1/k)$, and the extinction transformation S_d , applied to (90), produces

$$R = S_d(e^{A\tau}) = \frac{1}{(e^{k\tau}/2)(1 - a_1/k) + (e^{-k\tau}/2)(1 + a_1/k)} \cdot \begin{bmatrix} 1 & (a_2/2k)(e^{k\tau} - e^{-k\tau}) \\ (a_2/2k)(e^{k\tau} - e^{-k\tau}) & 1 \end{bmatrix} \quad (91)$$

Thus with the definition of R according to (65), we readily identify the transmission as

$$t = \frac{1}{e^{k\tau}/2(1 - a_1/k) + e^{-k\tau}/2(1 + a_1/k)} \quad (92)$$

and the reflectance as

$$r = \frac{a_2/2k(e^{k\tau} - e^{-k\tau})}{e^{k\tau}/2(1 - a_1/k) + e^{-k\tau}/2(1 + a_1/k)} \quad (93)$$

which correspond to the expressions given by Meador and Weaver [1980] for their model 2.

The extinction transformation of the n -stream model. For the n -stream model we use the eigenvalue decomposition,

which will be discussed in more detail later. Applying the S transformation to (105), we get

$$t = \left(u_- e^{-k\tau} z_- + u_+ e^{k\tau} z_+ \right)^{-1} \quad (94)$$

$$r = \left(u_+ e^{-k\tau} z_- + u_- e^{k\tau} z_+ \right) t^{-1} \quad (95)$$

where $u_{\pm}$, $z_{\pm}$ are defined accordingly to (106) and (107). Notice that (94) and (95) can be manipulated such that only negative exponents are present [Aronson and Yarmush, 1966; Aronson, 1970; Saastamoinen, 1980; Fryer and Frazer, 1984]. We will return to this aspect of (94) and (95) in our discussion on stability.

5. EIGENVECTOR ANALYSIS: APPLICATIONS TO THE RTE

The Method of Discrete Ordinates

One approach to evaluate the matrix exponential $\exp(A\tau)$ is to find the eigenvalues k_i and associated eigenvectors u_i of the matrix A . This is the essence of the discrete ordinate method of Chandrasekhar [1960], as discussed by Stamnes and Swanson [1981], Stamnes [1986], and Nakajima and Tanaka [1986] in recent literature. The method discussed in these papers is based on the factorization or decomposition of the matrix A . (The terminology "discrete ordinates" is in fact misleading, as the discreteness of the method which results by replacing the continuous angular dependence by a set of discrete directions is not unique to this method. We propose that this method be more appropriately referred to as the eigenvector method.)

The traditional derivation of the discrete ordinate method avoids finding an explicit expression for the propagator by imposing boundary conditions and solving for matching coefficients arising from the requirements of continuity of intensity across each of the boundaries. The boundary conditions are therefore an integral part of the solution scheme, and a new set of calculations are necessary for different set of boundary conditions. By contrast, the propagator is defined by the internal structure of the atmosphere and is not dependent in any way on boundary conditions. Therefore the fundamental solution is obtained first, and the boundary conditions are applied next.

The Propagator of a Two-Stream Model

We first consider the two-stream model as a relatively simple example of the eigenvector method. From the Cayley-Hamilton theorem [e.g., Graham, 1979] we know that some function of a $2n \times 2n$ matrix A can be represented by a polynomial $r(A)$ in A of the order $2n - 1$. For the case of a two-stream model, $n = 1$, and we can represent the propagator as

$$e^{A\tau} = \alpha I + \beta A \quad (96)$$

To get α and β , we first find the eigenvalues of

$$Ax = kx \quad (97)$$

which gives $k^2 = a_1^2 - a_2^2$, and since we require both $e^{A\tau}$ and $r(A)$ to possess the same eigenvalues [Pennisi, 1972; Graham, 1979], it follows that

$$e^{k\tau} = \alpha + \beta k \quad (98)$$

and

$$e^{-k\tau} = \alpha - \beta k \quad (99)$$

After simple algebra we finally arrive at

$$e^{A\tau} = \frac{e^{k\tau}}{2} \left(1 + \frac{A}{k} \right) + \frac{e^{-k\tau}}{2} \left(1 - \frac{A}{k} \right) \quad (100)$$

for the two-stream propagator where I is the 2×2 identity matrix.

The Eigenvalues and Eigenvectors of 2n Flow Model

Eigenvalues of the $2n \times 2n$ matrix A defined by (9) have been studied extensively by Aronson [1970], Aronson and Yarmush [1966] and, more recently, by Waterman [1981], Stamnes and Swanson [1981], Nakajima and Tanaka [1986], and Preisendorfer [1988]. Aronson [1971], studied relationship between the transfer matrix and Case's [Case and Zweifel, 1967] method of eigenfunctions. The structure of the eigenvectors is important when considering stability of numerical schemes. They occur in $\pm k$ pairs and are all real [Stamnes and Swanson, 1981; Aronson, 1970]. The eigenvalues are also invariant with respect to similarity transformations. Let us define the $2n \times 2n$ transformation matrix as

$$T = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad (101)$$

and note that $T^{-1} = \frac{1}{2}T$. Thus

$$\tilde{T} = TAT^{-1} = \begin{bmatrix} 0 & s \\ d & 0 \end{bmatrix} \quad (102)$$

where $s = a_1 - a_2$ and $d = a_1 + a_2$ and

$$\tilde{T}^2 = \begin{bmatrix} sd & 0 \\ 0 & ds \end{bmatrix} \quad (103)$$

Because matrix sd is ds transposed, it is enough to find eigenvectors of one of them. After Aronson [1970], let the diagonalization of sd be given by

$$k^2 = y^{-1}(sd)y \quad (104)$$

Thus it can be shown that

$$e^{A\tau} = \frac{1}{4} \begin{bmatrix} u_+ & u_- \\ u_- & u_+ \end{bmatrix} \begin{bmatrix} e^{-k\tau} & 0 \\ 0 & e^{k\tau} \end{bmatrix} \begin{bmatrix} z_+ & z_- \\ z_- & z_+ \end{bmatrix} \quad (105)$$

where

$$u_{\pm} = (y \pm x) \quad (106)$$

$$z_{\pm} = (y^{-1} \pm x) \quad (107)$$

and

$$x = dyk^{-1} = s^{-1}yk \quad (108)$$

For the $2n$ flow problem under consideration, u_+ , u_- , z_+ , z_- , s , d , a_1 , a_2 , x , y , and k are $n \times n$ dimensional matrices.

Invariant Imbedding

The more traditional discussion of invariant imbedding usually focuses on the Riccati equations, such as derived earlier. The earlier works of Bellman and Kalaba [1959], Redheffer [1962], and Preisendorfer [1958] and the review of

Scott [1975] provide ample illustration of the method. The method is a powerful tool for analyzing linear systems [e.g., Denman, 1979; 1986] and is frequently employed in current research on two-point boundary value problem for ODE's (see Mattheij and Staarink, [1984] among others).

While the method of invariant imbedding has been described in many different ways, we demonstrate here that the approach is a form of similarity transformation of matrix A , much in the same way as the eigenvector analysis described earlier. This connection is perhaps not surprising given that invariant imbedding techniques have been employed on certain eigenvalue problems (e.g., Scott, [1975] and Preisendorfer, [1973] among others). Under this transformation, the real virtue of invariant imbedding and the reason perhaps why it is popular in two-point boundary value problems is made apparent as we demonstrate that this transformation yields the matrix of block diagonal form and thus transforms the two-point boundary value problem to a more tractable and separable pair of initial value problems.

We start with a transformation T , which might be viewed as more general than that described by (103), as it is continuous in τ . We now apply this transformation to the propagator defined by (22), with the end result given by the similarity rule of (161), namely,

$$\begin{aligned} T^{-1}(\tau) \prod_{\tau_i}^{\tau} \exp[A(s)ds] T(\tau_i) \\ = \prod_{\tau_i}^{\tau} \exp \left[\left(T^{-1}(s)A(s)T(s) - T^{-1}(\tau) \frac{dT(\tau)}{ds} \right) ds \right] \end{aligned} \quad (109)$$

and desire that the resulting transformation matrix be block diagonal to provide a stable solution to (8). Let us define the transformation matrix $T(\tau)$ as

$$T(\tau) = \frac{1}{2} \begin{bmatrix} 1 & -r_u \\ r_d & -1 \end{bmatrix} \quad (110)$$

and impose the condition that r_u and r_d satisfy the matrix Riccati equations (85) and (86), then it can be shown that

$$\begin{aligned} T^{-1}(\tau)A(\tau)T(\tau) - T^{-1}(\tau) \frac{dT(\tau)}{d\tau} \\ = \begin{bmatrix} a_1 - a_2 r_d & 0 \\ 0 & -a_1 + a_2 r_u \end{bmatrix} \end{aligned} \quad (111)$$

and, by virtue of the block diagonal form of (111), the problem has been transformed into two uncoupled initial value problems, which are stable with respect to the direction of the solution.

Dichotomy, Stability, and Decoupling

We have already remarked that our general matrix A has a spectrum such that for every eigenvalue k_i there is an eigenvalue $-k_i$. The solution, in the form of the propagator $\exp(A\tau)$ is thus a combination of both growing and decaying exponentials as indicated by (105). For large optical thicknesses, growing exponentials will dominate the solution given in this form, and it follows that the naive application of the propagator will lead to numerical instability. In such circumstances the true solution is lost and cannot be recovered. The behavior just described is referred to as dichotomic and is the subject of vigorous ongoing research in

mathematical literature [Russell, 1985; vanLoon, 1985; de-Hook and Mattheij, 1985; Mattheij, 1985; Smith, 1987] and [Evans, 1986]. In the case of the two-stream model, this dichotomy means that there is one exponentially increasing and one exponentially decreasing fundamental solution component [Russell, 1985]. In the case of a $2n$ flow model, n growing and n decaying modes can be expected. The issue of numerical stability has been realized in the radiative transfer literature for some time. To illustrate the nature of this instability and the remedies introduced to overcome them, we consider the two-layer atmosphere. We confine our interests to the case of a sourceless atmosphere for brevity and desire to determine the fluxes at each of the boundaries including at the internal layer. We employ the two-stream formulations in this illustration, although the same arguments apply to the more general $2n$ stream model. The method commonly employed is exemplified in the two-stream work of Shettle and Weinman [1970] and Pollack and McKee [1985] and in the $2n$ stream work of Liou [1975] and Stamnes [1986] among others. In these studies the solutions for each individual layer are determined and the boundary conditions at the interface boundaries are matched, resulting in a system of simultaneous equations. In the present formulation the solutions for a two-layer atmosphere can be expressed as

$$I(\tau) = e^{A_2 \tau_2} e^{A_1 \tau_1} I(\tau_i) \quad (112)$$

where obviously, matrix multiplication serves as a matching condition between boundary of two layers. In Figure 3 we show each of the components of the propagator (denoted as P_{ij}) as a function of increasing optical thickness. One of the components (namely, P_{22}) becomes unbounded, while the others stay bounded. Thus the solution either in the form of the propagator or in the form of matching boundary conditions, as mentioned earlier will be numerically unstable. This can be overcome by employing the extinction formulation in the form of reflection and transmission functions, since they are well behaved and bounded.

6. THE CASE OF A VERTICALLY INHOMOGENEOUS ATMOSPHERE

We have so far described different ways of evaluating $\exp(A\tau)$ using small τ approximations and similarity trans-

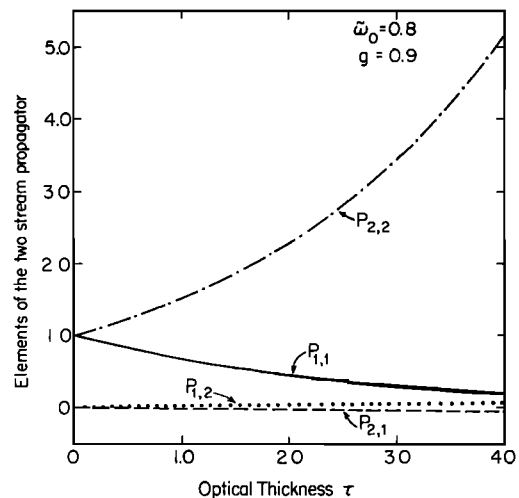


Fig. 3. Components of two-stream propagator as a function of increasing τ .

formations. We will now show, by a study of the properties of products of exponentials of a matrix, that the propagator can be readily used to construct solutions of RTE for an inhomogeneous atmosphere and arrive at the adding scheme as a result. The virtue of the adding scheme was actually made apparent in the earlier discussion of stability and is often used in radiative transfer studies. The relationship of the adding scheme to the propagator has already been realized in the atmospheric sciences literature by *Waterman* [1981], *Karp et al.* [1980], and *Stamnes* [1986]. *Peebles and Plesset* [1951] applied a similar scheme in gamma ray transfer. *Aronson and Yarmush* [1966] studied the transfer matrix solution in connection with neutron transfer. Scattering and transfer matrix methods are used in optimal control [e.g., *Denman*, 1986], while *Kennett* [1974] showed how this technique can be applied to seismic waves.

The Adding Method for a Sourceless Medium

We now treat a vertically contiguous atmosphere composed of a succession of overlying homogeneous layers and obtain composite expressions for reflectance and transmittance. We assume, for the moment, that there is no internal source, so that $F = 0$ and $G = 0$. Using (20) and (83) the extinction matrix for the layer (τ_i, τ_b) is

$$R(\tau_i, \tau_b) = S_d [P_d(\tau_i, \tau_b)] = S_d \left[\prod_{i=1}^k P_d(\tau_{i+1}, \tau_i) \right] \quad (113)$$

Since each component in the product of (113) can be expressed by the extinction matrix (65) through the extinction transformation, (113) can be written in the form

$$R(\tau_i, \tau_b) = S_d \left[\prod_{i=1}^k S_d [R(\tau_{i+1}, \tau_i)] \right] \quad (114)$$

Equation (114) actually represents the well-known adding scheme [e.g., *Grant and Hunt*, 1968 a, b, 1969 a, b]. It allows us to construct reflectances and transmittances of combined layers from our knowledge of reflectances and transmittances of individual layers, and it is equivalent to the star product composition rule of *Redheffer* [1962]. Consider, for illustration, an atmosphere composed of two layers extending from (τ_b, τ) and (τ, τ_i) . The extinction matrix for the two combined layers follows from (114) and (113) as

$$R(\tau_b, \tau_i) = S [S [R(\tau_b, \tau)] S [R(\tau, \tau_i)]] \quad (115)$$

With the notation $R(\tau_b, \tau) = R^*$, and $R(\tau, \tau_i) = R$ where the asterisk is used to indicate the lower layer properties and, after some algebra involving matrix multiplication and S transformations, we can write

$$t_u(\tau_i, \tau_b) = t_u \frac{1}{1 - r_d^* r_u} t_u^* \quad (116)$$

$$r_u(\tau_i, \tau_b) = r_u^* + t_d^* r_u \frac{1}{1 - r_d^* r_u} t_u^* \quad (117)$$

$$r_d(\tau_i, \tau_b) = r_d + t_u \frac{1}{1 - r_d^* r_u} r_d^* t_d \quad (118)$$

and

$$t_d(\tau_i, \tau_b) = t_d^* \frac{1}{1 - r_u r_d^*} t_d \quad (119)$$

which represents the adding formula for a two-layer atmosphere.

The Adding Scheme for an Inhomogeneous Atmosphere With Sources

Knowing the propagator, one can construct a particular solution for an arbitrary source function and write down the full solution as (33). For an inhomogeneous atmosphere the total propagator is given by product integral (20). In the same manner, it is natural to ask if the knowledge of F_k for individual, homogeneous layers is sufficient to reconstruct F for the entire inhomogeneous atmosphere. The answer is yes, and an equation similar to (20) can be derived as follows. Consider as above two layers (τ, τ_i) and (τ_b, τ) , then from (34) we write

$$I(\tau) = P(\tau, \tau_i) I(\tau_i) + F(\tau, \tau_i) \quad (120)$$

and

$$I(\tau_b) = P(\tau_b, \tau) I(\tau) + F(\tau_b, \tau) \quad (121)$$

Combining (120) and (121), we see that

$$F(\tau_b, \tau_i) = P(\tau_i, \tau) F(\tau, \tau_b) + F(\tau_i, \tau) \quad (122)$$

This is the adding formula for source terms in propagator formulation. Thus (84) and (122) may be used to obtain the adding of source terms in the extinction formulation.

Doubling method. Doubling can be viewed as a particular application of adding. In doubling we consider a homogeneous layer for which A is constant and the upward and downward components of the extinction matrix are the same. For the sake of discussion, we choose to use the property of matrix exponentials, such as defined by (152), to derive the doubling algorithm. Consider a layer of optical thickness τ for which the extinction matrix R , defined by (65), is given. From (152) and (114) we get

$$R(2\tau) = S_u [S_u (R(\tau)) S_u (R(\tau))] \quad (123)$$

Applying the S transformation to R and using (70), we obtain

$$S_u [R(2\tau)] = S_u [R(\tau)]^2 \quad (124)$$

Finally, from (68), it follows that

$$\begin{aligned} & \begin{bmatrix} t^{-1}(2\tau) & -t^{-1}(2\tau)r(2\tau) \\ r(2\tau)t^{-1}(2\tau) & t(2\tau) - r(2\tau)t^{-1}(2\tau)r(2\tau) \end{bmatrix} \\ &= \begin{bmatrix} t^{-1}(\tau) & -t^{-1}(\tau)r(\tau) \\ r(\tau)t^{-1}(\tau) & t(\tau) - r(\tau)t^{-1}(\tau)r(\tau) \end{bmatrix}^2 \end{aligned} \quad (125)$$

from which

$$t(2\tau) = t(\tau)(1 - r(\tau)^2)^{-1}t(\tau) \quad (126)$$

and

$$r(2\tau) = r(\tau) + t(\tau)r(\tau)(1 - r(\tau)^2)^{-1}t(\tau) \quad (127)$$

can be derived. This derivation defines the doubling scheme. It is usually employed to derive the extinction matrix for homogeneous layers. Clearly, an intimate relationship exists between *Ward's* [1977] algorithm for the calculation of a matrix exponent and the doubling formula.

Initialization methods. So far in the discussion of the extinction operator, it was assumed that the extinction matrix

$R(\tau)$ is known. We now discuss methods by which $R(\tau)$ is evaluated or "initialized", so that the composition rules described earlier can be employed. The method of initialization provides such an estimate of this matrix under the constraint that the medium is homogeneous. To this end, we could use, for example, the Taylor approximation (45), say, to the second order in τ , to approximate

$$e^{A\tau} \approx 1 + A\tau + \frac{A^2\tau^2}{2} + \dots \approx \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \tau \begin{bmatrix} a_1 & a_2 \\ -a_2 & -a_1 \end{bmatrix} + \frac{\tau^2}{2} \begin{bmatrix} a_1 & a_2 \\ -a_2 & -a_1 \end{bmatrix}^2 \quad (128)$$

Again using the S transformation (68), we obtain the transmittance function as

$$t = \left(1 - \tau a_1 + \frac{\tau^2}{2}(a_1^2 - a_2^2) \right)^{-1} = 1 + \tau a_1 + \frac{\tau^2}{2}(a_1^2 + a_2^2) \quad (129)$$

and the reflectance function as

$$r = a_2\tau + \frac{\tau^2}{2}(a_1a_2 + a_2a_1) \quad (130)$$

Equations (129) and (130) were derived by *Wiscombe* [1976] and are referred to as expanded diamond initialization (EDI). Independently, *Waterman* [1981] derived similar expressions up to third-order terms in τ . *Grant and Hunt* [1968a,b, 1969a,b] use a similar scheme, but only to a first order in τ and referred to this method as the infinitesimal generator initialization (IGI). As our analysis shows, EDI and IGI are both Taylor series decompositions of exponential. As we discussed previously, *Ward's* [1977] analysis indicates that Padé approximants may play some role in initialization schemes. It is clear that the conditions for small optical thickness are related to norm of A , namely, $\|A\|\tau/m \leq 1$, and the error analysis of initialization schemes should include such estimate.

The initialization schemes considered up to now apply to a homogenous atmosphere without sources. Consider an extension to this which allows us to initialize for sources. To this end, we need to evaluate integrals such as occur for the particular solution F given by (32), i.e.,

$$F = \int_{\tau_t}^{\tau} e^{A(\tau-s)} S ds \quad (131)$$

where both the $2n \times 2n$ matrix A and the $2n \times 1$ source vector S are assumed to be constant. Vector S is a $2n$ -dimensional equivalent of (37) or (38) evaluated for a particular sublayer. It can be seen from (84) that from F we can recover the source-related function G . After *van Loan* [1978], consider the $(2n+1) \times (2n+1)$ block triangular matrix

$$H = \begin{bmatrix} A & S \\ 0 & 0 \end{bmatrix} \quad (132)$$

and it can be proved that

$$e^{H\tau} = \begin{bmatrix} P & F \\ 0 & f \end{bmatrix} \quad (133)$$

where P and F follow our standard notation, with f a scalar function of τ . By equating submatrices in the identity (150) specified for matrix H and with boundary condition $\exp[H\tau]|_{\tau=0} = 1$, we get

$$\frac{d}{d\tau} P = AP$$

and

$$\frac{d}{d\tau} F = AF + S$$

and $f = 1$. The solution to these equations gives (133). Forming H and finding its matrix exponent with, for example, *Ward's* [1977] algorithm allows us to find both the fundamental solution and the source function integral F .

Splitting Methods and the Commutator

We begin our discussion by considering the fundamental solution for two combined layers extending from (τ_0, τ_1) and (τ_1, τ_2) . After (14), this solution requires the determination of the propagator

$$P_d(\tau_2, \tau_0) = e^{A_2(\tau_2-\tau_1)} e^{A_1(\tau_1-\tau_0)} \quad (134)$$

where A_1 and A_2 are matrices appropriately determined from the optical properties of each layer. It is tempting now to generalize (134) (and (21)) and replace them with

$$\exp \left(\int_{\tau_t}^{\tau} A(\tau) d\tau \right) \quad (135)$$

which is a possibility motivated by intuition from the Baker-Hausdorf-Campbell (BHC) exponential-type identity (59). Examining (59), we notice that additional terms to (135) appear, thus

$$P_d(\tau, \tau_t) = e^{\int_{\tau_t}^{\tau} A(\tau) d\tau} + \dots \quad (136)$$

where these unspecified additional terms involve integrals of commutators $[A(t), A(s)]$ and higher commutator terms. Although the commutator may seem only distantly relevant to radiative transfer, it conveniently describes several properties which we will now consider. We see that $\exp(\int_{\tau_t}^{\tau} A(t) dt)$ describes only part of the interaction of radiation with the medium. The presence of a nonvanishing commutator is a statement about asymmetry in the distribution of optical properties. In other words, two clouds (say, one composed of large droplets in the upper layer and small droplets in a bottom layer, and the second cloud with the reversed structure) may have the same $\int_{\tau_t}^{\tau} A(t) dt$, but they still will interact differently with radiation. This difference is characterized by the noncommutative property of matrices A , which tells us that two layers interact in a nonlinear way. Only in the small thickness limit is the interaction linear and do the matrices commute.

We will now explore the two-stream version of (136) to illustrate this feature. Before doing so, it is convenient to consider several variants of (136). Here we follow *Magnus* [1954] and *Wilcox* [1967] and assume that

$$P_d(\tau, \tau_t = 0) = e^{V(\tau)} \quad (137)$$

where $V(\tau)$ is a series

$$V(\tau) = \sum_{n=1}^{\infty} V_n(\tau) \quad (138)$$

Using exponential identities [e.g. *Stainberg*, 1988] one can derive the following formulas [*Wilcox*, 1967] for V

$$\mathbf{V}_1(\tau) = \int_0^\tau \mathbf{A}(s) ds \quad (139)$$

$$\mathbf{V}_2(\tau) = \frac{1}{2} \int_0^\tau ds \int_0^s dt [\mathbf{A}(s), \mathbf{A}(t)] \quad (140)$$

$$\mathbf{V}_3(\tau) = \frac{1}{6} \int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \int_0^{\tau_2} d\tau_3 ([[\mathbf{V}_1, \mathbf{V}_2], \mathbf{V}_3] + [[\mathbf{V}_3, \mathbf{V}_2], \mathbf{V}_1]) \quad (141)$$

⋮

where $\mathbf{A}_1 = \mathbf{A}(\tau_1)$, etc. and the higher-order terms can be calculated from recursive procedures.

The representation provided by (137) is of local nature as it applies to some local level τ . *Wei and Norman* [1964] discuss a more global approach based on product of exponentials

$$\mathbf{P}(\tau, \tau_i = 0) = \prod_{n=1}^k e^{\mathbf{V}_n(\tau)} \quad (142)$$

The advantage of the global representation (142) is that only finite amount of terms is required (see also *Sauter* [1979] and *Mulholland* [1971]).

Let us now consider an example of the commutator for the two-stream model. It follows from the definition of $\mathbf{A}$ for the two-stream model that (9) can be written in the form

$$\mathbf{A} = \mathbf{C} + \tilde{\omega} \mathbf{O} \quad (143)$$

where

$$\mathbf{C} = \begin{bmatrix} -1/4 & -7/4 \\ 7/4 & 1/4 \end{bmatrix} \quad (144)$$

and

$$\mathbf{O} = \frac{\tilde{\omega}}{4} \begin{bmatrix} 4 + 3g & 4 - 3g \\ -(4 - 3g) & -(4 + 3g) \end{bmatrix} \quad (145)$$

Consider two overlying homogeneous cloudy layers, one of optical thickness τ_1 and characterized by a single scatter albedo $\tilde{\omega}_1$ and the second layer characterized by properties τ_2 and $\tilde{\omega}_2$, and assume that the asymmetry parameter g is the same for both cloud layers. Such a situation might occur in reality, when, for instance, the upper portions of a cloud layer contain characteristically larger droplets (and hence smaller values of $\tilde{\omega}_0$) than the lower layers of the cloud. A relevant question to ask of such a case is whether or not the radiation reflected from the cloud is altered significantly when the positions of these layers are reversed. Some assessment of this problem can be made using (137) and (138). Suppose, for convenience, that $\tau_1 = \tau_2 = \tau$. Then it follows that

$$\mathbf{V}_1 = (\mathbf{A}_1 + \mathbf{A}_2)\tau \quad (146)$$

and

$$\mathbf{V}_2 = [\mathbf{A}_2, \mathbf{A}_1]\tau^2 \quad (147)$$

where, according to (143), the commutator becomes

$$\begin{aligned} [\mathbf{A}_1, \mathbf{A}_2] &= (\tilde{\omega}_2 - \tilde{\omega}_1) [\mathbf{C}, \mathbf{O}] \\ &= (\tilde{\omega}_2 - \tilde{\omega}_1) \begin{bmatrix} 0 & 3(g-1) \\ 3(g-1) & 0 \end{bmatrix} \end{aligned} \quad (148)$$

Applying now the S transformation (69), one can recover extinction matrix and, in turn, the reflection and transmission properties.

7. SUMMARY AND CONCLUSIONS

This paper outlines the general solution to the one-dimensional, azimuthally averaged radiative transfer equation in terms of a matrix exponential. This solution is developed for a vertically nonhomogeneous atmosphere. The link between the fundamental form of solution developed here to those more commonly used in radiative transfer (such as that of doubling/adding and Chandrasekhar's discrete ordinate approach) is established, and it is suggested that the matrix exponential formulations present the framework for the unification of the many different existing methods of solution. This paper demonstrates how the methods of invariant imbedding and discrete ordinates are in fact special forms of similarity transformation. It is apparent from discussions presented in this paper that the doubling and adding schemes provide a stable algorithm for the solution of the two-point boundary value problems typically encountered in radiative transfer. It was also further demonstrated how the approach might be made more numerically efficient by using Padé approximant. The paper furthermore provides examples of the two-stream solutions formulated as a matrix exponential and provides some new insight into the mathematical structure of the two-stream model. Some concepts, new to radiative transfer, which deal with the use of commutator and vertical structure equations, are described at the end of the paper.

APPENDIX: SOME PROPERTIES OF PRODUCT INTEGRAL AND MATRIX EXPONENT

Various properties of the product integral are used throughout this paper. We summarize some of these properties here. Refer to *Dollard and Friedman* [1979] for further discussion.

Property 1. For a matrix $\mathbf{A}(\tau)$ defined by (8) for optical thickness (τ, τ_i) we get derivative of product integral

$$\frac{d}{d\tau} \prod_{\tau_i}^{\tau} \exp[\mathbf{A}(s) ds] = \mathbf{A}(\tau) \prod_{\tau_i}^{\tau} \exp[\mathbf{A}(s) ds] \quad (149)$$

For constant $\mathbf{A}$, i.e., vertically homogeneous atmosphere, we get

$$\frac{d}{d\tau} e^{\mathbf{A}\tau} = \mathbf{A}e^{\mathbf{A}\tau} \quad (150)$$

Property 2. For two levels defined by optical thicknesses $\tau_b > \tau > \tau_i$ it follows from the definition of product integral (21) that

$$\prod_{\tau_i}^{\tau_b} \exp[\mathbf{A}(s) ds] = \prod_{\tau}^{\tau_b} \exp[\mathbf{A}(s) ds] \prod_{\tau_i}^{\tau} \exp[\mathbf{A}(s) ds] \quad (151)$$

This was already discussed in some length when deriving (20). The special case of constant $\mathbf{A}$ and same optical thicknesses gives (compare equation (159))

$$\exp[\mathbf{A}(s)\tau] = \{\exp[\mathbf{A}(s)\tau/2]\}^2 \quad (152)$$

and a simple extension to m layers gives

$$\exp[\mathbf{A}(s)\tau] = \{\exp[\mathbf{A}(s)\tau/m]\}^m \quad (153)$$

Property 3. Determinant of matrix exponent is given by

$$\det \left[\prod_{\tau_i}^{\tau} \exp[\mathbf{A}(s) ds] \right] = \exp \left[\int_{\tau_i}^{\tau} \text{tr} \mathbf{A}(s) ds \right] \quad (154)$$

Where tr indicates trace (sum of diagonal elements) of a matrix. Equation (154) shows that the propagator (22) is nonsingular, i.e. $\det \mathbf{P} \neq 0$.

Property 4. Upward and downward propagators P_d and P_u are related through matrix inversion by

$$\prod_{\tau_i}^{\tau_b} \exp[\mathbf{A}(s) ds] = \left(\prod_{\tau_i}^{\tau_b} \exp[\mathbf{A}(s) ds] \right)^{-1} \quad (155)$$

In particular, for the homogenous layer, where $\mathbf{A}$ is constant, we have

$$\mathbf{P}_d = e^{\mathbf{A}\tau} \quad \mathbf{P}_u = e^{-\mathbf{A}\tau} \quad (156)$$

which satisfies (156). Also,

$$e^{\mathbf{A}} e^{-\mathbf{A}} = e^{-\mathbf{A}} e^{\mathbf{A}} = \mathbf{I} \quad (157)$$

Thus in terminology of radiative transfer, downward propagation followed by upward propagation leaves intensities unchanged.

Property 5. If for all optical thicknesses τ, τ' matrices $\mathbf{A}$ commute, i.e., $\mathbf{A}(\tau)\mathbf{A}(\tau') = \mathbf{A}(\tau')\mathbf{A}(\tau)$, then the product integral of $\mathbf{A}$ can be evaluated as

$$\prod_{\tau_i}^{\tau_b} \exp[\mathbf{A}(s) ds] = \exp \left[\int_{\tau_i}^{\tau_b} \mathbf{A}(s) ds \right] \quad (158)$$

In particular, this formula is true for a homogeneous atmosphere, which gives

$$\mathbf{P}_d(\tau, \tau_i) = \exp[\mathbf{A}(\tau - \tau_i)] \quad (159)$$

Property 6. Certain bounds on the propagator can be established

$$\left\| \prod_{\tau_i}^{\tau_b} [\mathbf{A}(s) ds] \right\| \leq \exp \left[\int_{\tau_i}^{\tau_b} \|\mathbf{A}(s)\| ds \right] \quad (160)$$

Property 7 Similarity rule. Suppose matrix $\mathbf{T}(\tau)$ is defined for the layer and is nonsingular and has continuous derivative. Then

$$\begin{aligned} \mathbf{T}^{-1}(\tau) \prod_{\tau_i}^{\tau} \exp[\mathbf{A}(s) ds] \mathbf{T}(\tau_i) \\ = \prod_{\tau_i}^{\tau} \exp \left[\left(\mathbf{T}^{-1}(s) \mathbf{A}(s) \mathbf{T}(s) - \mathbf{T}^{-1}(\tau) \frac{d\mathbf{T}(s)}{ds} \right) ds \right] \end{aligned} \quad (161)$$

which is a consequence of transformation of variables in (8).

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