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DISCRETE ORDINATES ANGULAR QUADRATURE
OF THE NEUTRON TRANSPORT EQUATION

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DISCRETE ORDINATES ANGULAR QUADRATURE OF THE NEUTRON TRANSPORT EQUATION

by

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ABSTRACT

Methods of preparing discrete ordinates quadrature coefficients are described. Quadrature sets which satisfy complete symmetry conditions and various moment conditions are derived and tabulated, and critical thicknesses of one-dimensional slabs, spheres, and cylinders are calculated with these sets. Prescriptions for relaxing symmetry conditions and point location requirements are discussed, and orthogonal (Legendre-Tschebyschev) quadrature coefficients applicable in one-dimensional cylindrical or two-dimensional rectangular geometry are tabulated. Recipes are described for preparing biased direction sets, and a method of basing the bias upon material composition is outlined.

Preliminary computational results indicate that double Legendre and half-range moment satisfying quadrature sets are most accurate in one-dimensional plane geometry, while even-moment satisfying, completely symmetric sets are recommended for other geometries. At the present state of the art of discrete ordinates computations, results indicate that boundary condition treatment and, in curved geometries, the handling of the ray-to-ray transfer (streaming) terms can affect accuracy as much as further refinement of angular quadrature. Since computational results may depend upon all three of these quantities, further work is needed before an optimum quadrature method can be selected.

INTRODUCTION

The evolution of the selection of numerical quadrature sets for the numerical integration of the Boltzmann transport equation has been guided by two main principles:

1. Physical symmetry
2. The arrangement of discrete directions on latitudes on the unit sphere.

Selection of quadrature sets that satisfy the first principle guarantees that solutions will be independent of geometrical orientations. The first S_n quadrature set, which represented the angular variable, μ, by connected line segments, was equivalent to mechanical quadrature with abscissae, μ_i, located asymmetrically, with respect to $\mu = 0$, on the interval [-1,1] (see the Appendix). Although quite accurate in applications in homogeneous media,[1] this set did not give consistent results when, say, slabs of varying composition were geometrically inverted. Quadrature sets that are selected according to the second principle have the distinct advantage of permitting a double angular quadrature to be accomplished as a single direct sum. This report explores methods of selecting quadrature sets that satisfy symmetry conditions and also examines the relaxations of symmetry that are possible when geometric dimensionality permits.

COMPLETELY SYMMETRIC QUADRATURE SETS

Coordinate systems for rectangular, cylindrical, and spherical symmetries are shown in Figure 1. In each case the direction variable $\vec{\Omega}$ is defined with respect to an orthogonal rectangular coordinate frame (μ, η, ξ) which is locally aligned with respect to the unit vectors of the geometrical coordinate system. The possible orientations of the angular direction vector $\vec{\Omega}$ define a unit sphere in (μ, η, ξ) space. Complete symmetry requires that the (μ, η, ξ) coordinates of points on the unit sphere chosen to represent $\vec{\Omega}$ be invariant under all 90-degree rotations about the μ, η, or ξ axis. Hence, each set of coordinates must be symmetric with respect to the origin, and, further, the set of points on each axis must be the same. Thus, a description of one octant suffices to describe the arrangement of points on the unit sphere. For n points on each axis, [-1,1], there are $n(n + 2)/8$ points per octant on the unit sphere, $n = 2, 4, \ldots$. Figure 2 shows the arrangement for $n = 6$. Because these points lie on the unit sphere

$$\begin{aligned} \mu_3^2 + \eta_1^2 + \xi_1^2 &= 1 \\ \mu_2^2 + \eta_1^2 + \xi_2^2 &= 1 \\ &\vdots \end{aligned} \qquad (1)$$

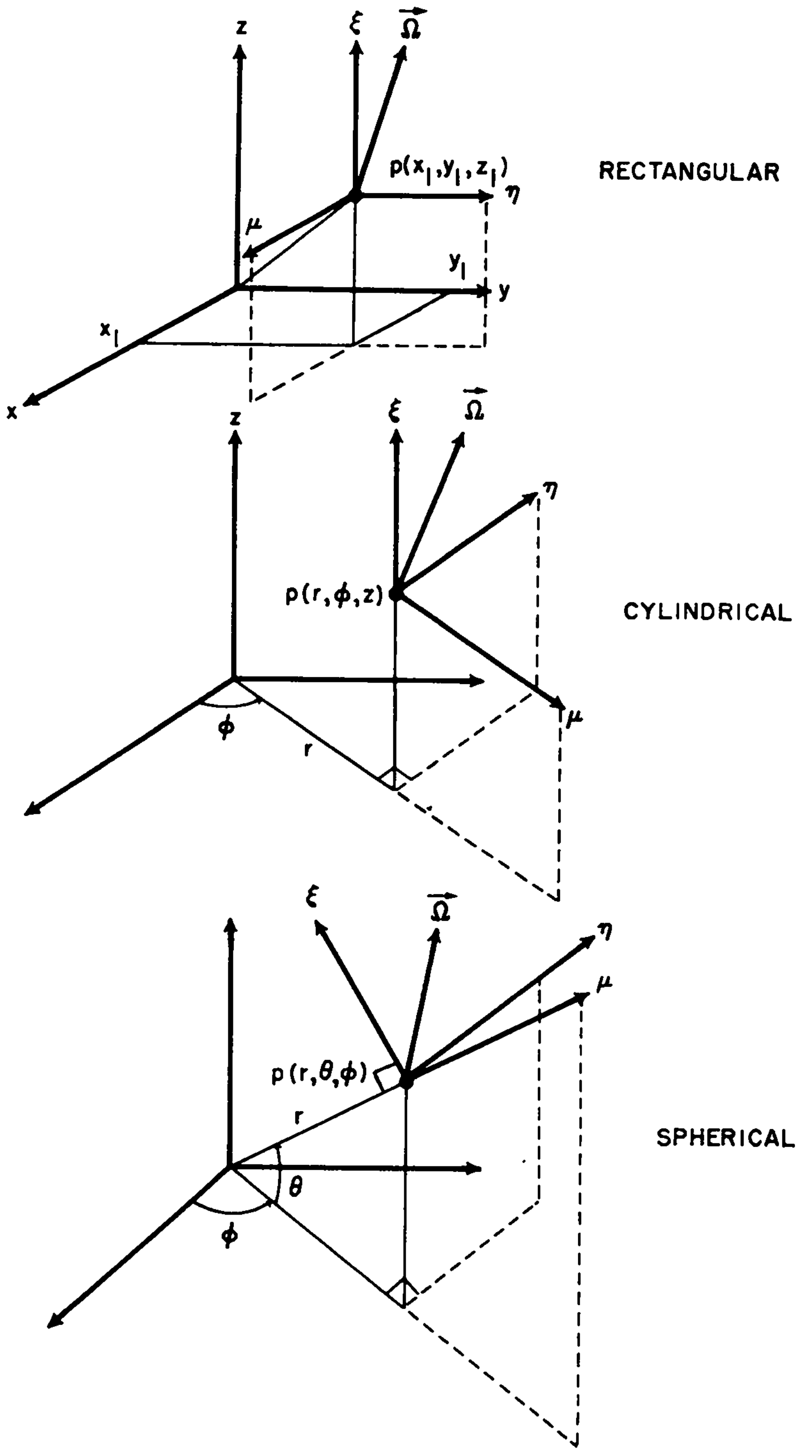

Fig. 1. Coordinate systems for rectangular, cylindrical, and spherical geometries.

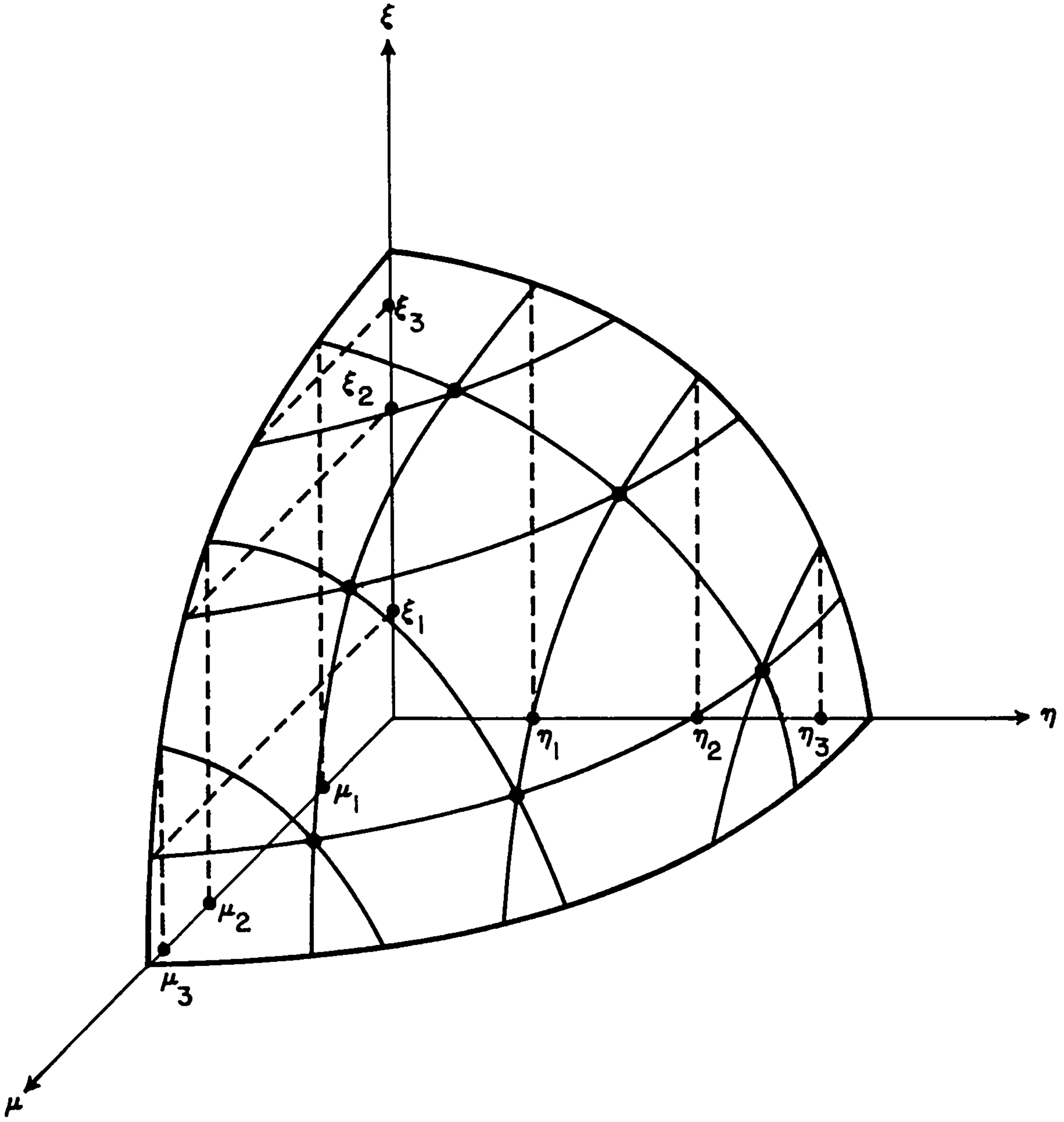

Fig. 2. Completely symmetric point arrangement, n = 6.

or, since the coordinates are from the same set,

$$\begin{aligned} \mu_3^{\,2} + 2\mu_1^{\,2} &= 1 \\ 2\mu_2^{\,2} + \mu_1^{\,2} &= 1 \\ &\vdots \end{aligned} \tag{2}$$

Because of the complete symmetry, the indices, i, j, k, of the coordinates of a point on the sphere sum to n/2 + 2. That is, in general,

$$\mu_i^{\,2} + \mu_j^{\,2} + \mu_{n/2+2-i-j}^{2} = 1.0 \tag{3}$$

where $i = 1,2,\ldots, n/2; \quad j = 1,2,\ldots,n/2 - i + 1$

The relation (3) is solved by [2,3]

$$\mu_i^{\,2} = \mu_1^{\,2} + (i - 1)\Delta \qquad i = 1,2,\ldots n/2 \tag{4}$$

where

$$\Delta = 2(1 - 3\mu_1^{\,2})/(n - 2) \tag{5}$$

Hence the requirement of complete symmetry fixes all μ_i except μ_1, and the freedom of Guassian quadrature is not present. In addition, rotational invariance dictates that weights for points on the unit sphere be chosen in a symmetric fashion. Diagrams showing points of equal weight are displayed in Figure 3. For a given latitude on the unit sphere, the sum of the point weights, p_i, defines a level weight, w_j.

n		
2	1	$w_1 = p_1$
4	1 1 1	$w_1 = 2p_1$ $w_2 = p_1$
6	1 2 2 1 2 1	$w_1 = 2p_1 + p_2$ $w_2 = 2p_2$ $w_3 = p_1$
8	1 2 2 2 3 2 1 2 2 1	$w_1 = 2p_1 + 2p_2$ $w_2 = 2p_2 + p_3$ $w_3 = 2p_2$ $w_4 = p_1$
10	1 2 2 3 4 3 2 4 4 2 1 2 3 2 1	$w_1 = 2p_1 + 2p_2 + p_3$ $w_2 = 2p_2 + 2p_4$ $w_3 = 2p_3 + p_4$ $w_4 = 2p_2$ $w_5 = p_1$
12	1 2 2 3 4 3 3 5 5 3 2 4 5 4 2 1 2 3 3 2 1	$w_1 = 2p_1 + 2p_2 + 2p_3$ $w_2 = 2p_2 + 2p_4 + p_5$ $w_3 = 2p_3 + 2p_5$ $w_4 = 2p_3 + p_4$ $w_5 = 2p_2$ $w_6 = p_1$
14	1 2 2 3 5 3 4 6 6 4 3 6 7 6 3 2 5 6 6 5 2 1 2 3 4 3 2 1	$w_1 = 2p_1 + 2p_2 + 2p_3 + p_4$ $w_2 = 2p_2 + 2p_5 + 2p_6$ $w_3 = 2p_3 + 2p_6 + p_7$ $w_4 = 2p_4 + 2p_6$ $w_5 = 2p_3 + p_5$ $w_6 = 2p_2$ and $p_3 + 2p_6 = p_4 + p_5 + p_7$ $w_7 = p_1$
16	1 2 2 3 5 3 4 6 6 4 4 7 8 7 4 3 6 8 8 6 3 2 5 6 7 6 5 2 1 2 3 4 4 3 2 1	$w_1 = 2p_1 + 2p_2 + 2p_3 + 2p_4$ $w_2 = 2p_2 + 2p_5 + p_7$ $w_3 = 2p_3 + 2p_6 + 2p_8$ $w_4 = 2p_4 + 2p_7 + p_8$ $w_5 = 2p_4 + 2p_6$ $w_6 = 2p_3 + p_5$ $w_7 = 2p_2$ $w_8 = p_1$ and $p_4 + p_5 + p_8 = p_3 + p_6 + p_7$

Fig. 3. Points of equal weight as a function of n. The equations are the relations between the point weights, p_i, and the level weights w_j.

These relations are also given in Figure 3, and the level weights are the weights corresponding to a one-dimensional angular quadrature. For $2 < n < 14$ there are $n/2 - 1$ different point weights. For $n \geq 14$ the number of different point weights increases rapidly. To fix the number of different point weights at $n/2 - 1$, it is assumed that point weights are chosen as a sum of a fundamental set of "axis" weights (a_i, a_j, a_k) with $i + j + k = n/2 + 2$. Then, enough additional relations among the p_j are provided to maintain $n/2 - 1$ different point weights. For example, the relation $p_3 + p_6 + p_6 = p_4 + p_5 + p_7$ $(n = 14)$ is established by noting that the point weights may be represented as

$$\begin{array}{ll} p_3 = a_5 + a_3 + a_1 & p_4 = a_4 + a_4 + a_1 \\ p_6 = a_3 + a_4 + a_2 & p_5 = a_5 + a_2 + a_2 \\ p_6 = a_4 + a_2 + a_3 & p_7 = a_3 + a_3 + a_3 \\ \hline \end{array}$$

$$\text{SUM} = a_1 + 2a_2 + 3a_3 + 2a_4 + a_5$$

Therefore, with complete symmetry, there are $n/2$ quantities, the $n/2 - 1$ p_j and μ_1, which can be selected, as opposed to n quantities in a Gaussian quadrature. However, it is not difficult to show[4] that if

$$\sum_{i=1}^{n(n+2)/8} p_i = \sum_{j=1}^{n/2} w_j = 1 \qquad (6)$$

that is, if the area of the octant is measured in units of $\pi/2$, then

$$\sum_{j=1}^{n/2} w_j \mu_j^2 = \frac{1}{3} \tag{7}$$

so that one moment condition is satisfied by any completely symmetric set. Hence, one can choose μ_1 and the w_j to satisfy the $n/2 + 1$ even-moment conditions

$$\int_{-1}^{1} \frac{\mu^{2i} d\mu}{2} = \int_{0}^{1} \mu^{2i} d\mu = \frac{1}{2i + 1} = \sum_{j=p}^{n/2} w_j \mu_j^{2i} \tag{8}$$

for $i = 0, 1, \ldots, n/2$. Completely symmetric quadrature sets (which automatically satisfy the odd moments over the entire range of μ because of symmetry) obtained by satisfying (8) are given in Table I. However, for $n > 22$, such sets lead to negative w_j which are undesirable because of numerical truncation errors.

As an alternative to matching even moments, all half-range moments

$$\int_{0}^{1} \mu^{i} d\mu = \frac{1}{i + 1} = \sum_{j=1}^{n/2} w_j \mu_j^{i} \tag{9}$$

$i = 0, 1, \ldots, n/2$, can be matched, but this procedure leads to negative weights for $n \geq 12$. Table II displays sets obtained by satisfying equation (9).

A method of moment matching which does not lead to negative weights is obtained by matching half-range level moments. Instead of satisfying successively higher moments by choice by level weight, sequences of lower order moments are matched by choosing point weights. For example, in

TABLE I

Completely Symmetric Quadrature Sets Satisfying Even Moment Conditions.[a]

	i	μ_i	μ_i^2	w_i	p_i
n = 4	1	0.3500212	0.1225148	0.3333333	0.3333333
	2	0.8688903	0.7549704	0.1666667	
n = 6	1	0.2666355	0.0710945	0.2547297	0.1761263
	2	0.6815076	0.4644527	0.1572071	0.1572071
	3	0.9261808	0.8578110	0.0880631	
n = 8	1	0.2182179	0.0476191	0.2117283	0.1209877
	2	0.5773503	0.3333333	0.1370370	0.0907407
	3	0.7867958	0.6190476	0.0907407	0.0925926
	4	0.9511897	0.9047619	0.0604938	
n = 12	1	0.1672126	0.0279601	0.1639814	0.0707626
	2	0.4595476	0.2111840	0.1190886	0.0558811
	3	0.6280191	0.3944080	0.0631890	0.0373377
	4	0.7600210	0.5776319	0.0624786	0.0502819
	5	0.8722706	0.7608559	0.0558811	0.0258513
	6	0.9716377	0.9440799	0.0353813	
n = 16	1	0.1389568	0.0193090	0.1371702	0.0489872
	2	0.3922893	0.1538909	0.1090850	0.0413296
	3	0.5370966	0.2884727	0.0442097	0.0212326
	4	0.6504264	0.4230545	0.0643754	0.0256207
	5	0.7467506	0.5576364	0.0400796	0.0360486
	6	0.8319966	0.6922183	0.0392569	0.0144589
	7	0.9092855	0.8268001	0.0413296	0.0344958
	8	0.9805009	0.9613820	0.0244936	0.0085179
n = 20	1	0.1206033	0.0145452	0.1195893	
	2	0.3475743	0.1208079	0.1026829	
	3	0.4765193	0.2270706	0.0282212	
	4	0.5773503	0.3333333	0.0739389	
	5	0.6630204	0.4395960	0.0181985	
	6	0.7388226	0.5458588	0.0471265	
	7	0.8075404	0.6521215	0.0313726	
	8	0.8708526	0.7583842	0.0270754	
	9	0.9298639	0.8646469	0.0332842	
	10	0.9853475	0.9709096	0.0185105	

[a]The weights given sum to 0.5. The point weights are those of Fig. 3.

TABLE II

Completely Symmetric Quadrature Sets Satisfying Odd Moment Conditions.[a]

	μ_i	μ_i^2	w_i	p_i
n = 4	0.2958759	0.0875425	0.3333333	0.3333333
	0.9082483	0.8249149	0.1666667	
n = 6	0.1838670	0.0338071	0.2178992	0.1024651
	0.6950514	0.4830964	0.2308682	0.2308682
	0.9656013	0.9323858	0.0512325	
n = 8	0.1422555	0.0202366	0.1721829	0.1090122
	0.5773503	0.3333333	0.2101402	0.0631708
	0.8040087	0.6464300	0.0631708	0.2939388
	0.9795543	0.9595267	0.0545061	
n = 12	0.0935899	0.0087591	0.1168911	
	0.4511138	0.2035036	0.2531215	
	0.6310691	0.3982482	-0.1410287	
	0.7700602	0.5929927	0.2658355	
	0.8875457	0.7877373	-0.0388597	
	0.9912022	0.9824819	0.0440403	

[a]The weights given sum to 0.5. The point weights are those of Fig. 3.

Figure 2, the normalized integral of η on the unit sphere along the latitude of μ_1 is $2\sqrt{1 - \mu_1^2}/\pi$. Defining this quantity as

$$2\sqrt{1 - \mu_1^2}/\pi = \Sigma p_i \mu_i / \Sigma p_i \tag{10}$$

where the point weights are those belonging to the μ_i, gives a sequence of low-order moment conditions, one for each μ level. These moment equations for Figure 2 are then

$$\begin{aligned} p_1\mu_1 + p_2\mu_3 + p_1\mu_3 &= (p_1 + p_2 + p_1)2\sqrt{1 - \mu_1^2}/\pi \\ p_2\mu_1 + p_2\mu_2 &= (p_2 + p_2)2\sqrt{1 - \mu_2^2}/\pi \\ p_1\mu_1 &= 2p_1\sqrt{1 - \mu_3^2}/\pi \end{aligned} \tag{11}$$

For general even n, the relations analogous to (11) give n/2 relations for the n/2 quantities p_i and μ_1. However, the last two relations

$$\mu_1 + \mu_2 = 2\sqrt{1 - \mu_{n/2-1}^2}/\pi \tag{12a}$$

$$\mu_1 = 2\sqrt{1 - \mu_{n/2}^2}/\pi \tag{12b}$$

cannot both be satisfied. To obtain a consistent set of equations, Eq. (12b), representing the smallest latitudinal area, is deleted and, instead, (6) is satisfied so that (7) is also satisfied. Thus the zeroth, second, and a sequence of first-order moments are matched. Then (12a) with (4) serves to define μ_1

$$\mu_1 = \frac{(n - 2)(1 - \sqrt{1 - \alpha}) - (n - 5)\alpha}{(n - 5)^2\alpha - (n - 2)(n - 8)} \qquad (13)$$

and hence all μ_i. Above, $\alpha = [(4/\pi)^2 - 1]^2$. The remaining $n/2 - 1$ p_j are found from equations analogous to (11). Sets obtained in this manner are displayed in Table III. Weights obtained in this manner are apparently always positive.

BIASED SYMMETRIC QUADRATURE SETS

Complete symmetry is required only in three-dimensional geometries. In lower dimensional geometries a relaxation of symmetry requirements allows additional degrees of freedom. A simple such relaxation is to keep the point and level arrangement of complete symmetry while allowing the points on each axis to be chosen from an independent set. In this case the requirement that points be on the unit sphere

$$\mu_i^2 + \eta_j^2 + \xi_k^2 = 1.0 \qquad (14)$$

is solved by

$$\begin{aligned} \mu_m^2 &= \mu_1^2 + (m - 1)\Delta \\ \eta_m^2 &= \eta_1^2 + (m - 1)\Delta \\ \xi_m^2 &= \xi_1^2 + (m - 1)\Delta \\ \Delta &= 2(1 - \mu_1^2 - \eta_1^2 - \xi_1^2)/(n - 2) \end{aligned} \qquad (15)$$

where $m = 1,2,\ldots,n/2$.

TABLE III

Completely Symmetric Quadrature Sets Satisfying Level Moment Conditions.[a]

	μ_i	μ_i^2	w_i	p_i
n = 4	0.3120418	0.0975949	0.3333333	0.3333333
	0.8971121	0.8048102	0.1666667	
n = 6	0.2390944	0.0571661	0.2582459	0.1831585
	0.6865981	0.4714169	0.1501748	0.1501748
	0.9410992	0.885668	0.0915792	
n = 8	0.2010510	0.0404215	0.2174330	0.1264098
	0.5773503	0.3333333	0.1283389	0.0910232
	0.7913565	0.6262452	0.0910220	0.0746315
	0.9587268	0.9191570	0.0632048	
n = 12	0.1596536	0.0254893	0.1726823	0.0781264
	0.4584710	0.2101957	0.1022793	0.0516366
	0.6284124	0.3949021	0.0738241	0.0429194
	0.7613203	0.5796086	0.0605145	0.0351903
	0.8742511	0.7643150	0.0516366	0.0309047
	0.9741773	0.9490214	0.0390632	
n = 16	0.1364305	0.0186133	0.1475402	0.0565552
	0.3917822	0.1534933	0.0874396	0.0361572
	0.5370040	0.2883733	0.0631648	0.0285758
	0.6505792	0.4232533	0.0519818	0.0262421
	0.7470832	0.5581334	0.0451381	0.0234298
	0.8324742	0.6930134	0.0402906	0.0188960
	0.9098865	0.8278934	0.0361672	0.0178932
	0.9812102	0.9627734	0.0282776	0.0156931

[a]The weights given sum to 0.5. The point weights are those of Fig. 3.

If complete symmetry is required, $\mu_1^2 = \eta_1^2 = \xi_1^2$, and equation (4) is obtained. Requiring rotational symmetry about the ξ axis means that $\mu_1^2 = \eta_1^2$ but ξ_1^2 is a free parameter, say $\xi_1^2 = b\mu_1^2$. Then

$$\mu_m^2 = \mu_1^2 + (m - 1)\Delta$$

$$\xi_m^2 = b\mu_1^2 + (m - 1)\Delta \qquad (16)$$

$$\Delta = 2\ [1 - (2 + b)\mu_1^2]/(n - 2)$$

Point weight diagrams for this case are given in Figure 4. Here, two different sets of level weights are defined by the point weights, one set corresponding to μ or η levels and one set corresponding to ξ levels. Again it is assumed that point weights are formed as a sum of basis weights (a_i, a_j, b_k) to maintain $2(\frac{n}{2} - 1)$ different point weights. There are now more conditions which can be satisfied and more ways in which they can be satisfied. Half-range moments similar to (9) could be matched along the ξ axis and whole-range conditions matched along the μ (and hence η) axis. Half-range, low-order moments could be satisfied in the two different directions. For example, for n = 6 the low-order moment conditions are

$$(p_1 + p_2 + p_3)2\sqrt{1 - \mu_1^2}/\pi = p_1\mu_1 + p_2\mu_2 + p_3\mu_3 \qquad (17a)$$

$$(p_2 + p_4)2\sqrt{1 - \mu_2^2}/\pi = p_2\mu_1 + p_4\mu_2 \qquad (17b)$$

$$p_3\ 2\sqrt{1 - \mu_3^2}/\pi = p_3\mu_1 \qquad (17c)$$

n

4

```
    1
   2 2
```

$w_1 = p_1 + p_2$

$w_2 = p_2 \qquad u_2 = 2p_2$

6

```
     1
    2 2
   3 4 3
```

$w_1 = p_1 + p_2 + p_3$

$w_2 = p_2 + p_4$

$w_3 = p_3 \qquad u_3 = 2p_3 + p_4$

8

```
      1
     2 2
    3 4 3
   5 6 6 5
```

$w_1 = p_1 + p_2 + p_3 + p_5$

$w_2 = p_2 + p_4 + p_6$

$w_3 = p_3 + p_6$

$w_4 = p_5 \qquad u_4 = 2p_5 + 2p_6$

10

```
       1
      2 2
     3 4 3
    5 6 6 5
   7 8 9 8 7
```

$w_1 = p_1 + p_2 + p_3 + p_5 + p_7$

$w_2 = p_2 + p_4 + p_6 + p_8$

$w_3 = p_3 + p_6 + p_9$

$w_4 = p_5 + p_8$

$w_5 = p_7 \qquad u_5 = 2p_7 + 2p_8 + p_9$

and

$p_3 + p_6 + p_8 = p_4 + p_5 + p_9$

12

```
              1
            2   2
          3   4   3
        5   6   6   5
      7   8   9   8   7
   10  11  12  12  11  10
```

$w_1 = p_1 + p_2 + p_3 + p_5 + p_7 + p_{10}$

$w_2 = p_2 + p_4 + p_6 + p_8 + p_{11}$

$w_3 = p_3 + p_6 + p_9 + p_{12}$

$w_4 = p_5 + p_8 + p_{12}$

$w_5 = p_7 + p_{11}$

$w_6 = p_{10} \qquad u_6 = 2(p_{10} + p_{11} + p_{12})$

and

$p_3 + p_6 + p_8 = p_4 + p_5 + p_9$

$p_5 + p_9 + p_{11} = p_6 + p_7 + p_{12}$

14

```
                 1
               2   2
             3   4   3
           5   6   6   5
         7   8   9   8   7
      10  11  12  12  11  10
   13   14   15   16   15   14   13
```

$w_1 = p_1 + p_2 + p_3 + p_5 + p_7 + p_{10} + p_{13}$

$w_2 = p_2 + p_4 + p_6 + p_8 + p_{11} + p_{14}$

$w_3 = p_3 + p_6 + p_9 + p_{12} + p_{15}$

$w_4 = p_5 + p_8 + p_{12} + p_{16}$

$w_5 = p_7 + p_{11} + p_{15}$

$w_6 = p_{10} + p_{14}$

$w_7 = p_{13} \qquad u_7 = 2(p_{13} + p_{14} + p_{15}) + p_{16}$

and

$p_3 + p_6 + p_8 = p_4 + p_5 + p_9$

$p_5 + p_9 + p_{11} = p_6 + p_7 + p_{12}$

$p_7 + p_{12} + p_{14} = p_8 + p_{10} + p_{15}$

$p_8 + p_{12} + p_{15} = p_9 + p_{11} + p_{16}$

Fig. 4. Point weight diagrams for half-symmetry. The level weights w_i apply to the μ or n levels, and the level weights u_i correspond to ξ levels. Only the different u level weights are shown for each n.

$$(2p_3 + p_4)2\sqrt{1 - \xi_1^2}/\pi = p_3\mu_1 + p_4\mu_2 + p_3\mu_3 \tag{18a}$$

$$2p_2\ 2\sqrt{1 - \xi_2^2}/\pi = p_2\mu_1 + p_2\mu_2 \tag{18b}$$

$$p_1\ 2\sqrt{1 - \xi_3^2}/\pi = p_1\mu_1 \tag{18c}$$

Keeping b as a free parameter gives **five** (n - 1) **quantities**, μ_1 and p_1, p_2, p_3, p_4 to be determined. Deleting (17c) and (18c) and satisfying the condition $\Sigma p_1 = 1$ gives five (n - 1) equations. ξ_1 ($\sqrt{b\mu_1}$) is then determined by (18b), and the remaining equations are linear in the p_j.
An alternative is to define accumulated weights

$$W_j = \sum_{i=1}^{j} w_i \qquad U_j = \sum_{i=1}^{j} u_j \tag{19}$$

so that $W_{j+1} - W_j = w_{j+1}$ and $U_{j+1} - U_j = u_{j+1}$ and assume that the W_j and U_j are separated by the same delta as the μ_j and ξ_j:

$$W_i = W_1 + (i - 1)\Delta$$
$$U_i = U_1 + (i - 1)\Delta \tag{20}$$
$$\Delta = 2\ [1 - (2 + b)\mu_1^2]/(n - 2)$$

Then the three independent quantities μ_1, W_1, and U_1 can be fixed by matching the **normalization** condition

$$\sum_{i=1}^{n/2} w_i = \sum_{i=1}^{n/2} u_i = 1 \tag{21}$$

and the two second-moment conditions

$$\sum_{i=1}^{n/2} w_i \mu_i^2 = \sum_{i=1}^{n/2} \mu_i \xi_i^2 = 1/3 \qquad (22)$$

for a given b. A consequence of equation (22) (but independent of the assumption (20)) is the simpler relation

$$\sum_{j=1}^{n/2-1} 2W_j + U_j = n - 2 \qquad (23)$$

Sets of quadrature coefficients have been prepared using the last-described receipe, and the resulting weights were found to be positive for the particular value of b = 2/3 used. Since such sets depend upon b, the spread of directions along the ξ axis can be varied relative to the μ and η axes direction spreads.

In the above, the number of independent point weights has been severely limited both by using the point arrangement of Figure 2 and by assuming various relationships among the point weights. A general method of choosing quadrature weights which removes these restrictions has been developed in the method of moments, described in **Reference** 5. In these methods, direction sets can be chosen so that discrete ordinates quadrature is equivalent to a generalized spherical harmonics method with a given boundary condition, say a Marshak boundary condition for no incoming flux. Once the direction sets are chosen, the quadrature weights are found by satisfying a general set of moments. Here, only the case in which points are arranged as in Figure 2 is discussed. Then, given a set of directions on each axis (with, however, $\mu_i^2 + \eta_j^2 + \xi_k^2 = 1$), the moment conditions for the $n(n + 2)/8$ point weights are given by the following triangular array[5]

$$
\begin{array}{lllll}
\psi_{00} & \psi_{02} & \psi_{04} & \cdot & \psi_{0,n-2} \\
\psi_{20} & \psi_{22} & \cdot & \cdot & \\
\psi_{40} & \cdot & \cdot & & \\
\cdot & \cdot & & & \\
\psi_{n-2,0} & & & &
\end{array}
$$

$n = 2, 4, 6, \ldots,$ where $\psi_{\ell m}$ symbolizes a moment of the form

$$\sum p_k \mu_i^{\ell} \eta_j^{m} = \frac{\frac{1}{2}\Gamma(\frac{\ell + 1}{2})\Gamma(\frac{m + 1}{2})}{\Gamma(\frac{1}{2})\Gamma(\frac{\ell + m + 3}{2})} \tag{24}$$

Above, p_k is a point weight corresponding to the point located by μ_i and η_j. To illustrate, consider $n = 2$. Then $p_1 = 1$ is the single equation to be satisfied. When $n = 4$ there are three weights and three equations

$$
\begin{array}{ll}
\psi_{00} & p_1 + p_2 + p_3 = 1 \\
\psi_{20} & p_1\mu_1^2 + p_2\mu_2^2 + p_3\mu_1^2 = 1/3 \\
\psi_{02} & p_1\eta_1^2 + p_2\eta_1^2 + p_3\eta_1^2 = 1/3
\end{array} \tag{25}
$$

Given the directions μ_i and η_j the above set can be solved for three point weights, that is for a completely unsymmetric choice of directions. The above formalism contains the half-symmetric case and the completely symmetric case. In particular, for the half-symmetric case only the diagonal and below-diagonal moments of the triangular array are needed. For n = 4 there are only two different point weights, and the moment equations become

$$\begin{aligned} &\psi_{00} \quad & p_1 + 2p_2 &= 1 \\ &\psi_{20} \quad & \mu_1^2 p_1 + (\mu_1^2 + \mu_2^2) p_2 &= 1/3 \end{aligned} \tag{26}$$

For n = 6 and four point weights in the half-symmetric case there are four equations

$$\begin{aligned} &\psi_{00} \quad & p_1 + 2p_2 + p_3 + 2p_4 &= 1 \\ &\psi_{20} \quad & \mu_1^2 p_1 + (\mu_1^2 + \mu_2^2) p_2 + \mu_2^2 p_3 + (\mu_1^2 + \mu_3^2) p_4 &= 1/3 \\ &\psi_{40} \quad & \mu_1^4 p_1 + (\mu_1^4 + \mu_2^4) p_2 + \mu_2^4 p_3 + (\mu_1^4 + \mu_3^4) p_4 &= 1/5 \\ &\psi_{22} \quad & \mu_1^2 \eta_1^2 p_1 + (\mu_1^2 \eta_2^2 + \mu_2^2 \eta_1^2) p_2 + \mu_2^2 \eta_2^2 p_3 + (\mu_1^2 \eta_3^2 + \mu_3^2 \eta_1^2) p_4 &= 1/15 \end{aligned} \tag{27}$$

For the n = 12 half-symmetric case there are 12 different point weights illustrating that the number of different point weights is not restricted to n - 2. For the completely symmetric case only the first column of the triangular array of moments need be used, indicating that even-moments matching is all that is required. The completely symmetric case is also contained in the half-symmetric case. For example, for n = 12 and the μ_i (and hence η_j) of Table I, solution of the 12 moment equations gives five different point weights, exactly equal to those of Table I. The above formulation is more general than previous methods since the direction sets can be determined independently, and, although not illustrated here, can be extended to more general point arrangements. Because of the generality, the above method is conveniently coded to produce quadrature sets (a general matrix formulation can be written). However, lacking any a priori choice of directions, meaningful comparisions of different quadrature sets are difficult to make.

Most of the above serves only to describe possible ways in which the additional degrees of freedom obtained by relaxing symmetry can be utilized, and no attempt has been made to exhaust possibilities or to determine, say, optimum moment conditions or procedures for choosing free parameters. Numerous additional symmetry relaxations are possible. The same number of points can be kept on each axis, but μ_1, η_1, and ξ_1 can be chosen independently; or different numbers of points can be chosen on each axis. Level conditions can be relaxed on one axis or all axes. The same number of points on each level can be used. One such scheme which is suited to orthogonal quadrature is the following. Suppose the quadrature of the surface of the unit sphere is accomplished by (for one octant)

$$A = \frac{2}{\pi} \int_0^1 d\xi \int_0^{\pi/2} d\omega \tag{28}$$

with ω defined as $\eta = \sqrt{1 - \xi^2} \sin \omega$ and $\mu = \sqrt{1 - \xi^2} \cos \omega$. Then

$$
\begin{aligned}
A &= \frac{2}{\pi} \int_0^1 d\xi \int_0^{\sqrt{1-\xi^2}} \frac{d\mu}{\sqrt{1 - \mu^2 - \xi^2}} \\
&= \frac{2}{\pi} \int_0^1 d\xi \int_0^1 \frac{d\mu}{\sqrt{1 - \mu^2}}
\end{aligned}
\tag{29}
$$

with $\mu = \sqrt{1 - \xi^2}\, y$. This suggests that the y integration be accomplished by Tschebyschev quadrature and the ξ integration by Legendre quadrature. Then, for example, for quadrature with three y points for each of three ξ points (Figure 5) there are nine points on the unit sphere octant, with the distribution of μ (and η) points being determined by the ξ point selection. Now points lie on the unit sphere on ξ levels but not on μ or η levels, and point weights are the product of Legendre and Tschebyschev weights. If it is argued that three y points are not needed on each ξ level, then a different order Tschebyschev quadrature can be used on each level as illustrated in Figure 6. This sort of scheme gives a significant improvement over completely symmetric quadrature when one-dimensional cylindrical critical radii are calculated.

For a given set of ξ levels $\{\xi_1, \xi_2, \ldots, \xi_{n/2}\}$ $\xi_1 < \xi_2 < \ldots < \xi_{n/2}$ and weights $\{w_1, w_2, \ldots, w_{n/2}\}$ corresponding to a Guassian quadrature on the ξ interval $[-1,1]$ the use of the same Tschebyschev quadrature on each ξ level gives the μ abscissae and point weights

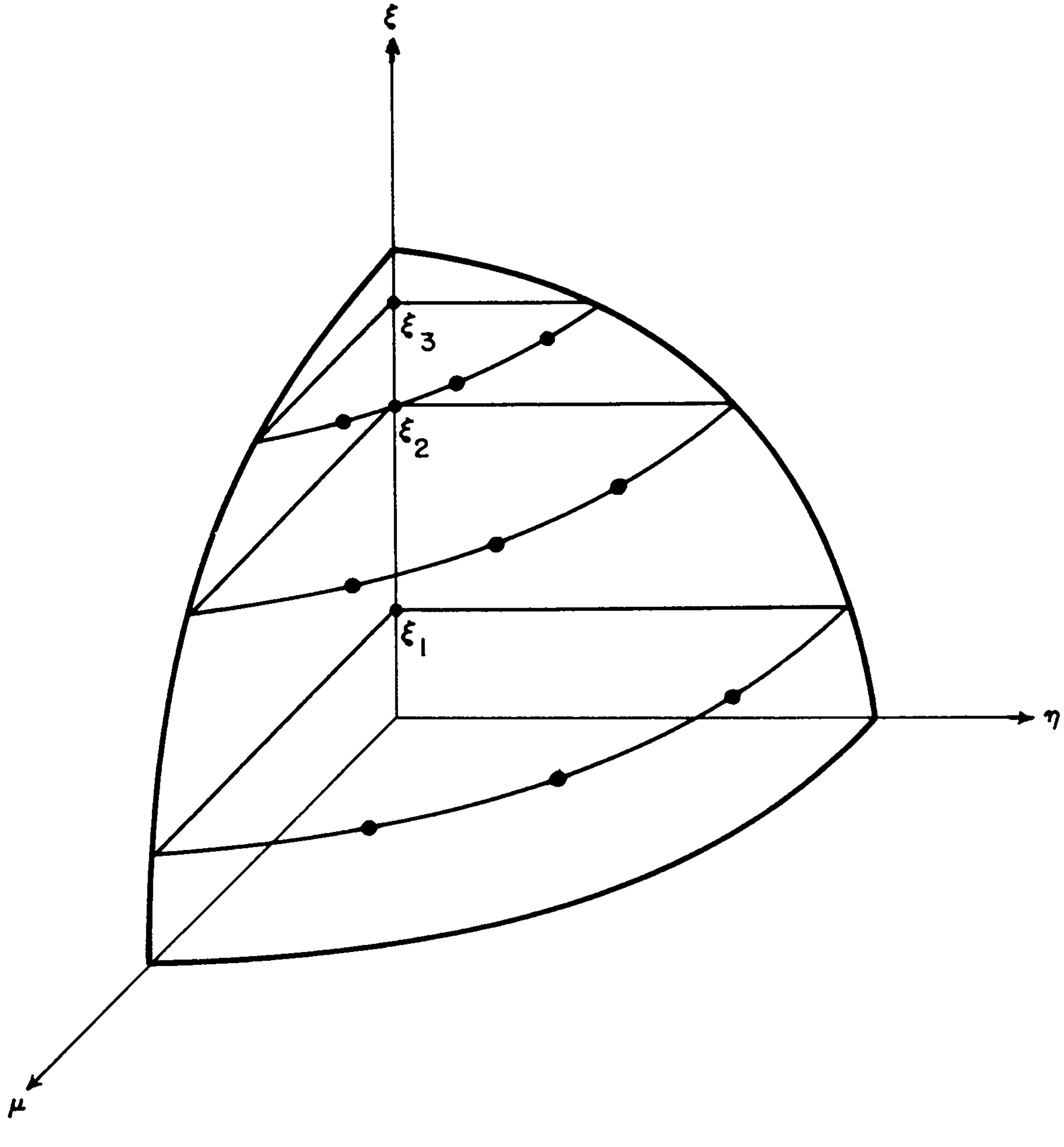

Fig. 5. Point arrangement for the same order of Tschebyschev quadrature on each ξ level. The order of the quadrature need not be the same as the number of ξ levels.

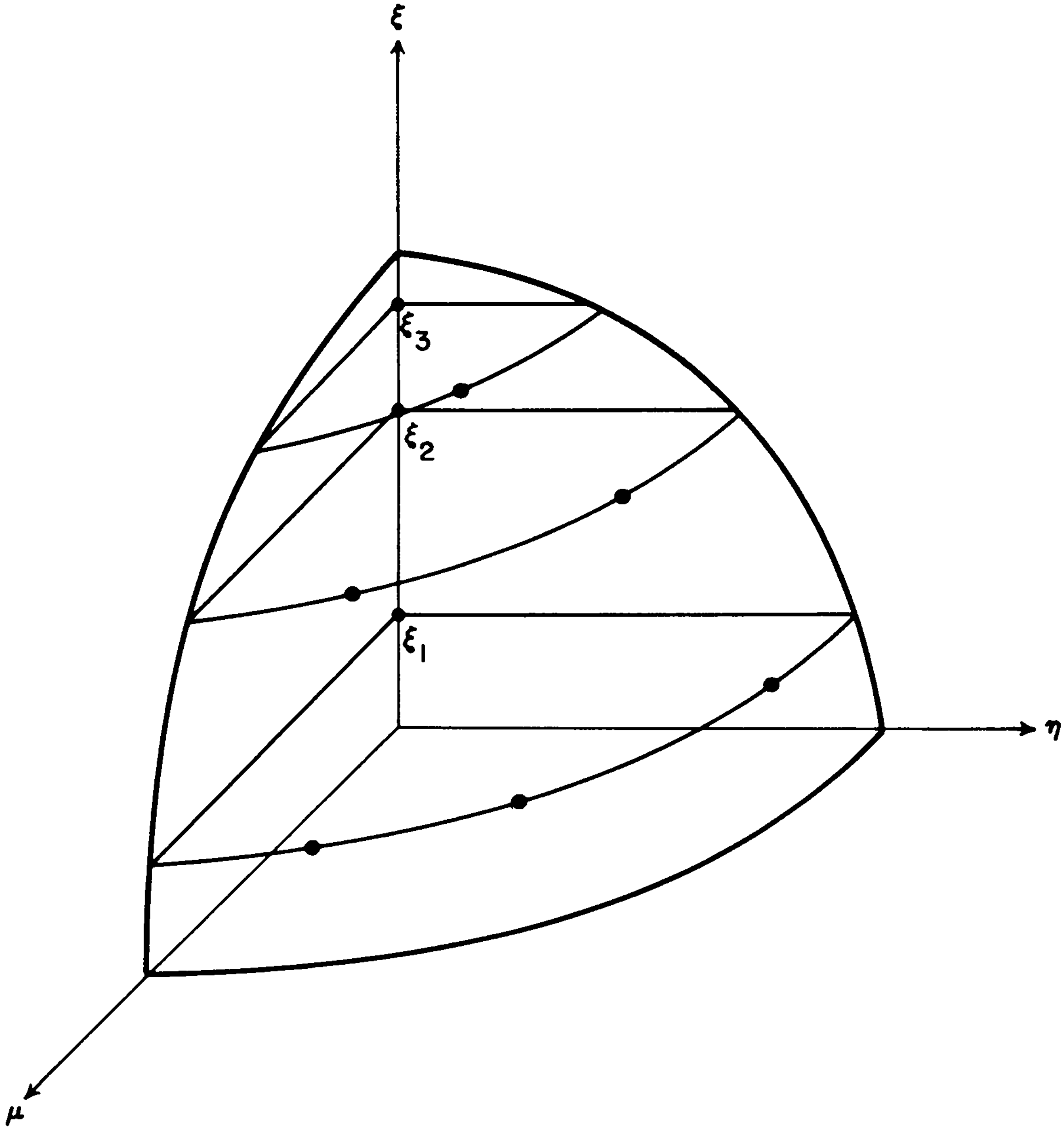

Fig. 6. Point arrangement for different order of Tschebyschev quadrature on each ξ level. Points do not all lie on the same η or μ levels as in a completely symmetric arrangement.

$$\mu_{i0} = -\sqrt{1 - \xi_i^{\,2}} \qquad\qquad p_i = 0$$

$$\mu_{ij} = \sqrt{1 - \xi_i^{\,2}}\,\cos\left(\frac{2n - 2j + 1}{2n}\pi\right) \quad p_i = \frac{w_i}{n} \tag{30}$$

$$i = 1,2,\ldots,n/2 \qquad j = 1,2,\ldots,n$$

Here the μ points with zero weights are those incoming directions used as starting directions in the current version of the S_n discrete ordinates transport code. The μ values are such that a complete quadrant is integrated, and the weights are such that the area of the quadrant is unity. For the same ξ_i and w_i the use of a different order Tschebyschev quadrature on each ξ level (as in Figure 6) gives the μ and point weights

$$\mu_{i0} = -\sqrt{1 - \xi_i^{\,2}} \qquad\qquad p_i = 0$$

$$\mu_{ij} = \sqrt{1 - \xi_i^{\,2}}\,\cos\left(\frac{2n - 4i - 2j + 5}{2n - 4i + 4}\pi\right) \quad p_i = \frac{w_i}{n + 2 - 2i} \tag{31}$$

$$i = 1,2,\ldots,n/2 \qquad j = 1,2,\ldots,(n + 2 - 2i)$$

These quadrature coefficients for the ξ_i corresponding to P_{n-1} and $DP_{n/2-1}$ quadrature are given in Table IV through Table VII for n = 4, 8, and 16.

Finally, quadrature schemes that are dependent upon material composition can be prepared. As a simple example consider the angular dependence of the flux of the monoenergetic transport equation in an

TABLE IV

$P_{n-1}(\xi)T_n(\mu)$ Quadrature Sets - Same Order

T_n Set On Each ξ Level.

	μ_{ij}	p_i	ξ_j
n = 4	-0.5083741	0.0	0.8611363
	0.1829577	0.0869637	
	0.4696763	0.0869637	
	-0.9404323	0.0	0.3399810
	0.3598878	0.1630363	
	0.8688459	0.1630363	
n = 8	-0.2790043	0.0	0.9602899
	0.0544310	0.01265357	
	0.1550065	0.01265357	
	0.2319836	0.01265357	
	0.2736433	0.01265357	
	-0.6044192	0.0	0.7966665
	0.1179163	0.02779763	
	0.3357973	0.02779763	
	0.5025562	0.02779763	
	0.5928054	0.02779763	
	-0.8507736	0.0	0.5255324
	0.16597767	0.0392133	
	0.4726644	0.0392133	
	0.7073924	0.0392133	
	0.8344262	0.0392133	
	-0.9830319	0.0	0.1834346
	0.1917800	0.0453355	
	0.5461432	0.0453355	
	0.8173612	0.0453355	
	0.9641432	0.0453355	

TABLE V

$DP_{n/2-1}(\xi)T_n(\mu)$ Quadrature Sets - Same Order T_n Set On Each ξ Level.[a]

	μ_{ij}	p_i	ξ_i
n = 4	-0.6148102	0.0	0.7886751
	0.2352776	0.125	
	0.5680104	0.125	
	-0.9774159	0.0	0.2113249
	0.3740408	0.125	
	0.9030143	0.125	
n = 8	-0.3661187	0.0	0.9305682
	0.0714262	0.0217409	
	0.2034046	0.0217409	
	0.3044166	0.0217409	
	0.3590838	0.0217409	
	-0.7423696	0.0	0.6699905
	0.1448291	0.0407591	
	0.4124384	0.0407591	
	0.6172578	0.0407591	
	0.7281052	0.0407591	
	-0.9439776	0.0	0.3300095
	0.1841609	0.0407591	
	0.5244458	0.0407591	
	0.7848887	0.0407591	
	0.9258394	0.0407591	
	-0.9975867	0.0	0.0694318
	0.1946195	0.0217409	
	0.5542294	0.0217409	
	0.8294630	0.0217409	
	0.9784184	0.0217409	

[a]For convenience the sets have been ordered as they would be entered in present S_n codes. For brevity the negative-weighted μ directions (same in magnitude as the positive directions) have been omitted.

TABLE VI

$P_{n-1}(\xi)T_n(\mu)$ Quadrature Sets - Different Order T_n Set On Each ξ Level.[a]

	μ_{ij}	p_i	ξ_i
n = 4	-0.5083741	0.0	0.7886751
	0.3594748	0.1739274	
	-0.9404323	0.0	0.2113247
	0.3598878	0.1630363	
	0.8688459		
n = 8	-0.2790043	0.0	0.9602899
	0.1972858	0.0506143	
	-0.6044192	0.0	0.7966665
	0.2313012	0.0555953	
	0.5584103	0.0555953	
	-0.8507736	0.0	0.5255324
	0.2201964	0.0522844	
	0.6015878	0.0522844	
	0.8217842	0.0522844	
	-0.9830319	0.0	0.1834346
	0.1917800	0.0453355	
	0.5461432	0.0453355	
	0.8173612	0.0453355	
	0.9641432	0.0453355	
n = 16	-0.1452095	0.0	0.9894009
	0.1026786	0.01357623	
	-0.3282956	0.0	0.9445750
	0.1256333	0.01556338	
	0.3033056	0.01556338	
	-0.5006822	0.0	0.8656312
	0.1295861	0.01585975	
	0.3540358	0.01585975	
	0.4836218	0.01585975	
	-0.6552589	0.0	0.7554044
	0.1278346	0.01557862	
	0.3640423	0.01557862	
	0.5448278	0.01557862	
	0.6426683	0.01557862	

TABLE VI (Continued)

n = 16 continued

μ_{ij}	p_i	ξ_i
-0.7862754	0.0	0.6178762
0.1230006	0.01495960	
0.3569615	0.01495960	
0.5559807	0.01495960	
0.7005765	0.01495960	
0.7765950	0.01495960	
-0.8889436	0.0	0.4580168
0.1160304	0.01409638	
0.3401839	0.01409638	
0.5411545	0.01409638	
0.7052463	0.01409638	
0.8212765	0.01409638	
0.8813385	0.01409638	
-0.9595308	0.0	0.2816036
0.1074405	0.01304310	
0.3169175	0.01304310	
0.5105032	0.01304310	
0.6784908	0.01304310	
0.8124567	0.01304310	
0.9056836	0.01304310	
0.9534967	0.01304310	
-0.9954761	0.0	0.0950125
0.0975737	0.01184066	
0.2889715		
0.4692641		
0.6315234		
0.7695135		
0.8779316		
0.9526112		
0.9906826		

[a]For convenience the sets have been ordered as they would be entered in present S_n codes. For brevity the negative-weighted μ directions (same in magnitude as the positive directions) have been omitted.

TABLE VII

$DP_{n/2-1}(\xi)T_n(\mu)$ Quadrature Sets - Different Order T_n Set On Each ξ Level.[a]

	μ_{ij}	p_i	ξ_j
n = 4	-0.6148102	0.0	0.7886751
	0.4347364	0.25	
	-0.9774159	0.0	0.2113249
	0.3740408	0.125	
	0.9030143	0.125	
n = 8	-0.3661187	0.0	0.9305682
	0.2588850	0.08696371	
	-0.7423696	0.0	0.6699905
	0.2840925	0.08151814	
	0.6858599	0.08151814	
	-0.94397762	0.0	0.3300095
	0.2443193	0.05434543	
	0.6674930	0.05434543	
	0.9118123	0.05434543	
	-0.9975867	0.0	0.0694318
	0.1946195	0.02174093	
	0.5542294	0.02174093	
	0.8294630	0.02174093	
	0.9784184	0.02174093	
n = 16	-0.1982824	0.0	0.98014493
	0.1402068	0.02530714	
	-0.4393147	0.0	0.89833324
	0.1681184	0.02779763	
	0.4058737	0.02779763	
	-0.6466744	0.0	0.76276620
	0.1673716	0.02614222	
	0.4572678	0.02614222	
	0.6246394	0.02614222	
	-0.8061455	0.0	0.59171732
	0.1572712	0.02266774	
	0.4478704	0.02266774	
	0.6702855	0.02266774	
	0.7906557	0.02266774	

TABLE VII (Continued)

n = 16 continued

μ_{ij}	p_i	ξ_j
-0.9128556	0.0	0.40828268
0.1428021	0.01813419	
0.4144277	0.01813419	
0.6454864	0.01813419	
0.8133602	0.01813419	
0.9016167	0.01813419	
-0.97145258	0.0	0.23723380
0.1268000	0.01307111	
0.3717588	0.01307111	
0.5913828	0.01307111	
0.7707051	0.01307111	
0.8975049	0.01307111	
0.9631417	0.01307111	
-0.9948151	0.0	0.10166676
0.1113917	0.00794218	
0.3285724	0.00794218	
0.5292775	0.00794218	
0.7304429	0.00794218	
0.8423356	0.00794218	
0.9389910	0.00794218	
0.9885625	0.00794218	
-0.9998029	0.0	0.01985507
0.0979998	0.00316339	
0.2902275	0.00316339	
0.4713038	0.00316339	
0.6342682	0.00316339	
0.7728581	0.00316339	
0.8817474	0.00316339	
0.9567517	0.00316339	
0.9949885	0.00316339	

[a]For convenience the sets have been ordered as they would be entered in present S_n codes. For brevity the negative-weighted μ directions (same in magnitude as the positive directions) have been omitted.

infinite medium (isotropic scattering)

$$\phi(\mu) = \frac{c/2}{1 + \mu\lambda_0}$$

$$\lambda_0 = c \tanh^{-1}\lambda_0 \tag{32}$$

$$c = (\Sigma_s + \nu\Sigma_f)/\Sigma_t$$

Picking a two-point quadrature such that this angular dependence is correctly integrated gives

$$w_1 = 1.0$$

$$\mu_1^2 = |1 - c|/\lambda_0^2 \tag{33}$$

which also correctly integrates $\mu\phi(\mu)$ and $\mu^2\phi(\mu)$. For $|c - 1| \ll 1$, $\lambda_0^2 \sim 3|1 - c|$ so that $\mu_1 \sim 1/\sqrt{3}$ which is the result obtained by requiring $w_1\mu_1^2 = \frac{1}{3}$ as in S_2 or diffusion theory quadrature. As $c \to 0$ (pure absorption), $\mu_1 \to 1.0$ indicating that to integrate a flux that is becoming more biased in the forward direction μ_1 should be chosen closer to unity. As $c \to \infty$ $\mu_1 \to 0$. Using μ_1 determined by (27) gave improved answers in critical slab thicknesses compared to using $\mu_1 = 1/\sqrt{3}$. Higher order quadratures can be obtained in a similar manner by requiring more moments of $\phi(\mu)$ to be satisfied. However, in a realistic problem, material properties change as a function of energy and position so that gains in accuracy obtained by using material dependent quadrature would seemingly be offset by the more complicated computation necessary for including the quadrature coefficient material dependence.

Although the completely symmetric quadrature sets are designed for three-dimensional geometries, one-dimensional monoenergetic critical thicknesses were calculated using the sets of Tables I through III. These results, for a variety of secondaries ratios $c = (\Sigma_s + \nu\Sigma_f)/\Sigma_t$, are displayed in Tables VIII through X. Comparable calculations for P_{n-1} and $DP_{n/2-1}$ sets are given in Reference 1 from which the exact results were taken. Of the three sets compared, the set prepared by satisfying even-moment conditions (Table I) is particularly good in cylindrical geometry and is better than the other two sets in spherical geometry. The set generated by matching odd moments (Table II) is effective only in plane geometry where the S_8 set is better than or comparable to the other two S_{16} sets. This behavior is analagous to that of $DP_{n/2-1}$ sets (half-range Gauss-Legendre quadrature) which, due to a combination of favorable circumstances, are particularly accurate in one-dimensional plane geometry. Although no complete test of the Legendre-Tschebyschev sets was made, for $c = 1.02$ in a cylinder the P_3T_4 set (Table VI) gave a critical radius of 9.0353 compared to a DP_1T_4 (Table VII) radius of 9.0264. These results bracket the S_4 results obtained using the quadrature set from Table I.

For the general use of quadrature sets it is recommended that the $DP_{n/2-1}$ sets always be used in one-dimensional plane geometry. In one-dimensional cylinders the completely symmetric sets of Table I or the

TABLE VIII

Monoenergetic Critical Thicknesses (MFP) Calculated Using Quadrature Sets of Table I.

Slabs (Half-Thickness)

c	S_4	S_8	S_{16}	Exact
1.02	5.68291	5.67065	5.66855	5.6655
1.05	3.32171	3.30659	3.30245	3.3002
1.10	2.13864	2.11998	2.11555	2.1134
1.20	1.32271	1.29710	1.29184	1.2893
1.40	0.78186	0.74758	0.73964	0.7366
1.60	0.56329	0.52656	0.51579	0.5120
1.80	0.44266	0.40637	0.39369	0.3887
2.00	0.36551	0.33091	0.31706	0.3108

Cylinders

c	S_4	S_8	---	Exact
1.02	9.03379	9.04364		9.0433
1.05	5.39784	5.40970		5.4118
1.10	3.56045	3.57335		3.5783
1.20	2.27052	2.28245		2.2884
1.40	1.38380	1.39215		1.3973
1.60	1.01122	1.01642		1.0209
1.80	0.80073	0.80356		0.8067
2.00	0.66414	0.66524		0.6673

Spheres

c	S_4	S_8	S_{16}	Exact
1.02	12.01730	12.02130	12.0229	12.0270
1.05	7.25660	7.26797	7.27197	7.2772
1.10	4.85011	4.86577	4.86982	4.8727
1.20	3.14533	3.16268	3.16887	3.1720
1.40	1.96022	1.97657	1.98206	1.9854
1.60	1.45371	1.46828	1.47316	1.4761
1.80	1.16338	1.17635	1.18072	1.1833
2.00	0.97267	0.98432	0.98826	0.9906

TABLE IX

Monoenergetic Critical Thicknesses (MFP) Calculated Using Quadrature Sets of Table II.

Slabs (Half-Thickness)

c	S_4	S_8	Exact
1.02	5.62241	5.66694	5.6655
1.05	3.25389	3.30066	3.3002
1.10	2.06750	2.11367	2.1134
1.20	1.25270	1.28847	1.2893
1.40	0.72152	0.73266	0.7366
1.60	0.51256	0.50665	0.5120
1.80	0.39934	0.38375	0.3887
2.00	0.32786	0.30716	0.3108

Cylinders

c	S_4	S_8	Exact
1.02	8.97433	9.02093	9.0433
1.05	5.34554	5.38904	5.4118
1.10	3.51360	3.55496	3.5783
1.20	2.22647	2.26442	2.2884
1.40	1.34377	1.37426	1.3973
1.60	0.97458	0.99820	1.0209
1.80	0.76735	0.78510	0.8067
2.00	0.63367	0.64674	0.6673

Spheres

c	S_4	S_8	Exact
1.02	11.97480	12.00510	12.0270
1.05	7.22652	7.25991	7.2772
1.10	4.82443	4.85785	4.8727
1.20	3.12868	3.15830	3.1720
1.40	1.94884	1.97416	1.9854
1.60	1.44513	1.46662	1.4761
1.80	1.15644	1.17508	1.1833
2.00	0.966837	0.98329	0.9906

TABLE X

Monoenergetic Critical Thicknesses (MFP) Calculated Using Quadrature Sets of Table III.

Slabs (Half-Thickness)

c	S_4	S_8	S_{16}	Exact
1.02	5.64343	5.65669	5.66343	5.6655
1.05	3.27617	3.28879	3.29616	3.3002
1.10	2.09044	2.10091	2.10884	2.1134
1.20	1.27495	1.27710	1.28446	1.2893
1.40	0.74089	0.72800	0.73171	0.7366
1.60	0.52880	0.50853	0.50796	0.5120
1.80	0.41322	0.39012	0.38617	0.3887
2.00	0.33990	0.31624	0.31004	0.3108

Cylinders

c	S_4	S_8	---	Exact
1.02	8.99519	9.0303		9.0433
1.05	5.36340	5.39658		5.4118
1.10	3.53025	3.56176		3.5783
1.20	2.24195	2.27073		2.2884
1.40	1.35734	1.38131		1.3973
1.60	0.98692	1.00622		1.0209
1.80	0.77853	0.79397		0.8067
2.00	0.64381	0.65619		0.6673

Spheres

c	S_4	S_8	S_{16}	Exact
1.02	11.99720	12.01610	12.01840	12.0270
1.05	7.24297	7.26417	7.26841	7.2772
1.10	4.83668	4.85924	4.86742	4.8727
1.20	3.13624	3.15837	3.16669	3.1720
1.40	1.95406	1.97387	1.98098	1.9854
1.60	1.44909	1.46633	1.47241	1.4761
1.80	1.15968	1.17482	1.18012	1.1833
2.00	0.96957	0.98307	0.98777	0.9906

P_nT_n sets are recommended. In one-dimensional spheres, the $DP_{n/2-1}$ or the sets of Table I seem best suited. In two- or three-dimensional geometries the completely symmetric sets of Table I or Table III would seem best, but more computational experience is needed. In special situations the biased half-symmetric sets and the material dependent sets can be useful. For the former, two-dimensional cylinders with small height-to-diameter ratios require accurate angular representation for directions nearly parallel to surfaces. The accurate representation can be obtained by proper choice of the parameter b. For neutron or photon transmission problems, accurate representation in the inward and outward directions is needed. In these problems either the half-symmetric or material dependent sets can be used to choose biased directions sets.

Finally, it should be mentioned that recent work[5] has indicated that proper treatment of the boundary conditions, and, in curved geometries, proper handling of the ray-to-ray transfer terms can be as important as choice of the angular quadrature. For example, in plane geometry, part of the accuracy of $DP_{n/2-1}$ sets is due to the fact that the Marshak boundary conditions for zero incoming flux are satisfied. Numerical experiments in which one of the Marshak boundary conditions was approximately satisfied have significantly improved P_3 results in plane geometry.

Thus, the problem of choosing numerical angular quadrature sets is indeed complicated. The work presented in this report should serve as a guide to future work and permit the intelligent preparation of quadrature sets tailored to specific needs.

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APPENDIX

The original S_n method(1) represented the angular flux in plane geometry by connected line segments. That is,

$$N(x,\mu) = \frac{n}{2}\left[(\mu - \mu_{j-1})N(x,\mu_j) + (\mu_j - \mu)N(r,\mu_{j-1})\right] \qquad \text{(A-1)}$$

with

$$\mu_j = -1 + 2j/n \qquad j = 0,1,2,\ldots,n \qquad \text{(A-2)}$$

Substituting (A-1) into the transport equation for plane geometry (isotropic sources)

$$\mu \frac{\partial N(x,\mu)}{\partial x} + \sigma N(x,\mu) = S(x) \qquad \text{(A-3)}$$

and integrating on μ from μ_{j-1} to μ_j gives the original S_n difference equation

$$\mu_j \frac{dN_j}{dx} + \sigma N_j = S(x) \qquad j = 0$$

$$\left(\frac{2\mu_j + \mu_{j-1}}{3}\right) \frac{dN_j}{dx} + \left(\frac{\mu_j + 2\mu_{j-1}}{3}\right) \frac{dN_{j-1}}{dx} + \sigma(N_j + N_{j-1}) \qquad \text{(A-4)}$$

$$= 2S(x) \qquad j > 0$$

where $N_j = N(x, \mu_j)$. To find a system of discrete ordinates equations equivalent to (A-4) with directions given by (A-2) let

$$\overline{N}_j = \sum_{i=0}^{j} b_{ji} N_{j-i} \tag{A-5}$$

and choose $b_{00} = 1$ so that $\overline{N}_0 = N_0$. Next form linear combinations of equations (A-4) with coefficients a_{jk} with $a_{j0} = 1$. That is, form a first equation by adding the $j = 1$ equation of (A-4) and a_{11} times the $j = 0$ equation of (A-4):

$$\frac{d}{dx}\left[\frac{2\mu_1 + \mu_0}{3} N_1 + \left(\frac{\mu_1 + 2\mu_0}{3} + a_{11}\mu_0\right) N_0\right] + \sigma(N_1 + (1 + a_{11})N_0) = (2 + a_{11})S \tag{A-6}$$

Then form a second equation by adding to the $j = 2$ equation of (A-4) a_{21} times the $j = 1$ equation and a_{22} times the $j = 0$ equation to obtain

$$\frac{d}{dx}\left\{\frac{2\mu_2 + \mu_1}{3} N_2 + \left[\frac{\mu_2 + 2\mu_1}{3} + \frac{a_{21}(2\mu_1 + \mu_0)}{3}\right] N_1 + \left[\frac{\mu_1 + 2\mu_0}{3} a_{21} + a_{22}\mu_0\right] N_0\right\} + \sigma\left[N_2 + (1 + a_{21})N_1 + (a_{21} + a_{22})N_0\right] = (2 + 2a_{21} + a_{22})S \tag{A-7}$$

Proceeding in this manner to form the j^{th} equation by adding to the j^{th} equation of (A-4) a_{jk} times the k^{th} preceeding equation, $k = 1, 2, \ldots, j$

gives

$$\frac{d}{dx}\left\{\frac{2\mu_j + \mu_{j-1}}{3} N_j + \sum_{i=1}^{j-1}\left[\frac{(\mu_{j+1-i} + 2\mu_{j-i})a_{j,i-1} + (2\mu_{j-i} + \mu_{j-i-1})a_{j,i}}{3}\right]N_{j-i}\right.$$

$$\left. + \left[\frac{\mu_1 + 2\mu_0}{3} a_{j,j-1} + \mu_0 a_{jj}\right]N_0\right\} \qquad \text{(A-8)}$$

$$+ \sigma\left[N_j + \sum_{i=1}^{j} (a_{j,i-1} + a_{j,i})N_{j-i}\right] = \left(a_{jj} + 2\sum_{i=1}^{j} a_{j,i-1}\right)S$$

For these equations to be equivalent to a discrete ordinates system in $\overline{N}_j$

$$\overline{\mu}_j \frac{d\overline{N}_j}{dx} + \sigma\overline{N}_j = S \qquad \text{(A-9)}$$

the coefficients a_{jk} must be chosen so that an equation of the above type is formed. For example, in equation (A-6)

$$(2 + a_{11})\,\overline{\mu}_1\overline{N}_1 = \left(\frac{2\mu_1 + \mu_0}{3}\right)N_1 + \left(\frac{\mu_1 + 2\mu_0}{3} + \mu_0 a_{11}\right)N_0 \qquad \text{(A-10)}$$

and

$$(2 + a_{11})\overline{N}_1 = N_1 + (1 + a_{11})N_0 \qquad \text{(A-11)}$$

Letting $\frac{2\mu_1 + \mu_0}{3} = \overline{\mu}_1$ gives the same coefficient for N_1 in (A-10) and (A-11). Then if a_{11} satisfies

$$\frac{\mu_1 + 2\mu_0}{3} + \mu_0 a_{11} = \left(\frac{2\mu_1 + \mu_0}{3}\right)(1 + a_{11}) = \overline{\mu}_1(1 + a_{11}) \qquad \text{(A-12)}$$

that is, if $a_{11} = -1/2$, the coefficients of N_0 are the same.
Finally, since $\overline{N}_1 = b_{10}N_1 + b_{11}N_0$, $b_{10} = 1/(2 + a_{11}) = 2/3$ and $b_{11} = (1 + a_{11})/(2 + a_{11}) = 1/3$. In general, with $\overline{\mu}_j = (2\mu_j + \mu_{j-1})/3$ the a_{jk} must satisfy the relations

$$\left[(\mu_{j+1-i} + 2\mu_{j-i})a_{j,i-1} + (2\mu_{j-1} + \mu_{j-i-1})a_{ji}\right] = 3\overline{\mu}_j \, (a_{j,i-1} + a_{j,i})$$

$$i = 1, 2, \ldots, j - 1 \qquad \text{(A-13)}$$

in addition to (A-12). The b_{jk} are given by

$$b_{j0} = 1\Big/\left(2 \sum_{i=1}^{j} a_{j,i-1} + a_{j,j}\right)$$

$$b_{jk} = \left(a_{j,k} + a_{j,k-1}\right)\Big/\left(2 \sum_{i=1}^{j} a_{j,i-1} + a_{jj}\right) \qquad \text{(A-14)}$$

Since the original quadrature was trapezoidal, that is,

$$\int_{-1}^{1} N d\mu = \left(N_0/2 + \sum_{i=1}^{n-1} N_i + N_n/2\right)/n \qquad \text{(A-15)}$$

the weights associated with the equivalent discrete ordinates quadrature are given by the identity

$$\frac{N_0}{2n} + \sum_{i=1}^{n-1} \frac{N_i}{n} + \frac{N_n}{2n} = \sum_{j=0}^{n} w_j \overline{N}_j$$

$$= \sum_{j=0}^{n} w_j \sum_{i=0}^{j} b_{ji} N_{j-i} \qquad \text{(A-16)}$$

Equating coefficients N_0, N_1, etc., gives a set of equations which may be solved for w_j:

$$\frac{1}{2n} = w_0 b_{00} + w_1 b_{11} + w_2 b_{22} \cdots w_n b_{nn}$$

$$\frac{1}{n} = w_1 b_{10} + w_2 b_{21} \cdots w_n b_{n,n-1}$$

$$\frac{1}{n} = w_2 b_{20} \cdots w_n b_{n,n-2} \qquad \text{(A-17)}$$

$$\frac{1}{2n} = w_n b_{n0}$$

Following this formalism through for n = 2, 4, 6 gives the following discrete ordinates weights and directions:

n = 2

j	$\bar{\mu}_j$	w_j
0	-1	1/10
1	-1/3	1/2
2	2/3	2/5

n = 4

j	$\bar{\mu}_j$	w_j
0	-1	23/440
1	-2/3	13/54
2	-1/6	11/45
3	1/3	19/72
4	5/6	59/297

$n = 6$

j	$\bar{\mu}_j$	w_j
0	-1	3/85
1	-7/9	116/729
2	-4/9	604/3645
3	-1/9	247/1458
4	2/9	118/729
5	5/9	257/1458
6	8/9	1640/12393

As is readily seen these weights are directions of an equivalent discrete ordinates system representing a nonsymmetric quadrature.