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Biorthogonal Angular Polynomial Expansions of the Boltzmann Transport Equation

by

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Abstract

A new system of biorthogonal polynomials is developed for the angular expansion of the directional flux in the linear Boltzmann transport equation. Recursion relations and an addition theorem are derived for a system of biorthogonal polynomials shown by Didon (1868) to be orthogonal over the unit hemisphere. These polynomials are applied to two dimensional forms of the Boltzmann equation. Equations for the coefficients of expansion are derived when the directional flux is expanded in a series of either system of polynomials. One of these systems of equations is shown to be a linear combination (with specific coefficients) of the equations obtained when the directional flux is expanded in spherical harmonic functions, and it is shown that this same system reduces to the spherical harmonics equations in one dimensional plane geometry.

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Introduction

One of the common methods of formulating mathematical approximations to the Boltzmann transport equation involves the expansion of the angular dependence of the directional flux in spherical harmonics. The expansion process results in an infinite system of coupled equations for the expansion coefficients, and this system is usually truncated by means of a terminating condition, which may be chosen almost arbitrarily. The approach has several advantages. It can be applied in general geometries[1,2] and is convenient because of the orthogonality properties of the spherical harmonic functions. If the particle sources include anisotropic scattering, the spherical harmonic addition theorem permits simple treatment of this kind of a source and minimizes the source coupling of the equations for the expansion coefficients. Further, particle conservation, a property of the exact transport equation, is maintained in the equations of the spherical harmonic approximations.

Despite these advantages, considerable effort has been expended in developing other angular expansion approximations. Part of this effort has been motivated by the desire to find simpler or more rapidly converging approximate systems. In one dimensional plane geometry, Aspelund[3] and Conkie[4] investigated Tschebyscheff angular expansions, and Mika[5] and Pomraning[6] considered expansions in terms of Jacobi polynomials. All of these efforts, which substitute classical orthogonal polynomials for the spherical harmonic functions, lead to approximations which are not readily generalized to other geometries and which, without modification, do not conserve particles. At the expense of the convenience of orthogonality and addition theorems, these latter two failings are eliminated by the very general expansion method proposed by Carlson.[7,8]

In this work still another expansion procedure is described, one which, although it may be applied to one or two dimensional cylindrical geometry, seems particularly adapted for use in two dimensional (x,y) rectangular geometry. In this method the angular dependence of the directional flux is expanded in terms of either of two systems of polynomials in two variables. The two systems of polynomials form a biorthogonal set and possess an addition theorem that permits simple treatment of anisotropic scattering. In (x,y) geometry the systems of equations for the expansion coefficients possess symmetry properties lacking in the usual spherical harmonic expansion. In the same geometry, expansion in terms of one system of polynomials of the biorthogonal set is a generalization of the Legendre polynomial expansion in plane geometry, and the system of equations for the expansion coefficients is easily reduced to the plane geometry case.

The work described here is preliminary in that no consideration is given to derivation of boundary conditions or to examination of terminating conditions. In addition, no attempt is made to solve the general systems of equations that are obtained. We content ourselves with deriving equations for expansion coefficients, examining some of the properties of these equations, and deriving the basic relations satisfied by the biorthogonal polynomials.

In the first section we formulate the Boltzmann equation in (x,y) rectangular geometry and describe the angular coordinate systems used throughout the work. In the second section we derive the two systems of coupled equations that result when the directional flux is expanded in each of the two systems of polynomials of the biorthogonal set. In the third section one of these systems is related to the usual spherical harmonic expansion, and in a fourth section certain elementary properties of the systems are examined. In a final section we discuss possibilities (of which there are many) for future investigations. Derivation of identities used in the text and of other useful relations are given in the appendices. In addition, the use of biorthogonal polynomials in cylindrical geometry and the expansion technique of Carlson are described in appendices.

The Boltzmann Equation in (x,y) Geometry

The general time-independent, monoenergetic Boltzmann equation is

$$\nabla\cdot(\underset{\sim}{\Omega}\psi) + \sigma(\underset{\sim}{r})\psi(\underset{\sim}{r},\Omega) = \int d\Omega'\psi(\underset{\sim}{r},\underset{\sim}{\Omega}')\sigma_s(\underset{\sim}{r})f(\underset{\sim}{\Omega}' \rightarrow \underset{\sim}{\Omega}) + \mathscr{S}(\underset{\sim}{r},\underset{\sim}{\Omega}) \qquad (1)$$

in which σ and σ_s are the macroscopic total and scattering cross sections, ψ is the particle flux (speed times density) at position $\underset{\sim}{r}$ traveling in the direction $\underset{\sim}{\Omega}$, f is the probability for transfer of a particle to $d\Omega$ about $\underset{\sim}{\Omega}$ after a scattering event in $d\Omega'$ about $\underset{\sim}{\Omega}'$, and $\mathscr{S}$ is the source of particles. For notational convenience we have restricted ourselves to the monoenergetic equation, but the expansions in the following sections are also applicable to the velocity dependent equation.

If the medium under consideration is infinite in the z direction, and if sources and cross sections do not depend on z, then ψ is independent of z, and Eq. (1) becomes

$$\mu\frac{\partial\psi}{\partial x} + \eta\frac{\partial\psi}{\partial y} + \sigma\psi = \sigma_s \int d\Omega'\psi(x,y,\underset{\sim}{\Omega}')f(\underset{\sim}{\Omega}' \rightarrow \underset{\sim}{\Omega}) + \mathscr{S}(x,y,\underset{\sim}{\Omega}) \qquad (2)$$

In Eq. (2) the angular coordinate system is such that $\underset{\sim}{\Omega}\cdot\underset{\sim}{e}_x = \mu$, $\underset{\sim}{\Omega}\cdot\underset{\sim}{e}_y = \eta$, and $\underset{\sim}{\Omega}\cdot\underset{\sim}{e}_z = \xi$ as depicted in Fig. 1. The variables μ, η, and ξ are the direction cosines of $\underset{\sim}{\Omega}$ and, hence,

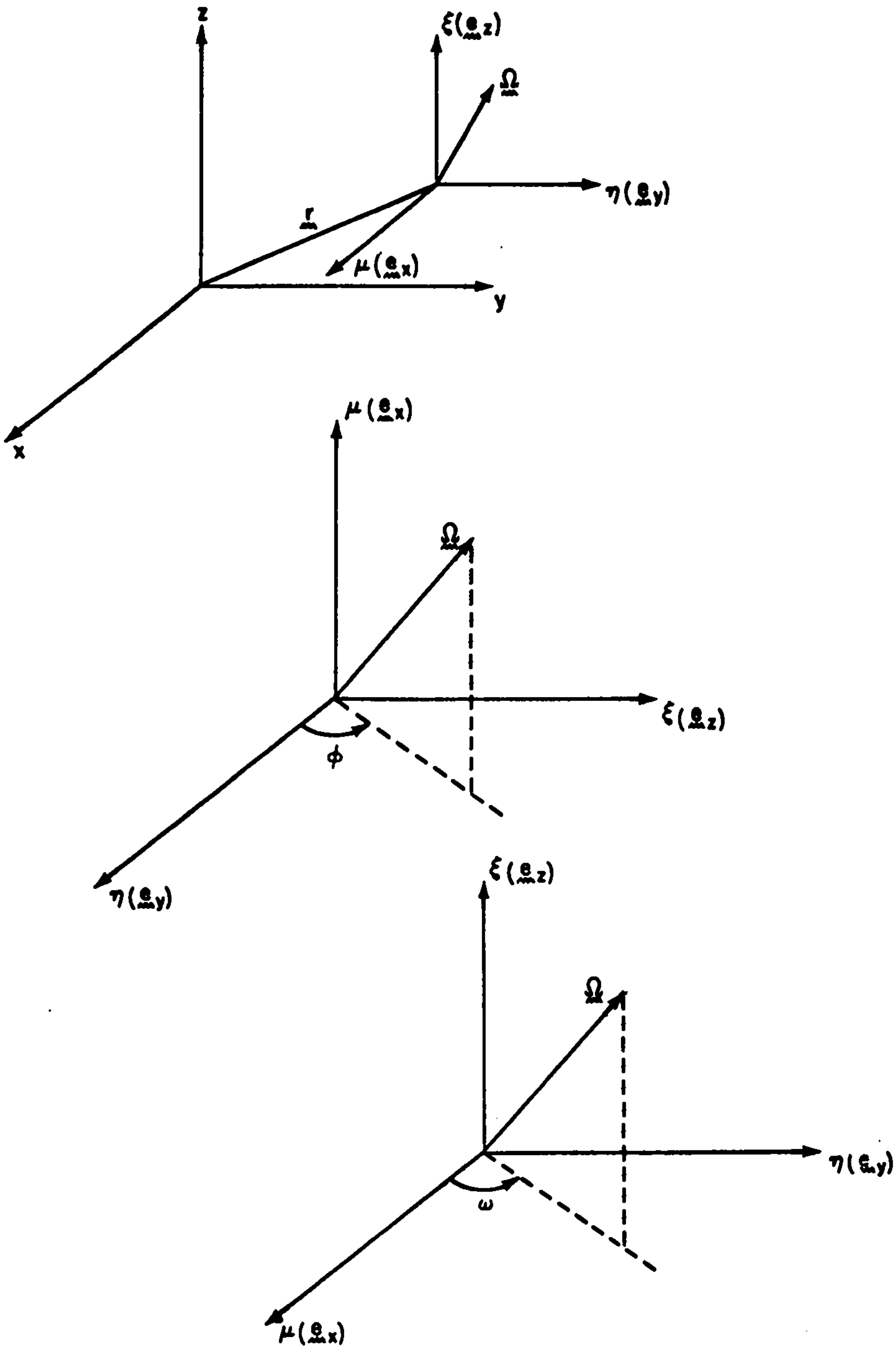

Fig. 1. Coordinate Systems.

$$\mu^2 + \eta^2 + \xi^2 = 1 \tag{3}$$

so that the unit vector $\underset{\sim}{\Omega} = \underset{\sim}{\Omega}(\mu, \eta, \xi)$ subject to Eq. (3). We shall have occasion to use two other representations of $\underset{\sim}{\Omega}$:

$$\text{a)} \quad \underset{\sim}{\Omega} = \underset{\sim}{\Omega}(\mu, \varphi) \qquad \begin{aligned} \eta &= (1 - \mu^2)^{\frac{1}{2}} \cos\varphi \\ \xi &= (1 - \mu^2)^{\frac{1}{2}} \sin\varphi \end{aligned} \tag{4}$$

$$\text{b)} \quad \underset{\sim}{\Omega} = \underset{\sim}{\Omega}(\xi, \omega) \qquad \begin{aligned} \mu &= (1 - \xi^2)^{\frac{1}{2}} \cos\omega \\ \eta &= (1 - \xi^2)^{\frac{1}{2}} \sin\omega \end{aligned} \tag{5}$$

These coordinates are also shown in Fig. 1. In terms of Eq. (4), the transport equation can be written

$$\begin{aligned} \mu \frac{\partial\psi}{\partial x} + \eta \frac{\partial\psi}{\partial y} + \sigma\psi(x, y, \mu, \varphi) &= \sigma_s \int_{-1}^{1} d\mu' \int_{-\pi}^{\pi} d\varphi' \psi(x, y, \mu', \varphi') f(\underset{\sim}{\Omega}' \rightarrow \underset{\sim}{\Omega}) \\ &\quad + \mathscr{S}(x, y, \mu, \varphi) \end{aligned} \tag{6}$$

Now, if $\mathscr{S}$ is an even function of φ and if $f(\underset{\sim}{\Omega}' \rightarrow \underset{\sim}{\Omega})$ is a function of $\underset{\sim}{\Omega}' \cdot \underset{\sim}{\Omega}$ only, then ψ is also an even function of φ, or what is the same thing, an even function of ξ, and hence a function of μ and η alone [because of Eq. (3)]. These statements can be verified by noting that

$$\begin{aligned} \underset{\sim}{\Omega}' \cdot \underset{\sim}{\Omega} \equiv \mu_o &= \mu\mu' + \eta\eta' + \xi\xi' \\ &= \mu\mu' + (1 - \mu^2)^{\frac{1}{2}}(1 - \mu'^2)^{\frac{1}{2}} \cos(\varphi - \varphi') \end{aligned} \tag{7}$$

and observing from Eq. (6) that $\psi(x,y,\mu,-\varphi)$ satisfies the same equation as $\psi(x,y,\mu,\varphi)$, assuming the boundary conditions are also even in φ. None of these assumptions is very restrictive and we use them in the remainder of the work, writing

$$\mu \frac{\partial\psi}{\partial x} + \eta \frac{\partial\psi}{\partial y} + \sigma\psi(x,y,\mu,\eta) = \sigma_s \int_{-1}^{1} d\mu' \int_{0}^{\pi} d\varphi' \psi(x,y,\mu',\eta')[f(\mu_o^+) + f(\mu_o^-)] + \mathcal{S}(x,y,\mu,\eta) \tag{8}$$

$$-1 \leq \mu \leq 1$$
$$0 \leq \varphi \leq \pi$$

where we have made use of evenness of ψ and used the notation

$$\mu_o^{\pm} = \mu\mu' + (1 - \mu^2)^{\frac{1}{2}}(1 - \mu'^2)^{\frac{1}{2}}\cos(\varphi \mp \varphi') \tag{9}$$

The variable of integration in the scattering integral can now be changed, giving

$$\int_{-1}^{1} d\mu \int_{0}^{\pi} d\varphi = \int_{-1}^{1} d\mu \int_{-(1-\mu^2)^{\frac{1}{2}}}^{(1-\mu^2)^{\frac{1}{2}}} d\eta \, (1 - \mu^2 - \eta^2)^{-\frac{1}{2}} \tag{10}$$

In the following derivations we do not display integration limits explicitly and adopt the convention that all integrals $d\mu d\varphi$ are over the hemisphere and that all integrals $d\mu d\eta$ are over the domain $\mu^2 + \eta^2 \leq 1$.

Biorthogonal Polynomial Expansion of the Flux

We first expand the directional flux in terms of polynomials $U_{nm}(\mu,\eta)$, which are defined by the generating function

$$G_1(a,b,\mu,\eta) = \frac{(1 - a\mu - b\eta)}{(1 - a\mu - b\eta)^2 + (a^2 + b^2)(1 - \mu^2 - \eta^2)} = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} a^n b^m U_{nm}(\mu,\eta) \tag{11}$$

assuming that a and b are small enough that the sum on the right converges, i.e., that $a^2 + b^2 \leq 1$. Equation (11) is the two variable analog of the generating function for the Tschebyscheff polynomials,[9] $T_n(\mu)$. The first few of the U_{nm} are displayed in Table I.

We let

$$\psi(x,y,\mu,\eta) = \sum_{\alpha=0}^{\infty} \sum_{\beta=0}^{\infty} \frac{2\alpha+2\beta+1}{2\pi} \binom{\alpha+\beta}{\beta}^{-1} U_{\alpha\beta}(\mu,\eta)\psi_{\alpha\beta}(x,y) \tag{12}$$

where the binomial coefficient is

$$\binom{\alpha+\beta}{\alpha} = \frac{(\alpha+\beta)!}{\alpha!\beta!} \tag{13}$$

The polynomials U are orthogonal over the unit circle with weight $(1 - \mu^2 - \eta^2)^{-\frac{1}{2}}$ to the polynomials V defined by the generating function

$$G_2(a,b,\mu,\eta) = (1 - 2a\mu - 2b\eta + a^2 + b^2)^{-\frac{1}{2}} = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} a^n b^m V_{nm}(\mu,\eta) \tag{14}$$

Table I

The Polynomials $U_{nm}(\mu,\eta)$

n/m	0	1	2	3	4
0	1	η	$2\eta^2+\mu^2-1$	$4\eta^3+3\mu^2\eta-3\eta$	$8\eta^4+8\mu^2\eta^2+\mu^4-8\eta^2-2\mu^2+1$
1	μ	$2\mu\eta$	$6\mu\eta^2+3\mu^3-3\mu$	$16\mu\eta^3+12\mu^3\eta-12\mu\eta$	
2	$2\mu^2+\eta^2-1$	$6\mu^2\eta+3\eta^3-3\eta$	$8\mu^4+8\eta^4+22\mu^2\eta^2-10\mu^2-10\eta^2+2$		
3	$4\mu^3+3\mu\eta^2-3\mu$	$16\mu^3\eta+12\mu\eta^3-12\mu\eta$			
4	$8\mu^4+8\mu^2\eta^2+\eta^4-8\mu^2-2\eta^2+1$				

The polynomials V are the two variable analog of the Legendre polynomials, $P_n(\mu)$. The first few of the V_{nm} are shown in Table II. In particular $V_{no}(\mu,\eta) = P_n(\mu)$ and $V_{om}(\mu,\eta) = P_m(\eta)$. The polynomials* U and V were first studied by Didon,[10] and in particular, he proved that

$$\iint d\mu d\eta V_{nm} U_{\alpha\beta}(1 - \mu^2 - \eta^2)^{-\frac{1}{2}} = \frac{2\pi}{2m+2n+1} \binom{m+n}{n} \delta_{n\alpha}\delta_{m\beta} \tag{15}$$

where $\delta_{n\alpha}$ and $\delta_{m\beta}$ are Kronecker symbols, e.g.,

$$\begin{aligned} \delta_{n\alpha} &= 0 \quad n \neq \alpha \\ &= 1 \quad n = \alpha \end{aligned} \tag{16}$$

The proof of Eq. (15) is reproduced in Appendix A. Multiplying Eq. (12) by V_{nm} and integrating, we have

$$\psi_{nm}(x,y) = \iint \frac{d\mu d\eta V_{nm}(\mu,\eta)\psi(x,y,\mu,\eta)}{(1 - \mu^2 - \eta^2)^{\frac{1}{2}}} \tag{17}$$

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*The authors discovered these polynomials independently. I (K.D.L.) had noticed in previous work[11] with the transport equation in (x,y) geometry that certain polynomials in μ and η occurred. By Gram-Schmidt orthogonalization I generated the first few V_{nm} and recognized that they were generated by G_2. However, the V_{nm} are not themselves orthogonal. Studying the Bateman[12] literature on orthogonal polynomials, I came to the conclusion that the polynomials U were generated by a generalization of the one variable Tschebyscheff polynomial generating function. However, I chose the logarithmic function (see Appendix B). Nelson DeMuth and I used this function to generate the first few U_{nm} and were attempting to prove orthogonality when he found the Didon reference. He recognized the applicability of the work when he saw a tabulation of the polynomials U_{nm}! The work of Didon (published 1868) seems to be the only existing description of the U and V polynomials.

Table II

The Polynomials $V_{nm}(\mu,\eta)$

n/m	0	1	2	3	4
0	1	η	$\frac{3\eta^2-1}{2}$	$\frac{5\eta^3-3\eta}{2}$	$\frac{35\eta^4-30\eta^2+8}{8}$
1	μ	$3\mu\eta$	$\frac{3\mu(5\eta^2-1)}{2}$	$\frac{5\mu\eta(7\eta^2-3)}{2}$	
2	$\frac{3\mu^2-1}{2}$	$\frac{3\eta(5\mu^2-1)}{2}$	$\frac{3(35\mu^2\eta^2-5\mu^2-5\eta^2+1)}{4}$		
3	$\frac{5\mu^3-3\mu}{2}$	$\frac{5\mu\eta(7\mu^2-3)}{2}$			
4	$\frac{35\mu^4-30\mu^2+8}{8}$				

It is shown in Appendix C that the scattering transfer function can be expanded as follows:

$$f(\mu_o^+) + f(\mu_o^-) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2\pi} b_\ell \sum_{j=0}^{\ell} \binom{\ell}{j}^{-1} V_{\ell-j,j}(\mu',\eta')U_{\ell-j,j}(\mu,\eta)$$

$$= \sum_{\ell=0}^{\infty} \sum_{j=0}^{\infty} \frac{2\ell+2j+1}{2\pi} b_{\ell+j} \binom{\ell+j}{j}^{-1} V_{\ell j}(\mu',\eta')U_{\ell j}(\mu,\eta) \tag{18}$$

where the b_ℓ are the same expansion coefficients as for the expansion of $f(\mu_o)$ in a series of the Legendre polynomials $P_\ell(\mu_o)$. When Eq. (18) is substituted in Eq. (8) and Eq. (17) is used, the transport equation becomes

$$\mu \frac{\partial\psi}{\partial x} + \eta \frac{\partial\psi}{\partial y} + \sigma\psi(x,y,\mu,\eta) = \sigma_s \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2\pi} b_\ell \sum_{j=0}^{\ell} \binom{\ell}{j}^{-1} \psi_{\ell-j,j}(x,y)U_{\ell-j,j}(\mu,\eta) + \mathcal{S}(x,y,\mu,\eta) \tag{19}$$

It is shown in Appendix B that the polynomials V satisfy the recursion relations

$$(2n + 2m + 1)\mu V_{nm} = (n + 1)(V_{n+1,m} - V_{n+1,m-2}) + (2m + n)V_{n-1,m}$$

$$(2n + 2m + 1)\eta V_{nm} = (m + 1)(V_{n,m+1} - V_{n-2,m+1}) + (2n + m)V_{n,m-1} \tag{20}$$

$$n,m = 0,1,2,\ldots$$

with the convention that polynomials with negative subscripts are zero. Multiplying Eq. (17) by $V_{nm}(1 - \mu^2 - \eta^2)^{-\frac{1}{2}}$ and integrating we have, with the use of Eqs. (15), (17), and (20), the following equations for the coefficients ψ_{nm}:

$$\frac{\partial}{\partial x}\left[(n+1)(\psi_{n+1,m} - \psi_{n+1,m-2}) + (2m+n)\psi_{n-1,m}\right]$$

$$+ \frac{\partial}{\partial y}\left[(m+1)(\psi_{n,m+1} - \psi_{n-2,m+1}) + (2n+m)\psi_{n,m-1}\right] \tag{21}$$

$$+ (\sigma - \sigma_s b_{n+m})(2n+2m+1)\psi_{nm} = (2n+2m+1)S_{nm}$$

$$m,n = 0,1,2,\ldots$$

In these equations we have defined

$$S_{nm}(x,y) = \iint \frac{d\mu d\eta \mathcal{S}(x,y,\mu,\eta)V_{nm}(\mu,\eta)}{(1-\mu^2-\eta^2)^{\frac{1}{2}}} \tag{22}$$

Because we have two systems of polynomials, we can also expand the flux in terms of the V polynomials, letting

$$\psi(x,y,\mu,\eta) = \sum_{\alpha=0}^{\infty}\sum_{\beta=0}^{\infty} \frac{2\alpha+2\beta+1}{2\pi}\binom{\alpha+\beta}{\beta}^{-1} V_{\alpha\beta}(\mu,\eta)\phi_{\alpha\beta}(x,y) \tag{23}$$

so that

$$\phi_{nm}(x,y) = \iint \frac{d\mu d\eta U_{nm}(\mu,\eta)\psi(x,y,\mu,\eta)}{(1-\mu^2-\eta^2)^{\frac{1}{2}}} \tag{24}$$

With this definition and Eq. (18) (interchanging primed and unprimed variables), Eq. (8) becomes

$$\mu \frac{\partial\psi}{\partial x} + \eta \frac{\partial\psi}{\partial y} + \sigma\psi(x,y,\mu,\eta) = \sigma_s \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2\pi} b_\ell \sum_{j=0}^{\ell} \binom{\ell}{j}^{-1} V_{\ell-j,j}(\mu,\eta)\phi_{\ell-j,j}(x,y) + \mathscr{S}(x,y,\mu,\eta) \tag{25}$$

As shown in Appendix B, the U polynomials satisfy the recursions

$$\begin{aligned}(2n + 2m + 1)\mu U_{nm} &= \frac{(n+1)(2m+n+1)}{m+n+1} U_{n+1,m} + (m + n)U_{n-1,m} - \frac{(m+2)(m+1)}{m+n+1} U_{n-1,m+2} \\ (2n + 2m + 1)\eta U_{nm} &= \frac{(m+1)(2n+m+1)}{m+n+1} U_{n,m+1} + (m + n)U_{n,m-1} - \frac{(n+2)(n+1)}{m+n+1} U_{n+2,m-1}\end{aligned} \tag{26}$$

$m,n = 0,1,2,\ldots$

Again, the convention is used that polynomials with negative subscripts are zero. When we multiply Eq. (25) by $U_{nm}(1 - \mu^2 - \eta^2)^{-\frac{1}{2}}$ and integrate, we obtain

$$\frac{1}{m+n+1} \frac{\partial}{\partial x} [(n + 1)(2m + n + 1)\phi_{n+1,m} + (m + n)(m + n + 1)\phi_{n-1,m} - (m + 2)(m + 1)\phi_{n-1,m+2}]$$

$$+ \frac{1}{m+n+1} \frac{\partial}{\partial y} [(m + 1)(2n + m + 1)\phi_{n,m+1} + (m + n)(m + n + 1)\phi_{n,m-1} - (n + 2)(n + 1)\phi_{n+2,m-1}]$$

$$+ (\sigma - \sigma_s b_{n+m})(2n + 2m + 1)\phi_{nm} = (2n + 2m + 1)\mathcal{S}_{nm} \tag{27}$$

with n,m = 0,1,2,... and

$$\mathcal{S}_{nm}(x,y) = \iint \frac{d\mu d\eta \mathcal{S}(x,y,\mu,\eta)U_{nm}(\mu,\eta)}{(1-\mu^2-\eta^2)^{\frac{1}{2}}} \tag{28}$$

Relation to the Spherical Harmonic Expansion

We define the spherical harmonic function Y_n^m as

$$Y_n^m(\mu,\varphi) = P_n^m(\mu)\cos m\varphi \tag{29}$$

anticipating the fact that no terms in $\sin m\varphi$ are needed because the flux ψ is assumed even in φ. In this definition the $P_n^m(\mu)$ are associated Legendre polynomials defined by*

$$P_n^m(\mu) = (1-\mu^2)^{\frac{m}{2}} \frac{d^m}{d\mu^m} P_n(\mu) \tag{30}$$

with $m \leq n$ and

$$P_n^{-m} = (-1)^m \frac{(n-m)!}{(n+m)!} P_n^m \tag{31}$$

The functions $\cos m\varphi$ are an orthogonal set on $0 \leq \varphi \leq \pi$ such that

$$\int_0^\pi \cos m\varphi \cos \beta\varphi d\varphi = \frac{\pi\delta_{m\beta}}{\epsilon_m} \tag{32}$$

where ϵ_m is the Neumann factor

$$\begin{aligned} \epsilon_m &= 1 \quad m = 0 \\ &= 2 \quad m > 0 \end{aligned} \tag{33}$$

*This definition differs by a factor of $(-1)^m$ from that given in the Bateman tables.[13]

The associated Legendre polynomials of the same superscript are orthogonal on $-1 \leq \mu \leq 1$ such that

$$\int_{-1}^{1} P_n^m(\mu) P_\alpha^m(\mu) d\mu = \frac{2}{2n+1} \frac{(n+m)!}{(n-m)!} \delta_{n\alpha} \tag{34}$$

Combining Eqs. (32) and (34) we have

$$\int_{-1}^{1} d\mu \int_{0}^{\pi} d\varphi \; Y_n^m(\mu,\varphi) Y_\alpha^\beta(\mu,\varphi) = \frac{2\pi(n+m)!}{2n+1(n-m)!} \frac{\delta_{n\alpha}\delta_{m\beta}}{\epsilon_m} \tag{35}$$

We therefore expand the flux as

$$\psi(x,y,\mu,\eta) = \sum_{\alpha=0}^{\infty} \frac{2\alpha+1}{2\pi} \sum_{\beta=0}^{\alpha} \frac{\epsilon_\beta(\alpha-\beta)!}{(\alpha+\beta)!} Y_\alpha^\beta(\mu,\varphi)\Phi_{\alpha\beta}(x,y) \tag{36}$$

so that

$$\Phi_{nm}(x,y) = \iint d\mu d\varphi Y_n^m(\mu,\varphi)\psi(x,y,\mu,\eta) \tag{37}$$

Now the scattering function $f(\mu_o)$ can be expanded in a Legendre polynomial series giving

$$f(\mu_o) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} b_\ell \; P_\ell(\mu_o) \tag{38}$$

where the b_ℓ are the same as in Eq. (18) and are given by

$$b_\ell = \int_{-\pi}^{\pi} d\varphi \int_{-1}^{1} d\mu_o \; P_\ell(\mu_o) f(\mu_o) \tag{39}$$

The addition theorem for spherical harmonics[14] permits the expansion of $P_\ell(\mu_o)$ as

$$P_\ell(\mu_o) = \sum_{j=0}^{\ell} \frac{\epsilon_j(\ell-j)!}{(\ell+j)!} P_\ell^j(\mu) P_\ell^j(\mu')\cos j(\varphi - \varphi') \tag{40}$$

Using Eqs. (40) and (38) we have

$$f(\mu_o^+) + f(\mu_o^-) = \sum_{\ell=0}^{\infty} \frac{(2\ell+1)b_\ell}{2\pi} \sum_{j=0}^{\ell} \frac{\epsilon_j(\ell-j)!}{(\ell+j)} Y_\ell^j(\mu,\varphi) Y_\ell^j(\mu',\varphi') \tag{41}$$

Therefore, Eq. (8) can be written

$$\mu \frac{\partial\psi}{\partial x} + \eta \frac{\partial\psi}{\partial y} + \sigma\psi = \sigma_s \sum_{\ell=0}^{\infty} \frac{(2\ell+1)b_\ell}{2\pi} \sum_{j=0}^{\ell} \frac{\epsilon_j(\ell-j)!}{(\ell+j)!} Y_\ell^j(\mu,\varphi)\Phi_{\ell j}(x,y) + \mathcal{S}(x,y,\mu,\eta) \tag{42}$$

The associated Legendre polynomials satisfy the recursion relations[15]

$$(2n + 1)\mu P_n^m(\mu) = (n + m)P_{n-1}^m(\mu) + (n + 1 - m)P_{n+1}^m(\mu) \tag{43}$$

and

$$\begin{aligned}(2n + 1)(1 - \mu^2)^{\frac{1}{2}} P_n^m(\mu) &= P_{n+1}^{m+1}(\mu) - P_{n-1}^{m+1}(\mu) \\ &= (n + 2 - m)(m - 1 - n)P_{n+1}^{m-1}(\mu) \\ &\quad + (n + m)(n + m - 1)P_{n-1}^{m-1}(\mu)\end{aligned} \tag{44}$$

These relations are valid for $n,m = 0,1,2,\ldots$ $m \leq n$ provided the definition of Eq. (31) is used.

By using Eq. (44) it is not difficult to show that

$$2(2n + 1)\eta Y_n^{\ m} = Y_{n+1}^{m+1} - Y_{n-1}^{m+1} + (n + 2 - m)(m - 1 - n)Y_{n+1}^{m-1}$$

$$+ (n + m - 1)(n + m)Y_{n-1}^{m-1} \qquad (45)$$

$$n,m = 0,1,\ldots \qquad m \leq n$$

We now multiply Eq. (42) by $Y_n^{\ m}$, integrate, and apply Eqs. (35), (37), (43), and (45) to find

$$\frac{\partial}{\partial x}\,[(n + m)\Phi_{n-1,m} + (n + 1 - m)\Phi_{n+1,m}]$$

$$+ \frac{1}{2}\frac{\partial}{\partial y}\,[\Phi_{n+1,m+1} - \Phi_{n-1,m+1} + (n + 2 - m)(m - 1 - m)\Phi_{n+1,m-1} +$$

$$(n + m)(n + m - 1)\Phi_{n-1,m-1}] + (2n + 1)(\sigma - \sigma_s b_n)\Phi_{nm} = (2n + 1)\tilde{\mathcal{S}}_{nm} \qquad (46)$$

$$n,m = 0,1,2,\ldots \qquad m \leq n$$

where the components of the source are given by

$$\tilde{\mathcal{S}}_{nm}(x,y) = \iint d\mu d\varphi Y_n^{\ m}(\mu,\varphi)\mathcal{S}(x,y,\mu,\eta) \qquad (47)$$

It is shown in Appendix C that the polynomials V_{nm} are linear combinations of the spherical harmonic functions, i.e., that

$$V_{nm}(\mu,\eta) = \sum_{k=0}^{\left[\frac{m}{2}\right]} A_k^{nm} P_{n+m}^{m-2k}(\mu)\cos[(m - 2k)\varphi] \tag{48}$$

with

$$A_k^{nm} = \frac{\epsilon_{m-2k}(n + 2k)!(-1)^k}{2^m n!(m - k)!k!} \tag{49}$$

Multiplying Eq. (48) by $\psi(x,y,\mu,\eta)$ and integrating, we have

$$\psi_{nm}(\mu,\eta) = \sum_{k=0}^{\left[\frac{m}{2}\right]} A_k^{nm} \Phi_{n+m,m-2k} \tag{50}$$

Therefore, the system of equations in Eq. (21) is a linear combination of the system of equations of Eq. (46). It is possible to verify this statement directly by letting, in Eq. (46), $m \to m - 2k$ and $n \to n + m$. If the resulting equations are multiplied by A_k^{nm} and summed, Eq. (20) is obtained. The process is straightforward except for the y derivative terms where considerable rearrangement of the sums is required.

It should be noted that the systems of equations in Eqs. (21) and (27) are symmetric with respect to the number of x and y derivatives while the spherical harmonics equations are not. This symmetry is a consequence of the symmetry of the polynomials U and V. That is, $V_{nm}(\mu,\eta) = V_{mn}(\eta,\mu)$ and $U_{nm}(\mu,\eta) = U_{mn}(\eta,\mu)$ so that if x and y and μ and η are interchanged the same systems of equations are obtained. Presumably, the presence of this symmetry in the systems of equations would facilitate numerical solution.

In Appendix A it is shown that

$$\int_0^{\pi} d\varphi U_{nm}(\mu,\eta) = \pi P_n(\mu)\delta_{no} \tag{51}$$

If it is assumed that the flux is independent of y, and if the expansion of Eq. (12) is integrated over φ, the result is

$$\begin{aligned} \psi(x,\mu) = \int_0^{\pi}\psi(x,\mu,\eta)d\varphi &= \sum_{\alpha=0}^{\infty}\sum_{\beta=0}^{\infty} \frac{(2\alpha + 2\beta + 1)}{2\pi} \binom{\alpha+\beta}{\beta}^{-1} \psi_{\alpha\beta}(x)\int_0^{\pi} d\varphi U_{\alpha\beta}(\mu,\eta) \\ &= \sum_{\alpha=0}^{\infty} \frac{2\alpha + 1}{2} \psi_{\alpha 0}(x)P_{\alpha}(\mu) \end{aligned} \tag{52}$$

In this case Eq. (21) becomes, with m = 0,

$$\begin{gathered} \frac{\partial}{\partial x}\left[(n + 1)\psi_{n+1,0} + n\psi_{n-1,0}\right] + (\sigma - \sigma_s b_n)(2n + 1)\psi_{n0} = (2n + 1)S_{n0} \\ n = 0,1,2,\ldots \end{gathered} \tag{53}$$

Because $V_{n0}(\mu,\eta)$ is just $P_n(\mu)$, these equations are the spherical harmonics equations in plane geometry.

Specific Forms of the Biorthogonal Moments Equations

The first few of the equations in Eq. (21) are:

n = m = 0

$$\frac{\partial\psi_{10}}{\partial x} + \frac{\partial\psi_{01}}{\partial y} + (\sigma - \sigma_s b_0)\psi_{00} = S_{00} \qquad (54)$$

n = 1, m = 0

$$\frac{2\partial\psi_{20}}{\partial x} + \frac{\partial\psi_{00}}{\partial x} + \frac{\partial\psi_{11}}{\partial y} + 3(\sigma - \sigma_s b_1)\psi_{10} = 3S_{10} \qquad (55)$$

n = 0, m = 1

$$\frac{\partial\psi_{11}}{\partial x} + \frac{2\partial\psi_{02}}{\partial y} + \frac{\partial\psi_{00}}{\partial y} + 3(\sigma - \sigma_s b_1)\psi_{01} = 3S_{01} \qquad (56)$$

n = m = 1

$$\frac{2\partial\psi_{21}}{\partial x} + \frac{3\partial\psi_{01}}{\partial x} + \frac{2\partial\psi_{12}}{\partial y} + \frac{3\partial\psi_{10}}{\partial y} + 5(\sigma - \sigma_s b_2)\psi_{11} = 5S_{11} \qquad (57)$$

Equation (54) is the system balance equation, because ψ_{10} is the current in the x direction and ψ_{01} is the current in the y direction ($V_{10} = \mu$ and $V_{01} = \eta$). Equations (55) and (56) are, with $\psi_{20} = \psi_{11} = \psi_{02} = 0$, just the current equations of diffusion theory. In this instance the system of Eqs. (54), (55), and (56) can be reduced to a second order partial differential equation in ψ_{00}. Equations (54) through (56) with

$\psi_{20} = \psi_{02} = \psi_{12} = \psi_{21} = 0$ is, with one exception, the system derived from a discrete ordinates representation by Lathrop[11] in the case of isotropic scattering. The exception is the coefficient of ψ_{11} and S_{11} in Eq. (57). In the discrete ordinates representation, the quadrature set is chosen to give a diffusion coefficient of $1/3\sigma$ (isotropic scattering) with the consequence that the coefficient of ψ_{11} and S_{11} is 3 instead of 5. If the equations of Eq. (21) are written up through $m + n = 2$ and truncated by setting $\psi_{nm} = 0$ for $n + m = 3$, the so-called P_2 equations are obtained. These equations can also be reduced to a second order partial differential equation in the scalar flux ψ_{00}. Although we have not examined the question thoroughly, we conjecture that the terminating condition $\psi_{nm} = 0$ for $n + m = N + 1$ results in a system of equations equivalent to the usual P_N spherical harmonics equations.

The first few of the equations in Eq. (27) are

<u>m = n = 0</u>

$$\frac{\partial \phi_{10}}{\partial x} + \frac{\partial \phi_{01}}{\partial y} + (\sigma - \sigma_s b_0)\phi_{00} = \mathcal{S}_{00} \tag{58}$$

<u>m = 0, n = 1</u>

$$\frac{2\partial \phi_{20}}{\partial x} + \frac{\partial \phi_{00}}{\partial x} - \frac{\partial \phi_{02}}{\partial x} + \frac{3}{2}\frac{\partial \phi_{11}}{\partial y} + 3(\sigma - \sigma_s b_1)\phi_{10} = 3\mathcal{S}_{10} \tag{59}$$

<u>m = 1, n = 0</u>

$$\frac{3}{2}\frac{\partial \phi_{11}}{\partial x} + \frac{2\partial \phi_{02}}{\partial y} + \frac{\partial \phi_{00}}{\partial y} - \frac{\partial \phi_{20}}{\partial y} + 3(\sigma - \sigma_s b_1)\phi_{01} = 3\mathcal{S}_{01} \tag{60}$$

m = n = 1

$$\frac{8}{3}\frac{\partial\phi_{21}}{\partial x} + \frac{2\partial\phi_{01}}{\partial x} - \frac{2\partial\phi_{03}}{\partial x}$$

$$+ \frac{8}{3}\frac{\partial\phi_{12}}{\partial y} + \frac{2\partial\phi_{10}}{\partial y} - \frac{2\partial\phi_{30}}{\partial x} + 5(\sigma - \sigma_s b_2)\phi_{11} = 5\mathcal{S}_{11} \tag{61}$$

Again, Eq. (58) is the system balance equation, and the truncation achieved by setting $\phi_{nm} = 0$ for $n + m > 1$ is the consistent P_1 approximation.

Possibilities for Future Investigations

In addition to the determination of suitable boundary conditions and possible truncation procedures, there are many avenues of research suggested by the biorthogonal expansions of this work. For example, since there are many systems of biorthogonal polynomials[12] is it possible to find a system applicable to more general geometries, in particular, (x,y,z) geometry? The properties of the U and V polynomials suggest that an expansion over each angular hemisphere ($\xi < 0$ or $\xi > 0$) is possible provided a simple recursion relation for $\xi V_{nm}(\mu,\eta)$ can be found. However, there are biorthogonal systems of polynomials in three variables that are orthogonal over the unit sphere $\mu^2 + \eta^2 + \xi^2 \leq 1$ that could be used. These systems would involve expansion coefficients with three subscripts [$P_{\ell mn}(\mu,\eta,\xi)$, say] some of which (those with even subscripts) would be related through Eq. (3).

Another interesting problem is the determination of discrete ordinates quadrature sets from the biorthogonal polynomials U and V. The question of mechanical quadrature is discussed briefly by Appell.[16] Perhaps such sets would be optimum, in the Gauss sense, for quadrature over the hemisphere and particularly applicable for numerical discrete ordinates solution of the transport equation. At present, there is no known "best" quadrature.[17]

Still another avenue of research is the determination of a solution to the system of equations of Eqs. (21) or (27). In the one dimensional case, e.g., Eq. (53), a solution of the form [using the notation of Eq. (53)]

$$\psi_{n0}(x) = g_{n0}(\nu)e^{\sigma x/\nu} \tag{62}$$

is postulated and substituted in the system. If the system is truncated, the consistency of the system determines permissible values of ν. The functions $g_n(\nu)$ can be found by making use of the properties of the recursion relation they must satisfy.[18] A similar substitution, say

$$\psi_{nm}(x,y) = g_{nm}(\nu,\tau)e^{\sigma x/\nu + \sigma y/\tau} \tag{63}$$

is possible in (x,y) geometry. Can the functions g_{nm} and values of ν and τ be determined? In the one dimensional case, the g_{n0} are determined from the properties of the functions which satisfy the same recursion relation as the g_{n0}, i.e., the Legendre polynomials and the associated Legendre functions. Presumably, if such a technique is applicable, there must be "singular" functions related to the U and V polynomials. Such functions might be determined from the partial differential equations, given by Didon,[10] satisfied by the U and V polynomials.

As a final and practical question, do the expansions in terms of the U or V polynomials offer any particular advantages, other than symmetry, over the spherical harmonic expansions?

Appendix A

Orthogonality Integral and Related Integrals

In each of the appendices, results are first stated and then verified. In this appendix we sketch the proof of:

$$\text{a)} \quad \iint d\mu d\eta V_{nm}(\mu,\eta)U_{\alpha\beta}(\mu,\eta)(1 - \mu^2 - \eta^2)^{-\frac{1}{2}} = \frac{2\pi}{2m + 2n + 1}\binom{m+n}{n}\delta_{n\alpha}\delta_{m\beta} \tag{A-1}$$

$$\text{b)} \quad \int_0^\pi d\phi U_{\alpha\beta}(\mu,\eta) = \pi P_\alpha(\mu)\delta_{\beta 0} \tag{A-2}$$

$$\text{c)} \quad \int_0^\pi d\phi V_{\alpha\beta}(\mu,\eta) = 0 \qquad \beta \text{ odd}$$

$$= \pi\, 2^{-\beta}(-1)^{\frac{\beta}{2}}\binom{\alpha+\beta}{\alpha}\binom{\beta}{\frac{\beta}{2}} P_{\alpha+\beta}(\mu) \qquad \beta \text{ even} \tag{A-3}$$

To prove Eq. (A-1) we follow Didon[10], and multiply the generating functions of Eqs. (11) and (14) and integrate, giving

$$\iint d\mu d\eta G_1(s,t,\mu,\eta)G_2(a,b,\mu,\eta)(1 - \mu^2 - \eta^2)^{-\frac{1}{2}}$$

$$= \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\sum_{\alpha=0}^{\infty}\sum_{\beta=0}^{\infty} a^n b^m s^\alpha t^\beta I_{nm\alpha\beta} \tag{A-4}$$

where $I_{nm\alpha\beta}$ is the integral on the left of Eq. (A-1). The integral on the left of Eq. (A-4) is

$$I = \iint \frac{d\mu d\eta (1 - \mu s - \eta t)(1 - \mu^2 - \eta^2)^{-\frac{1}{2}} (1 - 2a\mu - 2b\eta + a^2+b^2)^{-\frac{1}{2}}}{(1 - \mu s - \eta t)^2 + (s^2 + t^2)(1 - \mu^2 - \eta^2)} \quad \text{(A-5)}$$

With the following change of variables

$$\begin{aligned} \mu &= (a\lambda + b\tau)/r \\ \eta &= (b\lambda - a\tau)/r \\ r^2 &= a^2 + b^2 \qquad \zeta^2 = s^2 + t^2 \end{aligned} \quad \text{(A-6)}$$

for which $d\mu d\eta = d\lambda d\tau$, the integral becomes

$$I = \int d\lambda (1 - 2\lambda r + r^2)^{-\frac{1}{2}} \int \frac{d\tau (1 - \zeta\lambda\cos\theta - \zeta\tau\sin\theta)(1 - \lambda^2 - \tau^2)^{-\frac{1}{2}}}{(1 - \zeta\lambda\cos\theta - \zeta\tau\sin\theta)^2 + \zeta^2(1 - \lambda^2 - \tau^2)} \quad \text{(A-7)}$$

where

$$\begin{aligned} \cos\theta &= (as + bt)/r\zeta \\ \sin\theta &= (bs - at)/r\zeta \end{aligned} \quad \text{(A-8)}$$

and the domain of integration is $\lambda^2 + \tau^2 \leq 1$. When the change of variable $\tau = (1 - \lambda^2)^{\frac{1}{2}}\cos\varphi$ is made in the second integral, it becomes

$$I_2 = \int_0^{\pi} \frac{d\varphi (L - M\cos\varphi)}{(L - M\cos\varphi)^2 + N^2\sin^2\varphi} \quad \text{(A-9)}$$

where

$$\begin{aligned} L &= 1 - \zeta\lambda\cos\theta \\ M &= \zeta\sin\theta(1 - \lambda^2)^{\frac{1}{2}} \\ N &= \zeta(1 - \lambda^2)^{\frac{1}{2}} \end{aligned} \quad \text{(A-10)}$$

The integral of Eq. (A-9) can be rewritten as

$$I_2 = \frac{1}{2} \int_{-\pi}^{\pi} \frac{d\varphi}{L - M\cos\varphi - iN\sin\varphi} \quad \text{(A-11)}$$

which is an integral around the unit circle $z = e^{i\varphi}$ in the complex z plane. There is one simple pole inside the circle for which the residue is easily evaluated. The result is

$$I_2 = \pi(L^2 + N^2 - M^2)^{-\frac{1}{2}} \qquad \text{(A-12)}$$

$$= \pi(1 - 2\zeta\cos\theta\lambda + \zeta^2\cos^2\theta)^{-\frac{1}{2}}$$

The integral I is thus

$$I = \pi\int_{-1}^{1} d\lambda(1 - 2r\lambda + r^2)^{-\frac{1}{2}} (1 - 2\zeta\cos\theta\lambda + \zeta^2\cos^2\theta)^{-\frac{1}{2}}$$

$$= \pi \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} r^n(\zeta\cos\theta)^m \int_{-1}^{1} d\lambda P_n(\lambda)P_m(\lambda) \qquad \text{(A-13)}$$

$$= 2\pi \sum_{n=0}^{\infty} \frac{(r\zeta\cos\theta)^n}{2n+1}$$

where the generating function expansion for Legendre polynomials has been used and the sums converge for ζ and r less than unity. When $(r\zeta\cos\theta)^n$ is expanded the result is

$$I_1 = 2\pi \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \binom{n+m}{m} \frac{(as)^n(bt)^m}{2m+2n+1} \qquad \text{(A-14)}$$

which is equal to the right side of Eq. (A-4). Equation (A-14) is invariant under the transformation $a \to a/p$, $s \to ps$, $b \to b/q$, $t \to qt$, which is true of the right side of Eq. (A-4) only if Eq. (A-1) is valid. Didon also discusses the integral in the case when ζ and r are not both less than unity.

The integral of Eq. (A-2) is evaluated in a similar manner. Integrating G_1 we have, after the substitution $\eta = (1 - \mu^2)^{\frac{1}{2}} \cos\varphi$,

$$\int_0^{\pi} d\varphi \frac{L - M\cos\varphi}{(L - M\cos\varphi)^2 + N^2 \sin^2\varphi} =$$

$$= \sum_{\alpha=0}^{\infty} \sum_{\beta=0}^{\infty} s^{\alpha} t^{\beta} \int_0^{\pi} d\varphi U_{\alpha\beta}(\mu,\eta) \tag{A-15}$$

where, on the left,

$$L = 1 - s\mu$$

$$M = (1 - \mu^2)^{\frac{1}{2}} t \tag{A-16}$$

$$N = (1 - \mu^2)(s^2 + t^2)$$

so that, when Eq. (A-12) is applied, Eq. (A-15) becomes

$$\pi(1 - 2s\mu + s^2)^{-\frac{1}{2}} = \pi \sum_{\alpha=0}^{\infty} s^{\alpha} P_{\alpha}(\mu) = \sum_{\alpha=0}^{\infty} s^{\alpha} t^{\beta} \int_0^{\pi} d\varphi U_{\alpha\beta}(\mu,\eta) \tag{A-17}$$

from which Eq. (A-2) follows.

Equation (A-3) follows immediately by integration of Eq. (48), which is derived in Appendix C.

Appendix B

Generating Functions, Rodrigues-Type Formulas, and Recursion Relations

The generating functions are

$$G_1(a,b,\mu,\eta) = \frac{(1-a\mu-b\eta)}{(1-a\mu-b\eta)^2 + (a^2+b^2)(1-\mu^2-\eta^2)} = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} a^n b^m U_{nm}(\mu,\eta) \qquad \text{(B-1)}$$

$$\begin{aligned} G_3(a,b,\mu,\eta) &= 1 - \ln[(1 - a\mu - b\eta)^2 + (a^2 + b^2)(1 - \mu^2 - \eta^2)] \\ &= U_{00} + 2 \sum_{n}^{\infty} \sum_{m}^{\infty} \frac{a^n b^m U_{nm}(\mu,\eta)}{n+m} \end{aligned} \qquad \text{(B-2)}$$

In the sum on the right, $n = m = 0$ is excluded.

$$G_2(a,b,\mu,\eta) = (1 - 2a\mu - 2b\eta + a^2 + b^2)^{-\frac{1}{2}} = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} a^n b^m V_{nm}(\mu,\eta) \qquad \text{(B-3)}$$

The functions G_1 and G_3 are generalizations of Tschebyscheff polynomial generating functions and G_2 is a generalization of the Legendre polynomial generating function. Just as in the case of the classical polynomials, there are undoubtedly other generating functions.

Didon[10] derives the Rodrigues formulas

$$V_{nm}(\mu,\eta) = \frac{(-1)^{m+n}(1+u^2+v^2)^{\frac{m+n+1}{2}}}{m!n!} \frac{\partial^{n+m}}{\partial u^n \partial v^m} (1 + u^2 + v^2)^{-\frac{1}{2}} \qquad \text{(B-4)}$$

where

$$u = \mu(1 - \mu^2 - \eta^2)^{-\frac{1}{2}}$$
$$v = \eta(1 - \mu^2 - \eta^2)^{-\frac{1}{2}} \qquad \text{(B-5)}$$

and

$$U_{nm}(\mu,\eta) = \frac{(-1)^{m+n}\binom{m+n}{n}(1-\mu^2-\eta^2)^{\frac{1}{2}}}{1.3.5\ldots(2m+2n-1)} \; \frac{\partial^{n+m}(1-\mu^2-\eta^2)^{n+m-\frac{1}{2}}}{\partial\mu^n\partial\eta^m} \qquad \text{(B-6)}$$

Equation (B-4) is also given in the Bateman Tables.[19]

There seems to be many recursion relations among the polynomials and Didon obtained only $U_{n1} = (n + 1)\eta U_{n0}$, which is a special case of Eq. (B-17) below. We outline the derivation of the following:

$$(n + 1)(V_{n+1,m} + V_{n+1,m-2}) + nV_{n-1,m} = (2n + 1)\mu V_{nm} + 2(n + 1)\eta V_{n+1,m-1} \qquad \text{(B-7)}$$

$$(n + m + 1)V_{n+1,m} + (n + m)(V_{n+1,m-2} + V_{n-1,m}) = (2n + 2m + 1)(\mu V_{nm} + \eta V_{n+1,m-1}) \qquad \text{(B-8)}$$

$$(2n + 2m + 1)\mu V_{nm} = (n + 1)(V_{n+1,m} - V_{n+1,m-2}) + (n + 2m)V_{n-1,m} \qquad \text{(B-9)}$$

$$(2n + 2m + 1)\eta V_{nm} = (m + 1)(V_{n,m+1} - V_{n-2,m+1}) + (2n + m)V_{n,m-1} \qquad \text{(B-10)}$$

$$(n + 1)V_{n+1,m} + (n + m)V_{n-1,m} = (2n + m + 1)\mu V_{nm} + (n + 1)\eta V_{n+1,m-1} \qquad \text{(B-11)}$$

$$(m + 1)V_{n,m+1} + (n + m)V_{n,m-1} = (m + 1)\mu V_{n-1,m+1} + (n + 2m + 1)\eta V_{nm} \quad \text{(B-12)}$$

$$m(\mu V_{n-1,m} - V_{n-2,m}) = n(\eta V_{n,m-1} - V_{n,m-2}) \quad \text{(B-13)}$$

$$U_{n+1,m} + (1 - \eta^2)U_{n-1,m} + 2\mu\eta U_{n,m-1} + (1 - \mu^2)U_{n+1,m-2} =$$
$$2\mu U_{nm} + 2\eta U_{n+1,m-1} - \mu\delta_{n0}\delta_{m0} \quad \text{(B-14)}$$

$$\frac{(n+1)(n+m-1)}{n+m+1} U_{n+1,m} + (n - 1)(1 - \eta^2)U_{n-1,m} + n2\mu\eta U_{n,m-1} +$$
$$(n + 1)(1 - \mu^2)U_{n+1,m-2} = \frac{2(n+m-1)}{n+m} [n\mu U_{nm} +$$
$$(n + 1)\eta U_{n+1,m-1}] - \mu\delta_{n0}\delta_{m0} \quad \text{(B-15)}$$

$$(n + m + 1)(2m + 2n + 1)\mu U_{nm} = (n + 1)(2m + n + 1)U_{n+1,m} +$$
$$(m + n)(m + n + 1)U_{n-1,m} - (m + 2)(m + 1)U_{n-1,m+2} \quad \text{(B-16)}$$

$$(n + m + 1)(2m + 2n + 1)\eta U_{nm} = (m + 1)(2n + m + 1)U_{n,m+1} +$$
$$(n + m)(n + m + 1)U_{n,m-1} - (n + 2)(n + 1)U_{n+2,m-1} \quad \text{(B-17)}$$

$$\frac{\partial V_{n,m-1}}{\partial \mu} = \frac{\partial V_{n-1,m}}{\partial \eta} \quad \text{(B-18)}$$

$$\eta \frac{\partial V_{nm}}{\partial \mu} - \frac{\partial V_{n,m-1}}{\partial \mu} = (m + 1)V_{n-1,m+1} \quad \text{(B-19)}$$

$$\mu \frac{\partial V_{nm}}{\partial \eta} - \frac{\partial V_{n-1,m}}{\partial \eta} = (n + 1)V_{n+1,m-1} \tag{B-20}$$

$$\frac{\partial V_{nm}}{\partial \omega} \equiv \mu \frac{\partial V_{nm}}{\partial \eta} - \eta \frac{\partial V_{nm}}{\partial \mu} = (n + 1)V_{n+1,m-1} - (m + 1)V_{n-1,m+1} \tag{B-21}$$

In general, these equations hold for, $n,m = 0,1,2,\ldots,$ and polynomials with negative subscripts are assumed equal to zero. The symmetric relations obtained by interchanging μ, η, and subscripts also hold. For example, in Eq. (B-15) the term $(n + 1)(1 - \mu^2)U_{n+1,m-2}(\mu,\eta)$ is replaced by $(m + 1)(1 - \eta^2)U_{n-2,m+1}(\mu,\eta)$. With similar transpositions in the remaining terms a different recursion is obtained. Equations (B-9) and (B-10) are such a symmetric pair as are other of the relations displayed. Six other recursions involving five U polynomials can be obtained by eliminating a polynomial from Eqs. (B-14) and (B-15). In such manipulations the Kronecker delta term can be neglected.

Equation (B-7) is derived by equating coefficients in the identity

$$(1 - 2a\mu - 2b\eta + a^2 + b^2) \frac{\partial G_2}{\partial a} = (\mu - a)G_2 \tag{B-22}$$

Equation (B-8) is derived by following a procedure described by Appell.[16] From Eq. (B-3) we have

$$\begin{aligned} [1 - 2(a\mu + b\eta) + a^2 + b^2]^{-\frac{1}{2}} &= \sum_{n=0}^{\infty} (a^2 + b^2)^{\frac{n}{2}} P_n\left[\frac{a\mu+b\eta}{(a^2+b^2)^{\frac{1}{2}}}\right] \\ &= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} a^{n-m} b^m V_{n-m,m}(\mu,\eta) \end{aligned} \tag{B-23}$$

from which

$$S_n \equiv \sum_{m=0}^{n} a^{n-m} b^m V_{n-m,m}(\mu,\eta) = (a^2 + b^2)^{\frac{n}{2}} P_n(z) \qquad \text{(B-24)}$$

where $z = (a\mu + b\eta)/(a^2 + b^2)^{\frac{1}{2}}$. From the recursion relation for Legendre polynomials,

$$(n + 1)P_{n+1}(z) = (2n + 1)zP_n(z) - nP_{n-1}(z) \qquad \text{(B-25)}$$

we form, by multiplying by $(a^2 + b^2)^{n+1/2}$,

$$(n + 1)S_{n+1} = (2n + 1)(a\mu + b\eta)S_n - n(a^2 + b^2)S_{n-1} \qquad \text{(B-26)}$$

Equating coefficients of powers of a and b gives Eq. (B-8). Equations (B-9) through (B-13) are derived by eliminating one of the polynomials from (B-7) and (B-8).

Equation (B-14) is obtained by equating coefficients in the identity

$$D \frac{\partial G_1}{\partial a} = - \mu - \frac{\partial D}{\partial a} G_1 \qquad \text{(B-27)}$$

where D is the denominator of G_1. When Appell's procedure is applied to G_1, the same recursion is obtained. The procedure does give the interesting relation

$$\alpha^n T_n(z) = \sum_{m=0}^{n} a^{n-m} b^m U_{n-m,m} \qquad \text{(B-28)}$$

where $\alpha^2 = (1 - x^2 - y^2)(a^2 + b^2) + (ax + by)^2$, $z = (ax + by)/\alpha$, and T_n is a Tschebyscheff polynomial as defined in the Bateman tables.[9] Equation (B-15) is obtained from the identity

$$D \frac{\partial G_1}{\partial a} = - \mu + (1 - a\mu + b\eta) \frac{\partial G_3}{\partial a} \tag{B-29}$$

Equations (B-16) and (B-17) are derived from the Rodrigues relation of Eq. (B-6). For example, we postulate $AU_{n+1,m} + B\mu U_{nm} + CU_{n-1,m} + DU_{n-1,m+2} = 0$, where A, B, C, and D are functions of n and m. After the application of Eq. (B-6) and some rather tedious rearrangement, enough equations are obtained to determine A, B, C, and D. This procedure is not entirely satisfactory because it is based on the assumption of the general form of the relation to be verified. In this case we were led to the assumed form by manipulations of the lower degree polynomials and the desire to represent μU_{nm} (and ηU_{nm}) in terms of other polynomials with coefficients independent of μ and η. In general, relations among the U polynomials are more difficult to obtain than relations among the V polynomials. There are possibly three other relations among the U polynomials analogous to Eqs. (B-11), (B-12), and (B-13).

Equations (B-18), (B-19), and (B-20) are derived from the identities

$$b \frac{\partial G_2}{\partial \mu} = a \frac{\partial G_2}{\partial \eta} \tag{B-30}$$

$$(\eta - b) \frac{\partial G_2}{\partial \mu} = a \frac{\partial G_2}{\partial b} \tag{B-31}$$

and

$$(\mu - a) \frac{\partial G_2}{\partial \eta} = b \frac{\partial G_2}{\partial a} \tag{B-32}$$

Equation (B-21), which is needed in expansions in cylindrical geometry, is obtained by combining Eqs. (B-18), (B-19), and (B-20).

Appendix C

Addition Theorem for the Polynomials U and V

We wish to show that

$$f(\mu_o^+) + f(\mu_o^-) = \sum_{\ell=0}^{\infty} \frac{(2\ell+1)b_\ell}{2\pi} \sum_{j=0}^{\ell} \binom{\ell}{j}^{-1} V_{\ell-j,j}(\mu',\eta')U_{\ell-j,j}(\mu,\eta) \qquad \text{(C-1)}$$

where $\mu_o^{\pm}$ is defined by Eq. (9). By comparing this equation with Eq. (41)

$$f(\mu_o^+) + f(\mu_o^-) = \sum_{\ell=0}^{\infty} \frac{(2\ell+1)b_\ell}{2\pi} \sum_{j=0}^{\ell} \frac{\epsilon_j(\ell-j)!}{(\ell+j)!} Y_\ell^j(\mu,\varphi)Y_\ell^j(\mu',\varphi') \qquad \text{(C-2)}$$

we see that we need only prove that

$$\sum_{j=0}^{\ell} \binom{\ell}{j}^{-1} V_{\ell-j,j}(\mu',\eta')U_{\ell-j,j}(\mu,\eta) = \sum_{j=0}^{\ell} \frac{\epsilon_j(\ell-j)!}{(\ell+j)!} Y_\ell^j(\mu,\varphi)Y_\ell^j(\mu',\varphi') \qquad \text{(C-3)}$$

To verify this identity we first show that

$$V_{nm}(\mu,\eta) = \sum_{k=0}^{\left[\frac{m}{2}\right]} \frac{\epsilon_{m-2k}(n+2k)!(-1)^k}{2^m n!(m-k)!k!} Y_{n+m}^{m-2k}(\mu,\varphi) \qquad \text{(C-4)}$$

and that

$$Y_\ell^j(\mu,\varphi) = \frac{(\ell+j)!}{2^j \ell!} \sum_{k=0}^{\left[\frac{\ell-j}{2}\right]} \frac{(-1)^k}{2^{2k}} \binom{j+2k}{k} U_{\ell-j-2k,\,j+2k}(\mu,\eta) \qquad \text{(C-5)}$$

In these equations $Y_\ell^j(\mu,\varphi) = P_\ell^j(\mu)\cos j\varphi$.

We start from a relation derived in Appendix B:

$$(a^2 + b^2)^{n/2} P_n[(a\mu + b\eta)/(a^2 + b^2)^{\frac{1}{2}}] = \sum_{m=0}^{n} a^{n-m} b^m V_{n-m,m}(\mu,\eta) \tag{C-6}$$

On the left of this equation, we write the argument of the Legendre polynomial as $\mu\mu' + \eta\eta' + \xi\xi'$ with

$$\begin{aligned} \mu' &= a/(a^2 + b^2)^{\frac{1}{2}} \\ \eta' &= b/(a^2 + b^2)^{\frac{1}{2}} \\ \xi' &= (1 - \mu'^2 - \eta'^2)^{\frac{1}{2}} = 0 \end{aligned} \tag{C-7}$$

Using the spherical harmonic addition theorem we have, with $\xi' = 0$,

$$P_n[(a\mu + b\eta)/(a^2 + b^2)^{\frac{1}{2}}] = \sum_{j=0}^{n} \frac{\epsilon_j (n-j)!}{(n+j)!} P_n^j(\mu') Y_n^j(\mu,\varphi) \tag{C-8}$$

Letting $t = b/a$ we combine this relation with Eq. (C-6), obtaining

$$\sum_{m=0}^{n} t^m V_{n-m,m} = (1 + t^2)^{\frac{n}{2}} \sum_{j=0}^{n} \frac{\epsilon_j (n-j)!}{(n+j)!} P_n^j[(1 + t^2)^{-\frac{1}{2}}] Y_n^j(\mu,\varphi) \tag{C-9}$$

From the relation between P_n^j and the Gegenbauer polynomials[20] we have

$$(1 + t^2)^{\frac{n}{2}} P_n^j[(1 + t^2)^{-\frac{1}{2}}] = \frac{t^j}{2^n} \sum_{\ell=0}^{\left[\frac{n-j}{2}\right]} \frac{(-1)^\ell (2n-2\ell)!(1+t^2)^\ell}{\ell!(n-j-2\ell)!(n-\ell)!} \tag{C-10}$$

By expanding $(1 + t^2)^{\ell}$ in a binomial series, rearranging the sums on the right of Eq. (C-9), and equating coefficients of powers of t in the finite sums we have

$$V_{n-m,m}(\mu,\eta) = \sum_{k=0}^{\left[\frac{m}{2}\right]} \sum_{j=0}^{\left[\frac{n-m}{2}\right]} \frac{\epsilon_{m-2k}(n-m+2k)!(-1)^{j+k}(2n-2k-2j)!}{2^n(n+m-2k)!(n-m-2j)!(n-j-k)!k!j!} Y_n^{m-2k}(\mu,\varphi) \quad \text{(C-11)}$$

The rearrangement of sums is complicated, and we sketch the process showing only the powers of t and neglecting coefficients. Starting from

$$\sum_{j=0}^{n} \sum_{\ell=0}^{\left[\frac{n-j}{2}\right]} t^j(1 + t^2)^{\ell} \quad \text{(C-12)}$$

we interchange order of summation and expand, obtaining

$$\sum_{\ell=0}^{\left[\frac{n}{2}\right]} \sum_{k=0}^{\ell} \sum_{j=0}^{n-2\ell} t^{j+2k} \quad \text{(C-13)}$$

again neglecting coefficients. Letting $j \rightarrow j - 2k$ and interchanging order of summation we have

$$\sum_{j=0}^{n} t^j \sum_{\ell=0}^{\left[\frac{n}{2}\right]} \sum_{k=\max(0,\left[\frac{j-n+2\ell}{2}\right])}^{k=\min(\left[\frac{j}{2}\right],\ell)} \quad \text{(C-14)}$$

At this point, we equate coefficients of powers of t and then interchange the order of the last two sums giving, with $j \rightarrow m$,

$$\sum_{k=0}^{\left[\frac{m}{2}\right]} k + \sum_{\ell=k}^{\left[\frac{n-m}{2}\right]} \tag{C-15}$$

which, with $\ell = j + k$ gives the two sums of Eq. (C-11). The j summation of this equation can be expressed in closed form by first letting $n \rightarrow n + m$ giving

$$V_{nm}(\mu,\eta) = \sum_{k=0}^{\left[\frac{m}{2}\right]} \frac{\epsilon_{m-2k}(n+2k)!(-1)^k Y_{n+m}^{m-2k}(\mu,\varphi)}{2^m(n+2m-2k)!k!} \sum_{j=0}^{\left[\frac{n}{2}\right]} \frac{(-1)^j(2n+2m-2k-2j)!}{2^n j!(n-2j)!(n+m-j-k)!} \tag{C-16}$$

then noting that[21]

$$C_n^{m-k+\frac{1}{2}}(1) = \sum_{j=0}^{\left[\frac{n}{2}\right]} \frac{(-1)^j(2n+2m-2k-2j)!}{2^n j!(n-2j)!(m+n-j-k)!} \frac{(m-k)!}{(2m-2k)!} \tag{C-17}$$

and then using the value[22]

$$C_n^{m-k+\frac{1}{2}}(1) = \binom{n+2m-2k}{n} \tag{C-18}$$

Combining this result with Eqs. (C-17) and (C-16) gives Eq. (C-4).

Equation (C-5) is obtained by direct expansion. We let

$$\begin{aligned} Y_n{}^j(\mu,\varphi) &= \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} B_{pq}^{nj} U_{pq}(\mu,\eta) \\ &= \sum_{p=0}^{\infty} \sum_{q=0}^{p} B_{p-q,q}^{nj} U_{p-q,q}(\mu,\eta) \end{aligned} \tag{C-19}$$

where the coefficients B are to be determined. That is,

$$\frac{2\pi\binom{p+q}{p}}{2p+2q+1} B_{pq}^{nj} = \iint d\mu d\varphi V_{pq}(\mu,\eta) Y_n^{\,j}(\mu,\varphi) \tag{C-20}$$

using the orthogonality properties of the U and V polynomials. We now use Eq. (C-4) on the right of this equation to obtain

$$B_{pq}^{nj} = \frac{(2p+2q+1)}{2\pi} \binom{p+q}{p}^{-1} \sum_{k=0}^{\left[\frac{q}{2}\right]} A_k^{\,pq} \iint d\mu d\varphi\, Y_{p+q}^{q-2k}(\mu,\varphi) Y_n^{\,j}(\mu,\varphi) \tag{C-21}$$

where $A_k^{\,pq}$ is the coefficient of the expansion of Eq. (C-4). Using the orthogonality properties of the spherical harmonic functions and simplifying, we have

$$B_{p-q,\,q}^{nj} = \frac{\delta_{np} p!\,q!}{2^q} \sum_{k=0}^{\left[\frac{q}{2}\right]} \frac{(-1)^k (p+q-2k)!\,\delta_{j,\,q-2k}}{k!\,(q-k)!} \tag{C-22}$$

When the properties of the second Kronecker delta are used, we find that

$$B_{p-q,\,q}^{nj} = \frac{\delta_{np}(-1)^{\frac{q-j}{2}} (n+j)!}{n!\,2^q} \binom{q}{\frac{q-j}{2}} \tag{C-23}$$

for q-j even and that the coefficients are zero otherwise. Substituting this result in Eq. (C-19) gives

$$Y_n^{\,j}(\mu,\varphi) = \sum_{q=0}^{n} \frac{(-1)^{\frac{q-j}{2}} (n+j)!}{n!\,2^q} \binom{q}{\frac{q-j}{2}} U_{n-q,\,q} \tag{C-24}$$

provided q-j is even. The lower limit of this sum is effectively $q = j$ since $[(q-j)/2]!$ is infinite for $q < j$. Substituting $q = j+2k$ gives Eq. (C-5).*

We now substitute Eq. (C-4) on the left of Eq. (C-3) obtaining

$$\sum_{j=0}^{\ell} U_{\ell-j,j}(\mu,\eta) \sum_{k=0}^{\left[\frac{j}{2}\right]} \frac{\epsilon_{j-2k} j!(\ell-j+2k)! Y_{\ell}^{j-2k}(\mu',\varphi')}{2^{j} \ell!(j-k)!k!} \tag{C-25}$$

$$\overset{?}{=} \sum_{j=0}^{\ell} \frac{\epsilon_j(\ell-j)!}{(\ell-j)!} Y_{\ell}^{j}(\mu,\varphi) Y_{\ell}^{j}(\mu',\varphi')$$

On the left of this equation we interchange the order of summation, let $j \to j + 2k$ and interchange the order of summation once more, obtaining, after subtraction of the left side,

$$\sum_{j=0}^{\ell} \frac{\epsilon_j(\ell-j)!}{(\ell+j)!} Y_{\ell}^{j}(\mu',\varphi') \tag{C-26}$$

$$\left[\sum_{k=0}^{\left[\frac{\ell-j}{2}\right]} \frac{(-1)^k (j+2k)! U_{\ell-j-2k,\,j+2k}(\mu,\varphi)(\ell+j)!}{2^{j+2k} \ell!(j+k)!k!} - Y_{\ell}^{j}(\mu,\varphi)\right] \overset{?}{=} 0$$

---

*We have not been able to find the inverse relations expressing Y_n^m as a sum of the V polynomials or expressing the U polynomials as a sum of the Y functions. Either one of these relations would serve to determine the other, and in addition would provide the information to evaluate the integrals

$$S_{nm\alpha\beta} = \iint d\mu d\varphi V_{nm}(\mu,\eta) V_{\alpha\beta}(\mu,\eta)$$

$$T_{nm\alpha\beta} = \iint d\mu d\varphi U_{nm}(\mu,\eta) U_{\alpha\beta}(\mu,\eta)$$

which are zero unless $n + m = \alpha + \beta$.

But the quantity in brackets is identically zero by Eq. (C-5) so that the addition theorem is verified.

In the proof we have stated a not too obvious identity [Eq. (C-3)] and then verified it. We actually were led to the left side of Eq. (C-3) by conjecture based on the values for $\ell = 0,1,2,3$. However, this form can be established by a procedure used by Mathews[23] in a heuristic proof of the spherical harmonic addition theorem. If a function $g(\mu,\eta)$ is expanded in terms of the polynomials U,

$$g(\mu,\eta)=\sum_{\ell=0}^{\infty}\sum_{j=0}^{\infty} A_{\ell j}U_{\ell j}(\mu,\eta) \tag{C-27}$$

the expansion coefficients are given by

$$A_{\ell j} = \frac{2\ell+2j+1}{2\pi}\binom{\ell+j}{j}^{-1}\iint d\mu' d\varphi' V_{\ell j}(\mu',\eta')g(\mu',\eta') \tag{C-28}$$

When this relation is substituted in Eq. (C-27) the result

$$g(\mu,\eta) = \iint d\mu' d\varphi' g(\mu',\eta')\sum_{\ell=0}^{\infty}\sum_{j=0}^{\infty}\frac{2\ell+2j+1}{2\pi}\binom{\ell+j}{j}^{-1}V_{\ell j}(\mu',\eta')U_{\ell j}(\mu,\eta) \tag{C-29}$$

implies that

$$\begin{aligned}\delta(\mu-\mu')\delta(\varphi-\varphi') &= \sum_{\ell=0}^{\infty}\sum_{j=0}^{\infty}\frac{2\ell+2j+1}{2\pi}\binom{\ell+j}{j}^{-1}V_{\ell j}(\mu',\eta')U_{\ell j}(\mu,\eta) \\ &= \sum_{\ell=0}^{\infty}\frac{2\ell+1}{2\pi}\sum_{j=0}^{\ell}\binom{\ell}{j}^{-1}V_{\ell-j,j}(\mu',\eta')U_{\ell-j,j}(\mu,\eta)\end{aligned} \tag{C-30}$$

But for $0 \leq \varphi, \varphi' \leq \pi$ the delta functions on the left are a function of μ_o^+ only and can be expanded as

$$\delta(\mu - \mu')\delta(\varphi - \varphi') = \sum_{\ell=0}^{\infty} D_\ell P_\ell(\mu_o^+) \tag{C-31}$$

The expansion coefficients D_ℓ are given by

$$\iint d\mu_o^+ d\varphi \sum_{k=0}^{\infty} D_k P_k(\mu_o^+) P_\ell(\mu_o^+) = \iint d\mu_o^+ d\varphi P_\ell(\mu_o^+) \delta(\mu - \mu')\delta(\varphi - \varphi) \tag{C-32}$$

or

$$\frac{2\pi D_\ell}{2\ell+1} = 1 \tag{C-33}$$

since the integral on the right is equal to $P_\ell(1) = 1$. Therefore,

$$\delta(\mu - \mu')\delta(\varphi - \varphi') = \sum_{P=0}^{\infty} \frac{2\ell+1}{2\pi} P_\ell(\mu_o^+) \tag{C-34}$$

or, letting $\varphi' \rightarrow -\varphi'$

$$\delta(\mu - \mu')\delta(\varphi + \varphi') = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2\pi} P_\ell(\mu_o^-) \tag{C-35}$$

But in Eq. (C-30), when $\varphi' \rightarrow -\varphi'$ on the left, the right side is unchanged since η' is an even function of φ'. Therefore,

$$\delta(\mu - \mu')\left[\frac{\delta(\varphi-\varphi')+\delta(\varphi+\varphi')}{2}\right] = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2\pi}\left[\frac{P_\ell(\mu_o^{+})+P_\ell(\mu_o^{-})}{2}\right]$$

$$= \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2\pi} \sum_{j=0}^{\ell} \binom{\ell}{j}^{-1} V_{\ell-j,j}(\mu',\eta')U_{\ell-j,j}(\mu,\eta) \tag{C-36}$$

When the coefficients of $(2\ell+1)/2\pi$ are equated, the desired form of the addition theorem is obtained.

Appendix D

Power Series Expansion of the U and V Polynomials, Special Values and Miscellaneous Results

By expanding the generating functions and equating coefficients of powers of a and b we find

$$V_{nm}(\mu,\eta) = \sum_{j=0}^{\left[\frac{n}{2}\right]} \sum_{k=0}^{\left[\frac{m}{2}\right]} \frac{(-1)^{j+k}}{2^{n+m}} \binom{j+k}{k} \binom{2n+2m-2j-2k}{n+m-j-k} \binom{n+m-j-k}{j+k} \binom{n+m-2j-2k}{m-2k} \mu^{n-2j} \eta^{m-2k} \tag{D-1}$$

which reduces, as it should, to the known sum for the Legendre polynomials[24] when n or m is equal to zero. Similarly, we have

$$U_{nm}(\mu,\eta) = \sum_{j=0}^{\left[\frac{n}{2}\right]} \sum_{k=0}^{\left[\frac{m}{2}\right]} \binom{j+k}{k} \binom{n+m}{2j+2k} \binom{n+m-2j-2k}{m-2k} (\mu^2 + \eta^2 - 1)^{j+k} \mu^{n-2j} \eta^{m-2k} \tag{D-2}$$

Directly from these results we find the following

$$\begin{aligned} U_{nm}(0,0) &= 0 \qquad n \text{ or } m \text{ odd} \\ &= (-1)^{\frac{n+m}{2}} \binom{\frac{n+m}{2}}{\frac{n}{2}} \qquad n \text{ and } m \text{ even} \end{aligned} \tag{D-3}$$

$$U_{nm}(1,0) = \delta_{mo} \tag{D-4}$$

$$U_{nm}(0,1) = \delta_{no} \tag{D-5}$$

$$V_{nm}(0,0) = 0 \qquad n \text{ or } m \text{ odd}$$

$$= \frac{(-1)^{\frac{n+m}{2}} \Gamma\left(\frac{n+m+1}{2}\right)}{\Gamma\left(\frac{1}{2}\right)\left(\frac{n}{2}\right)! \left(\frac{m}{2}\right)!} \qquad n \text{ and } m \text{ even} \tag{D-6}$$

$$V_{nm}(\mu,0) = 0 \qquad m \text{ odd} \tag{D-7}$$

$$V_{n,2m}(\mu,0) = \frac{(-1)^m}{2^{2m}} \binom{2m}{m} C_n^{m+\frac{1}{2}}(\mu) \tag{D-8}$$

In this equation, $C_n^{m+\frac{1}{2}}$ is a Gegenbauer polynomial.[22] Consequently,

$$V_{n,2m}(1,0) = \frac{(-1)^m}{2^{2m}} \binom{2m}{m} \binom{n+2m}{n} \tag{D-9}$$

Combining this result with the addition theorem in the form ($\mu' = 1$, $\eta' = 0$, $\mu_o = \mu$)

$$P_\ell(\mu) = \sum_{j=0}^{\ell} \binom{\ell}{j}^{-1} U_{\ell-j,j}(\mu,\eta) V_{\ell-j,j}(1,0) \tag{D-10}$$

gives

$$P_\ell(\mu) = \sum_{j=0}^{\left[\frac{\ell}{2}\right]} \frac{(-1)^j \binom{2j}{j}}{2^{2j}} U_{\ell-2j,2j}(\mu,\eta) \tag{D-11}$$

which is a special case of Eq. (C-5). Many similar relations can be found in this manner.

By manipulating Eq. (D-2) it is possible to show that

$$2U_{om} = \left[\eta + (\mu^2 + \eta^2 - 1)^{\frac{1}{2}}\right]^m + \left[\eta - (\mu^2 + \eta^2 - 1)^{\frac{1}{2}}\right]^m \qquad \text{(D-12)}$$

and that $U_{1m} = (m + 1)\mu U_{om}$.

Appendix E

Biorthogonal Expansions in Cylindrical Geometry

In two dimensional cylindrical geometry (r,θ) the Boltzmann equation is[15]

$$\frac{\mu\partial(r\psi)}{r\partial r} + \frac{\eta\partial\psi}{r\partial\theta} - \frac{1}{r}\frac{\partial(\eta\psi)}{\partial\omega} + \sigma\psi(r,\theta,\mu,\eta) =$$

$$\sigma_s \int_{-1}^{1} d\mu' \int_{0}^{\pi} d\varphi'\psi(x\ y,\mu',\eta')[f(\mu_o^+) + f(\mu_o^-)] + \mathcal{S}(r,\theta,\mu,\eta) \tag{E-1}$$

where ω is defined in Eq. (5) and where the same symmetries assumed in Eq. (8) have been used. Expanding the angular flux as in Eq. (12)

$$\psi(r,\theta,\mu,\eta) = \sum_{\alpha=0}^{\infty}\sum_{\beta=0}^{\infty} \frac{2\alpha+2\beta+1}{2\pi}\binom{\alpha+\beta}{\beta}^{-1} U_{\alpha\beta}(\mu,\eta)\psi_{\alpha\beta}(r,\theta) \tag{E-2}$$

gives the relation

$$\psi_{nm}(r,\theta) = \iint d\mu d\varphi V_{nm}(\mu,\eta)\psi(r,\theta,\mu,\eta) \tag{E-3}$$

With the application of this relation and the expansion of Eq. (18), the Boltzmann equation becomes

$$\frac{\mu\partial(r\psi)}{r\partial r} + \frac{\eta\partial\psi}{r\partial\theta} - \frac{1}{r}\frac{\partial(\eta\psi)}{\partial\omega} + \sigma\psi = \sigma_s \sum_{\ell=0}^{\infty}\frac{2\ell+1}{2\pi} b_\ell \sum_{j=0}^{\ell}\binom{\ell}{j}^{-1} \psi_{\ell-j,j}(r,\theta)U_{\ell-j,j}(\mu,\eta)$$

$$+ \mathcal{S}(r,\theta,\mu,\eta) \tag{E-4}$$

From this point, the expansion proceeds as in (x,y) geometry except for the angular derivative term. We consider this term alone, which when multiplied by $V_{nm}(\mu,\eta)$ and integrated is

$$\iint d\mu d\varphi V_{nm}(\mu,\eta)\,\frac{\partial(\eta\psi)}{\partial\omega} \tag{E-5}$$

The integral over μ and φ is equivalent to the integral over $\xi(0 \leq \xi \leq 1)$ and $\omega(-\pi \leq \omega \leq \pi)$ so that

$$\begin{aligned}\iint d\mu d\varphi V_{nm}(\mu,\eta)\,\frac{\partial(\eta\psi)}{\partial\omega} &= \iint d\xi d\omega V_{nm}(\mu,\eta)\,\frac{\partial(\eta\psi)}{\partial\omega}\\ &= \int d\xi\left\{V_{nm}\eta\psi\Big|_{\omega=-\pi}^{\omega=\pi} - \int d\omega\eta\psi\,\frac{\partial V_{nm}}{\partial\omega}\right\}\\ &= -\iint d\xi d\omega\psi\eta\,\frac{\partial V_{nm}}{\partial\omega}\\ &= -\iint d\mu d\varphi\psi\eta\,\frac{\partial V_{nm}}{\partial\omega}\end{aligned} \tag{E-6}$$

where the fact that $\eta = 0$ at $\omega = \pm\pi$ has been used. Combining this term with the rest of the transport equation, we have, after differentiation of the first term,

$$\begin{aligned}&\frac{\partial}{\partial r}\iint d\mu d\varphi\mu V_{nm}\psi + \frac{1}{r}\frac{\partial}{\partial\theta}\iint d\mu d\varphi\eta V_{nm}\psi\\ &\quad + \frac{1}{r}\iint d\mu d\varphi\left(\mu V_{nm} + \eta\,\frac{\partial V_{nm}}{\partial\omega}\right)\psi + \cdots\end{aligned} \tag{E-7}$$

When the recursion relations derived in Appendix B are applied, we find the following equation for the expansion coefficients

$$
\begin{aligned}
&\frac{\partial}{\partial r}\left[(n+1)(\psi_{n+1,m}-\psi_{n+1,m-2})+(n+2m)\psi_{n-1,m}\right] \\
&+\frac{1}{r}\frac{\partial}{\partial\theta}\left[(m+1)(\psi_{n,m+1}-\psi_{n-2,m+1})+(2n+m)\psi_{n,m-1}\right] \\
&+\frac{1}{r}\{(n+1)(m+1)\psi_{n+1,m}+(n+1)(2n+m)\psi_{n+1,m-2} \\
&-(m+1)(m+2)(\psi_{n-1,m+2}-\psi_{n-3,m+2})+[(m-n+1)-m(m+3n)]\psi_{n-1,m}\} \\
&+(\sigma-\sigma_s b_{n+m})(2n+2m+1)\psi_{nm}=(2n+2m+1)\mathcal{S}_{nm}(r,\theta)
\end{aligned}
\tag{E-8}
$$

where

$$\mathcal{S}_{nm}(r,\theta)=\iint d\mu d\varphi\,\mathcal{S}(r,\theta,\mu,\eta)V_{nm}(\mu,\eta) \tag{E-9}$$

Equation (E-8) can be reduced to one dimensional cylindrical geometry by assuming that ψ is independent of θ. In this case certain moments can be removed by making use of additional symmetry properties of the angular flux.

The presence of five expansion coefficients necessary to account for the angular derivative may indicate that the biorthogonal expansion is not optimum for cylindrical geometry, but we are not convinced that we have found the simplest recursion for $\eta\partial V_{nm}/\partial\varpi$.

Appendix F

A General Method of Moments

In this appendix, for the sake of completeness, we describe the general moments formulation of Carlson[7,8] as it is applied to the transport equation in (x,y) geometry. We consider the transport equation, Eq. (8), restricted to anisotropic scattering and an isotropic source, writing

$$\mu \frac{\partial\psi}{\partial x} + \eta \frac{\partial\psi}{\partial y} + \sigma\psi(x,y,\mu,\eta) = \frac{\sigma_s}{2\pi} \iint d\mu' d\varphi' \psi(x,y,\mu',\varphi') \tag{F-1}$$

$$+ \frac{3\sigma_s b_1}{2\pi} [\mu \iint d\mu' d\varphi' \mu' \psi + \eta \iint d\mu' d\varphi' \eta' \psi] + \frac{S(x,y)}{2\pi}$$

We now define the operator

$$\tilde{M}_{nm} = \int_{-1}^{1} d\mu \int_{0}^{\pi} d\varphi \cdot \mu^n \eta^m \tag{F-2}$$

such that

$$\tilde{M}_{nm}\psi = \int_{-1}^{1} d\mu \int_{0}^{\pi} d\varphi \psi(x,y,\mu,\eta) \mu^n \eta^m \equiv \psi_{nm}(x,y) \tag{F-3}$$

Thus, Eq. (F-1) is

$$\mu \frac{\partial\psi}{\partial x} + \eta \frac{\partial\psi}{\partial y} + \sigma\psi(x,y,\mu,\eta) = \frac{\sigma_s \psi_{00}}{2\pi} + \frac{3\sigma_s b_1}{2\pi} [\mu\psi_{10} + \eta\psi_{01}] + \frac{S(x,y)}{2\pi} \tag{F-4}$$

Applying $\widetilde{M}_{nm}$ to this equation we have

$$\frac{\partial \psi_{n+1,m}}{\partial x} + \frac{\partial \psi_{n,m+1}}{\partial y} + \sigma \psi_{nm} = \sigma_s \psi_{00} \tau_{nm} + 3\sigma_s b_1 \psi_{10} \tau_{n+1,m}$$

$$+ 3\sigma_s b_1 \psi_{10} \tau_{n,m+1} + \mathcal{S}(x,y) \tau_{nm} \tag{F-5}$$

where

$$\tau_{nm} = \frac{\int_{-1}^{1} d\mu \int_{0}^{\pi} d\varphi \mu^n \eta^m}{2\pi} = 0 \quad \text{n odd or m odd}$$

$$= \frac{\Gamma\left(\frac{n+1}{2}\right) \Gamma\left(\frac{m+1}{2}\right)}{2\Gamma\left(\frac{1}{2}\right) \Gamma\left(\frac{m+n+3}{2}\right)} \quad \text{m and n even} \tag{F-6}$$

In this general formulation the angular flux is not defined explicitly in terms of the moments ψ_{nm}. Rather, any assumed angular behavior may be postulated with undetermined coefficients and the coefficients related to the moments by Eq. (F-3). For example, suppose

$$\psi(x,y,\mu,\eta) = \sum_{\alpha=0}^{1} \sum_{\beta=0}^{1} \frac{a_{\alpha\beta}}{2\pi} \mu^\alpha \eta^\beta \tag{F-7}$$

Then,

$$\psi_{nm} = \sum_{\alpha=0}^{1} \sum_{\beta=0}^{1} a_{\alpha\beta} \tau_{\alpha+m,\beta+m} \tag{F-8}$$

and enough of these equations can be used to determine the four coefficients a_{00}, a_{01}, a_{10}, and a_{11}. Once these coefficients are determined, it follows that the ψ_{nm}, $n,m > 1$ can be expressed in terms of the ψ_{nm} for $n,m \leq 1$. Therefore, a consistent set of equations can be formed from the set of Eq. (F-5) by writing these equations for $n,m = 0,1$ and then eliminating the higher moments. Thus, the general formulation of Carlson permits a very general choice of angular representation, leads to a very simple system of moments equations, and makes possible the consistent truncation of the system of equations. However, the treatment of a general scattering source is cumbersome and the coupling of the scattering source is different than in the spherical harmonic or biorthogonal expansions. For example, in Eq. (F-5), the scalar flux, ψ_{00}, appears in every equation for which m and n are even in contrast to Eqs. (21), (27), or (46) in which the scalar flux appears only in the $n = m = 0$ equations. Whether this coupling and the similar coupling of the anisotropic terms is a computational disadvantage, is an unexplored question.

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