PERGAMON

Journal of Quantitative Spectroscopy & Radiative Transfer 64 (2000) 219–226

Journal of Quantitative Spectroscopy & Radiative Transfer

www.elsevier.com/locate/jqsrt

Particular solutions for the discrete-ordinates method

L.B. Barichello[a], R.D.M. Garcia[b], C.E. Siewert[c]

[a] Instituto de Matemática, Universidade Federal do Rio Grande do Sul, 91509-900 Porto Alegre, RS, Brazil
[b] Centro Técnico Aeroespacial, Instituto de Estudos Avançados, 12231-970 São José dos Campos, SP, Brazil
[c] Mathematics Department, North Carolina State University, Raleigh, NC 27695-8205, USA

Received 12 October 1998

Abstract

A full-range orthogonality relation is developed and used to construct the infinite-medium Green's function for a general form of the discrete-ordinates approximation to the transport equation in plane geometry. The Green's function is then used to define a particular solution that is required in the solution of inhomogeneous versions of the discrete-ordinates equations. © 1999 Elsevier Science Ltd. All rights reserved.

1. Introduction

In a series of papers [1–3] concerning radiation-transport problems in plane geometry, linear-algebra techniques were used to develop particular solutions to be used with the spherical-harmonics method when solving problems based on an inhomogeneous version of the equation of transfer. In this work, we use the elementary solutions of the homogeneous discrete-ordinates equations to develop the infinite-medium Green's function, which is then used to construct a particular solution of a general form of the inhomogeneous discrete-ordinates equations.

As we wish to include in this work a model [4, 5] used in studies of scattering with complete energy redistribution, we start with the equation of transfer

$$\xi \frac{\partial}{\partial \tau} G(\tau, \xi) + G(\tau, \xi) = \sum_{l=0}^{L} f_l \Pi_l(\xi) \int_{-\gamma}^{\gamma} \Psi(\xi') \Pi_l(\xi') G(\tau, \xi') \, d\xi' + Q(\tau, \xi) \tag{1}$$

for $\tau \in (0, \tau_0)$ and $\xi \in [-\gamma, \gamma]$. As we also wish to include here all of the Fourier-component ($m \geq 0$) problems basic to the general azimuth-dependent transport equation [6], and since the details are not required for what we do here, we do not specify the functions $\Pi_l(\xi)$ and $\Psi(\xi)$ or the constants $\{f_l\}$ that appear in Eq. (1). However, we do exclude from our

PII: S0022-4073(98)00146-0

current development the conservative case which we define in Section 5 of this work. To complete our discussion of Eq. (1), we note that the inhomogeneous term $Q(\tau, \xi)$ is considered to be known.

To have a set of discrete-ordinates equations we use an N-point quadrature scheme with nodes $\{\xi_i\}$ and weights $\{w_i\}$ and rewrite Eq. (1) as

$$\xi_i \frac{\mathrm{d}}{\mathrm{d}\tau} G(\tau, \xi_i) + G(\tau, \xi_i) = \sum_{l=0}^{L} f_l \Pi_l(\xi_i) \sum_{n=1}^{N} w_n \Psi(\xi_n) \Pi_l(\xi_n) G(\tau, \xi_n) + Q(\tau, \xi_i) \tag{2}$$

for $i = 1, 2, \dots, N$. As we do not put any restrictions on our quadrature scheme, we clearly include the possibility of using a composite scheme where the full-range integration interval $[-\gamma, \gamma]$ is subdivided into any number of sub-intervals with an equal or unequal number of quadrature points in each of them.

2. The elementary solutions of the discrete-ordinates equations

Our goal here is to find a particular solution of Eq. (2); however to do that we first want to construct the infinite-medium Green's function in terms of solutions to the homogeneous version of Eq. (2). So, seeking exponential solutions, we substitute

$$G(\tau, \xi_i) = \phi(\nu, \xi_i) \mathrm{e}^{-\tau/\nu} \tag{3}$$

into the homogeneous version of Eq. (2) to obtain

$$\left(1 - \frac{\xi_i}{\nu}\right) \phi(\nu, \xi_i) = \sum_{l=0}^{L} f_l \Pi_l(\xi_i) g_l(\nu), \tag{4}$$

where we have defined

$$g_l(\nu) = \sum_{i=1}^{N} w_i \Psi(\xi_i) \Pi_l(\xi_i) \phi(\nu, \xi_i). \tag{5}$$

We consider that $\nu \notin \{\xi_i\}$ so that we can solve Eq. (4) to find

$$\phi(\nu, \xi_i) = \frac{\nu}{\nu - \xi_i} \sum_{l=0}^{L} f_l \Pi_l(\xi_i) g_l(\nu). \tag{6}$$

Now upon multiplying Eq. (6) by $w_i \Psi(\xi_i) \Pi_\alpha(\xi_i)$, for $\alpha = 0, 1, \dots, L$, and summing over i, we find

$$[\mathbf{I} - \mathbf{M}(\nu)]\mathbf{g}(\nu) = \mathbf{0}, \tag{7}$$

where the components of the vector $\mathbf{g}(\nu)$ are $g_0(\nu), g_1(\nu), \dots, g_L(\nu)$ and where the elements of the matrix $\mathbf{M}(\nu)$ are given by

$$M_{\alpha,l}(\nu) = \nu f_l \sum_{i=1}^{N} \frac{w_i \Psi(\xi_i)}{\nu - \xi_i} \Pi_\alpha(\xi_i) \Pi_l(\xi_i). \tag{8}$$

It is clear that

$$\Omega(v) = \det[\mathbf{I} - \mathbf{M}(v)] = 0 \tag{9}$$

will define the acceptable collection of separation constants or eigenvalues $\{v_k\}$. It is also clear that once we have found these eigenvalues, the components of $\mathbf{g}(v_k)$ can be found from Eq. (7), and so in this way we can, in principle, complete the definition of the elementary solutions listed as Eq. (6).

We note that there is an important class of problems [6] where special properties of the defining functions $\Psi(\xi)$ and $\Pi_l(\xi)$, along with particular values of the constants γ and $\{f_l\}$ and certain choices for the quadrature scheme, make it possible to simplify greatly the use of Eqs. (9) and (7) to find the eigenvalues $\{v_k\}$ and the required components of the vector $\mathbf{g}(v_k)$. However, since we wish to keep our formulation general, we do not pursue that line of analysis here.

It is clear that, while the condition $\Omega(v) = 0$ does define the spectrum, trying to find the eigenvalues (or even the number of eigenvalues) from Eq. (9) is not, in general, very attractive from a computational point of view. However, we have another way. Considering Eq. (4) for $i = 1, 2, \dots, N$, we can write that collection of equations in the form

$$\Xi^{-1}(\mathbf{I} - \mathbf{W})\mathbf{\Phi}(v) = \frac{1}{v}\mathbf{\Phi}(v), \tag{10}$$

where $\mathbf{I}$ is the identity matrix, and where the components of $\mathbf{\Phi}(v)$ are $\phi(v, \xi_i)$, for $i = 1, 2, \dots, N$,

$$\Xi = \text{diag}\{\xi_1, \xi_2, \dots, \xi_N\} \tag{11}$$

and the elements of the $\mathbf{W}$ matrix are given by

$$W_{i,j} = w_j \Psi(\xi_j) \sum_{l=0}^{L} f_l \Pi_l(\xi_i) \Pi_l(\xi_j). \tag{12}$$

Now since Eq. (10) is in the standard form of an eigenvalue problem, we see that there are exactly N eigenvalues and that they can be computed by using, for example, the driver program RG from the EISPACK collection [7]. In addition, we note that while computing $\mathbf{g}(v_k)$ from Eq. (7) and using the components of these vectors in Eq. (6) to establish the required elementary solutions can be efficient for cases where $L \ll N$, one should consider, when this is not the case, computing the elementary solutions directly as the eigenvectors defined by Eq. (10).

It is usually the case in transport calculations [6, 8] that the eigenvalue spectrum $\{v_k\}$ is such that the eigenvalues occur in plus–minus pairs; however, since we do not wish to impose any special properties on the defining functions or assign any special values to the constants in Eq. (1), and since we wish to allow the possibility that our discrete-ordinates solution can be based on a composite quadrature scheme, that need not even be symmetric about the origin, then we cannot assume that the eigenvalues occur in pairs. So to maintain as much generality as possible, we assume only that the eigenvalue problem as defined by Eq. (10) yields J positive and $N - J$ negative, distinct and real eigenvalues and that the intersection of $\{v_k\}$ and $\{\xi_i\}$ is null.

We consider that we have found the eigenvalues $\{v_k\}$, and so we now want to prove that these elementary solutions $\phi(v_k, \xi_i)$ satisfy a full-range orthogonality relation. To see this we first evaluate Eq. (4) at $v = v_j$ and then multiply the resulting equation by $w_i \Psi(\xi_i) \phi(v_k, \xi_i)$ and sum over i to find

$$\sum_{i=1}^{N} w_i \Psi(\xi_i) \phi(v_k, \xi_i) \left(1 - \frac{\xi_i}{v_j}\right) \phi(v_j, \xi_i) = \sum_{l=0}^{L} f_l g_l(v_k) g_l(v_j). \tag{13}$$

If we subtract Eq. (13) from a version of Eq. (13) that has j and k interchanged we find the classical form

$$(v_j - v_k) \sum_{i=1}^{N} w_i \xi_i \Psi(\xi_i) \phi(v_j, \xi_i) \phi(v_k, \xi_i) = 0, \tag{14}$$

and so, since we have assumed the eigenvalues to be distinct,

$$\sum_{i=1}^{N} w_i \xi_i \Psi(\xi_i) \phi(v_j, \xi_i) \phi(v_k, \xi_i) = 0, \quad j \neq k. \tag{15}$$

We note that elementary linear-algebra techniques can also be used to derive this orthogonality condition from Eq. (10).

To complete this part of our work, we note that the functions $\phi(v_j, \xi_i)$, as defined by Eqs. (4) and (5), can be scaled by an arbitrary constant, and so we choose to normalize these solutions by taking

$$\sum_{i=1}^{N} w_i \Psi(\xi_i) \phi(v_j, \xi_i) = 1. \tag{16}$$

3. The infinite-medium Green's function

Since we have developed the elementary solutions of the homogeneous version of Eq. (2), we can use those solutions to construct the Green's function we seek. We therefore consider

$$\xi_i \frac{\mathrm{d}}{\mathrm{d}\tau} \mathrm{G}(\tau, \xi_i : x, \xi_\alpha) + G(\tau, \xi_i : x, \xi_\alpha) = \sum_{l=0}^{L} f_l \Pi_l(\xi_i) \sum_{n=1}^{N} w_n \Psi(\xi_n) \Pi_l(\xi_n) \times G(\tau, \xi_n : x, \xi_\alpha) + \delta(\tau - x) \delta_{i,\alpha} \tag{17}$$

for $i, \alpha = 1, 2, \ldots, N$. Here we take the "source location" to be $x \in (0, \tau_0)$ and the "source direction" to be $\xi_\alpha \in \{\xi_i\}$. We note that $\delta(\tau - x)$ is the Dirac delta "function" and that $\delta_{i,\alpha}$ is the Kronecker delta.

To develop the desired solution for $G(\tau, \xi_k : x, \xi_\alpha)$ we can, as discussed for example by Case and Zweifel [8], write one solution valid for $\tau > x$ (and bounded as $\tau \to \infty$) and another solution valid for $\tau < x$ (and bounded as $\tau \to -\infty$); we can then match-up these two solutions with the "jump condition"

$$\xi_i \lim_{\varepsilon \to 0} [G(x + \varepsilon, \xi_i : x, \xi_\alpha) - G(x - \varepsilon, \xi_i : x, \xi_\alpha)] = \delta_{i,\alpha} \tag{18}$$

for $i = 1, 2, \ldots, N$.

We now wish to use the elementary solutions derived in the previous section of this work to construct the Green's function; however, we must first distinguish between the positive and the negative eigenvalues. So from this point in our work onward, we use ν_j for $j = 1, 2, \dots, J$ to denote the positive eigenvalues and we use $-\nu_j$ for $j = J+1, J+2, \dots, N$ to denote the negative eigenvalues. We therefore can express the desired solution as

$$G(\tau, \xi_i\colon x, \xi_\alpha) = \sum_{j=1}^{J} A_{j,\alpha}\phi(\nu_j, \xi_i)\mathrm{e}^{-(\tau - x)/\nu_j}, \quad \tau > x, \tag{19a}$$

and

$$G(\tau, \xi_i\colon x, \xi_\alpha) = -\sum_{j=J+1}^{N} B_{j,\alpha}\phi(-\nu_j, \xi_i)\mathrm{e}^{-(x-\tau)/\nu_j}, \quad \tau < x. \tag{19b}$$

Substituting Eqs. (19) into Eq. (18) we find

$$\xi_i \sum_{j=1}^{J} A_{j,\alpha}\phi(\nu_j, \xi_i) + \xi_i \sum_{j=J+1}^{N} B_{j,\alpha}\phi(-\nu_j, \xi_i) = \delta_{i,\alpha}, \tag{20}$$

and so we multiply Eq. (20) by $w_i\Psi(\xi_i)\phi(\nu_\beta, \xi_i)$, sum, for $1 \le \beta \le J$, over i from 1 to N and use Eq. (15) to find

$$A_{\beta,\alpha} = \frac{w_\alpha \Psi(\xi_\alpha)\phi(\nu_\beta, \xi_\alpha)}{N(\nu_\beta)}. \tag{21a}$$

In a similar manner we multiply Eq. (20) by $w_i\Psi(\xi_i)\phi(-\nu_\beta, \xi_i)$, $J+1 \le \beta \le N$, sum over i from 1 to N and use Eq. (15) to find

$$B_{\beta,\alpha} = \frac{w_\alpha \Psi(\xi_\alpha)\phi(-\nu_\beta, \xi_\alpha)}{N(-\nu_\beta)}. \tag{21b}$$

Here

$$N(\pm\nu_\beta) = \sum_{i=1}^{N} w_i \xi_i \Psi(\xi_i)[\phi(\pm\nu_\beta, \xi_i)]^2. \tag{22}$$

4. The particular solution: general and special cases

Having found the Green's function, we can immediately express the desired particular solution to Eq. (2) as

$$G_{\mathrm{p}}(\tau, \xi_i) = \int_0^{\tau_0} \sum_{\alpha=1}^{N} G(\tau, \xi_i\colon x, \xi_\alpha) Q(x, \xi_\alpha)\,\mathrm{d}x \tag{23}$$

which can, after we make use of Eqs. (19), be written as

$$G_{\mathrm{p}}(\tau, \xi_i) = \sum_{j=1}^{J} \mathscr{A}_j(\tau)\phi(\nu_j, \xi_i) + \sum_{j=J+1}^{N} \mathscr{B}_j(\tau)\phi(-\nu_j, \xi_i), \tag{24}$$

where

$$\mathscr{A}_j(\tau) = \int_0^{\tau} \left\{ \sum_{\alpha=1}^{N} Q(x, \xi_\alpha)\, A_{j,\alpha} \right\} \mathrm{e}^{-(\tau - x)/\nu_j}\,\mathrm{d}x \tag{25a}$$

and

$$\mathscr{B}_j(\tau) = -\int_{\tau}^{\tau_0} \left\{ \sum_{\alpha=1}^{N} Q(x, \xi_\alpha)\, B_{j,\alpha} \right\} \mathrm{e}^{-(x-\tau)/v_j}\, \mathrm{d}x, \tag{25b}$$

and where the $A_{j,\alpha}$ and $B_{j,\alpha}$ are defined by Eqs. (21). Equation (24) is our particular solution for the general case; so we now look at two cases of interest where that result can be simplified.

The first special case we consider is defined by the source term in Eq. (2) being independent of ξ_i, so that $Q(x, \xi_i)$ can be replaced by $Q(x)$ in Eqs. (25), and so we can use Eqs. (21) and the normalization condition given by Eq. (16) to write

$$\mathscr{A}_j(\tau) = \frac{1}{N(v_j)} \int_0^{\tau} Q(x) \mathrm{e}^{-(\tau - x)/v_j}\, \mathrm{d}x \tag{26a}$$

and

$$\mathscr{B}_j(\tau) = -\frac{1}{N(-v_j)} \int_{\tau}^{\tau_0} Q(x) \mathrm{e}^{-(x-\tau)/v_j}\, \mathrm{d}x. \tag{26b}$$

For our second special case we consider

$$Q(\tau, \xi_i) = F(\xi_i) \mathrm{e}^{-\tau/\xi_0} \tag{27}$$

which is encountered [6] in radiation-transport problems when the radiation due to an incident beam is separated from the "diffuse field" in order to avoid some complications that can arise when generalized functions are used to define the boundary conditions of the problem. For this case we find we can write Eqs. (25) as

$$\mathscr{A}_j(\tau) = \frac{\xi_0 v_j}{N(v_j)}\, C(\tau\colon v_j, \xi_0) \sum_{\alpha=1}^{N} w_\alpha \Psi(\xi_\alpha) \phi(v_j, \xi_\alpha) F(\xi_\alpha) \tag{28a}$$

and

$$\mathscr{B}_j(\tau) = -\frac{\xi_0 v_j}{N(-v_j)} \mathrm{e}^{-\tau/\xi_0} S(\tau_0 - \tau\colon v_j, \xi_0) \sum_{\alpha=1}^{N} w_\alpha \Psi(\xi_\alpha) \phi(-v_j, \xi_\alpha) F(\xi_\alpha), \tag{28b}$$

where

$$S(\tau\colon x, y) = \frac{1 - \mathrm{e}^{-\tau/x} \mathrm{e}^{-\tau/y}}{x + y} \tag{29a}$$

and

$$C(\tau\colon x, y) = \frac{\mathrm{e}^{-\tau/x} - \mathrm{e}^{-\tau/y}}{x - y}. \tag{29b}$$

5. The conservative case

We now would like to discuss briefly the conservative case, which we have implicitly excluded from our analysis in the preceding sections of this work. While it is possible that the term conservative case can be interpreted in various ways, we use the term here to mean those values of the parameters $\{f_l\}$, for a given L, which allow the separation constant v in Eq. (3) to be unbounded. Continuing, we see from Eq. (3) that allowing v to be unbounded implies that the homogeneous version of Eq. (2) can be satisfied by a solution of the form

$$G(\tau, \xi_i) = \phi(\xi_i). \tag{30}$$

So now if we substitute Eq. (30) into the homogeneous version of Eq. (2) we find

$$\phi(\xi_i) = \sum_{l=0}^{L} f_l \Pi_l(\xi_i) g_l \tag{31}$$

for $i = 1, 2, \ldots, N$. Here

$$g_l = \sum_{n=1}^{N} w_n \Psi(\xi_n) \Pi_l(\xi_n)\, \phi(\xi_n). \tag{32}$$

We now multiply Eq. (31) by $w_i \Psi(\xi_i)\Pi_\alpha(\xi_i)$, for $\alpha = 0, 1, \ldots, L$, and sum the resulting equation over the index i to obtain

$$g_\alpha = \sum_{l=0}^{L} a_{\alpha,l} g_l, \tag{33}$$

where

$$a_{\alpha,l} = f_l \sum_{n=1}^{N} w_n \Psi(\xi_n) \Pi_\alpha(\xi_n) \Pi_l(\xi_n). \tag{34}$$

Finally, we can rewrite Eq. (33), for $\alpha = 0, 1, \ldots, L$, as

$$[\mathbf{I} - \mathbf{A}]\mathbf{g} = \mathbf{0}, \tag{35}$$

where the $(L+1) \times (L+1)$ matrix $\mathbf{A}$ has elements $a_{\alpha,l}$ and the vector $\mathbf{g}$ has elements g_l for $l = 0, 1, 2, \ldots, L$. Clearly any combination of the parameters $\{f_l\}$ that makes the coefficient matrix $\mathbf{I} - \mathbf{A}$ singular will yield what we have defined to be a conservative case.

From an analytical and computational point of view, the problem with the conservative case is that the largest separation constant becomes infinite, and so the exponential solution, introduced by Eq. (3), does not always generate the two independent forms of the solution that are needed. Rather than develop the modifications to our particular solution for non-conservative cases to include all possible conservative cases, we note that these modifications have been developed and used [9] for the classical azimuth-dependent model of radiative transfer [6].

6. Concluding comments

Particular solutions, of course, are not unique since to any given particular solution we can always add arbitrary multiples of solutions of the homogeneous equation. And so in some cases results simpler than the ones we have found here can be obtained; however, these simpler forms (see for example the one used by Chandrasekhar [6] to solve the classical albedo problem) can have singularities for certain values of the defining parameters.

While we have focused our attention in this work on finding a particular solution for use with the discrete-ordinates method, we have found that the methods used here can also be used to obtain the particular solutions for the spherical-harmonics method that are reported in Refs. [1–3].

Acknowledgements

It is noted that the work of L.B.B. and R.D.M.G. was supported in part by CNPq of Brazil.

References

[1] Siewert CE, Thomas Jr JR. JQSRT 1990;43:433.
[2] McCormick NJ, Siewert CE. JQSRT 1991;46:519.
[3] Siewert CE, McCormick NJ. JQSRT 1993;50:531.
[4] Hummer DG. Mon Not R Astr Soc 1968;138:73.
[5] McCormick NJ, Siewert CE. Astrophys J 1970;162:633.
[6] Chandrasekhar S, Radiative transfer. London: Oxford University Press, 1950.
[7] Smith BT, Boyle JM, Dongarra JJ, Garbow BS, Ikebe Y, Klema VC, Moler CB. Matrix eigensystem routines — EISPACK guide, Berlin: Springer, 1976.
[8] Case KM, Zweifel PF. Linear transport theory. Reading, MA: Addison-Wesley, 1967.
[9] Siewert CE. JQSRT 2000;64:227.