Optimal Numerical Integration on a Sphere

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1. **Introduction and Summary.** This paper discusses the approximation of integrals over the surface of a sphere by formulas of the following form.

$$\sum_{i=1}^{N} a_i\, f(\theta_i\,,\, \phi_i) \sim \int f(\theta, \phi)\, dS.$$

Little has been published on this subject or on its extension to the solid sphere. The literature is surveyed briefly in Section 7. Most of our space is devoted to formulas invariant with respect to a finite group of rotations of the sphere. We study such formulas by means of the group characters, as does Sobolev [12, 13].

The criterion by which integration formulas are usually judged is that of *efficiency*. It is defined like this. Consider a system of functions over the domain of integration such as polynomials in Euclidean space or surface harmonics on the sphere. They have properties of completeness and they are ordered in a natural way. Suppose that the integration formula is exact for the first L independent functions and therefore for all linear combinations of them. The efficiency E is the ratio of L to the number of arbitrary constants in the formula. The latter is a fixed multiple (one more than the dimensionality of the domain of integration) of the number N of points at which the integrand is evaluated.

A linear combination of surface harmonics (of degree not more than p) will be called a spherical polynomial (of degree p). If we choose to embed the surface of the sphere in Euclidean space of three dimensions, we find that the trace left on the surface by an ordinary polynomial in x, y and z is a spherical polynomial of the same degree. For the surface of the sphere a pth degree integration formula (exact for spherical polynomials of degree p) has

$$L = \sum_{m=0}^{p} (2m + 1) = (p + 1)^2$$

and

$$E = \frac{(p + 1)^2}{3N}.$$

Efficiency is a useful yardstick and the main part of this paper is written with reference to it. It is not beyond criticism as we shall see later. One suspects that efficiency is used for higher-dimensional regions, largely because it is the natural way of expressing the classical results of mechanical quadrature for the line segment. It is these results that we first attempt to generalize to the surface of the sphere. Generalization from the line segment to the circumference of the unit circle is achieved by replacing the classical arguments [14, Theorem 3.4.1] by their analogues for a complex variable and using the theory of polynomials orthogonal on the unit circle [14, chapter XI]. The classical arguments do not extend to the sphere but we may continue as follows.

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In the case of unit weight function the points of the integration formula for the circumference are evenly spaced. In other words, the set of points is invariant under a finite group of rotations of the unit circle. In the case of the sphere we are considering only unit weight function so that it is natural to study sets of points invariant under one of the finite groups of rotations associated with the regular solids. Sections 2–6 are concerned with this.

Let g be the order of the group. Then we shall see that, apart from any intrinsic merit, the use of an invariant formula reduces by a factor of approximately g the number of independent surface harmonics for which the formula must be made exact. This enables us to find some efficient formulas. They are listed in Table 2. The most spectacular is accurate to the 14th degree, that is exact for 225 independent functions, and uses only 72 points so that $E > 1$.

In the case of the circle it is possible to determine an infinite sequence of formulas of increasing accuracy and with E near unity. As far as the writer is aware, no one has shown that this can be done for the sphere or any other two-dimensional region; although $E = \frac{2}{3}$ has been obtained for the sphere by cartesian product methods (see Section 7). There is no evidence yet that $E = 1$ is a fruitful target in more than one dimension unless we are content with limited accuracy. Nor is $E = 1$ a strict upper bound to what may be achieved, as shown by the 14th degree formula cited above. It may be better to seek to generalize the classical results of mechanical quadrature without reference to the efficiency E.

In a sequel to this paper it will be shown how restatement in probabilistic terms leads to a concrete problem of minimization with respect to disposition of the sample points (cf. Section 7.1). This method applies also to the circle and yields the classical result.

If approximate integration is to be programmed the number of sample points may be unimportant. To meet this case a sequential procedure based solely on symmetry is outlined in Section 7.2.

The subject of this paper is essentially the wide dispersal of points on the surface of a sphere. It is relevant to interpolation and to certain problems of mathematical statistics, as well as to numerical integration.

2. Existence of Formulas. Properties of group representations assumed here are given by Heine [4, Appendix C.].

The three finite groups $\mathcal{G}_4$, $\mathcal{S}_4$, $\mathcal{G}_5$ of rotations of the sphere are associated respectively with the regular tetrahedron, octahedron-cube and icosahedron-dodecahedron. Let G be a realization of one of these groups, of order g, and let $\omega(R)$ be the set of n positions on the sphere that an arbitrary point R takes up under the different rotations of G. In general $n = g$, but if R coincides with a vertex of the regular solid, the centroid of a face (vertex of the dual solid) or the mid-point of an edge, then $n < g$.

Now there is induced on the set $\omega(R)$ an n-dimensional permutation representation $\{D\}$ of G. This may be split into its component irreducible unitary representations $\{D_\lambda\}$; that is, the carrier space Ω of dimension n, is a direct sum

$$\Omega = \oplus \, \Omega_\lambda \, ; \qquad\qquad\qquad \lambda = 1, \cdots, r$$

of subspaces Ω_λ, each invariant under G. The dimension of Ω_λ is that of $\{D_\lambda\}$ multi-

plied by the number of times the latter appears in $\{D\}$, which may be zero. The Ω_λ are *mutually orthogonal*, because permutations are unitary transformations. Now e, the vector with equal components, is invariant under all permutations and so belongs to Ω_1, the subspace subject to the identical representation $\{D_1\}$.

We turn next, for reasons given in the Introduction, to the surface harmonics of fixed degree m. These form a $(2m + 1)$-dimensional function-space V invariant under all rotations of the sphere, and therefore under those of G. So a $(2m + 1)$-dimensional representation $\{\Delta\}_m$ of G is obtained, and V is a direct sum

$$V = \oplus V_\lambda ; \qquad\qquad \lambda = 1, \cdots, r$$

where the subspaces V_λ comprise functions which transform under G according to the inequivalent representations $\{D_\lambda\}$. Consider now the natural projection of V into Ω

$$V \to \Omega$$

whereby every function of V is identified with the n-vector of its values at the points of $\omega(R)$. Because G operates both on V and on Ω then further

$$V_\lambda \to \Omega_\lambda ; \qquad\qquad \lambda = 1, \cdots, r.$$

If

$$M \equiv \oplus V_\lambda ; \quad \lambda \neq 1, \quad \dim V_\lambda \neq 0, \quad \dim \Omega_\lambda \neq 0$$

$$N \equiv \oplus V_\lambda ; \quad \lambda \neq 1, \quad \dim V_\lambda \neq 0, \quad \dim \Omega_\lambda = 0$$

then

$$V = V_1 \oplus M \oplus N$$

and the functions of N vanish at every point of $\omega(R)$; while the functions of M are orthogonal, over $\omega(R)$, to Ω_1 and thus orthogonal to e, that is their average over $\Omega(R)$ is zero. The functions of V_1 are constant over $\omega(R)$.

The point of this decomposition is that the true value of the integral of any surface harmonic of degree m is zero, except when $m = 0$. Now V_1 does not depend on the particular invariant set $\omega(R)$ under consideration so that an integration formula which assigns equal weights to points in the same invariant set is accurate for the whole of V if it is accurate for V_1. This statement is trivial when $m = 0$ for then $V = V_1$. From now on we shall distinguish different values of m by writing $V^{(m)}$ for V and $V_1^{(m)}$ for V_1.

The dimension of $V_1^{(m)}$ is the number of times the identical representation appears in $\{\Delta\}_m$. Let this be $d_1^{(m)}$, for $m = 0, 1, 2, \cdots$. Then an integration formula accurate to the pth degree may be found using just

$$C_p \equiv \sum_{m=0}^{p} d_1^{(m)}$$

invariant sets. In fact almost any C_p sets will do, by the following

THEOREM. *The set of points $R_1, R_2, \cdots, R_h$ on the sphere is said to be a p-adequate h-tuple if there exists a pth degree integration formula, invariant under G, which uses only $\omega(R_j)$; $j = 1, \cdots, h$. Then the set of C_p-tuples which are not p-adequate has measure zero (with respect to the natural C_p-fold product measure).*

Proof. Let a basis of linearly independent functions of

$$U_p \equiv \oplus V_1^{(m)}; \qquad\qquad m = 0, 1, \cdots, p$$

be $f_i(\theta, \phi)$; $i = 1, \cdots, C_p$. Then the C_p-tuple (R_j); $j = 1, \cdots, C_p$ is certainly p-adequate if the $C_p \times C_p$ matrix whose (i, j)th element is the sum of the values of $f_i(\theta, \phi)$ at the points of $\omega(R_j)$ is non-singular. Now $V_1^{(m)}$ contains only functions that are constant over any $\omega(R)$, so that the determinant that must not vanish is simply

$$\det A \equiv \|f_i(R_j)\|.$$

The proof is by induction: we assume that $R_1, \cdots, R_h$ have been chosen, where $1 \leq h < C_p$, so that the first h columns of A are linearly independent and show that almost any choice of R_{h+1} will do. Let β_i $(i = 1, \cdots, C_p)$ be constants, not all zero, such that

$$\sum_{i=1}^{C_p} \beta_i f_i(R_j) = 0; \qquad\qquad j = 1, \cdots, h.$$

If R is any point on the sphere such that the column $f.(R)$ is linearly dependent on the first h columns $f.(R_j), j = 1, \cdots, h$, then

$$\sum_{i=1}^{C_p} \beta_i f_i(R) = 0.$$

Now this finite sum of surface harmonics is not identically zero because the $f_i(\cdot)$ are the linearly independent functions of U_p. Hence the set on which it vanishes has measure zero. Thus for almost any R_{h+1} the first $(h + 1)$ columns of A are linearly independent. It follows by induction that det. A is non-zero *p.p.*

3. Calculation of C_p. Before this theorem can be put to work the numbers C_p must be calculated.

The decomposition of $\{\Delta\}_m$ is a straightforward matter involving the characters of the $\{D_\lambda\}$ and of $\{\Delta\}_m$ itself: see for example Heine [4, page 119]. Consider a rotation of the sphere through an angle ψ about any axis: with this as axis of co-ordinates the tesseral harmonics

$$e^{is\phi} P_m^s(\cos \theta); \qquad\qquad s = 0, \pm 1, \cdots, \pm m$$

are eigenfunctions of the rotation, with eigenvalues $e^{is\psi}$. So the character of $\{\Delta\}_m$ is

$$\sum_{s=-m}^{m} e^{is\psi} = \frac{\sin (m + \frac{1}{2})\psi}{\sin \frac{1}{2}\psi}.$$

Hence

(1) $$d_1^{(m)} = \frac{1}{g} \sum_{k=1}^{g} \frac{\sin (m + \frac{1}{2})\psi_k}{\sin \frac{1}{2}\psi_k}$$

where the kth group element is a rotation through an angle ψ_k. The results are

quite simple because

$$\delta^{(m)} \equiv d_1^{(m)} - \frac{1}{g}(2m + 1)$$

is periodic in m, with period $\frac{1}{2}g$.

An ingenious alternative for (1) is obtained by Sobolev [12]: let q_1, q_2, q_3 be the orders of the subgroups of G which give rise respectively to the vertices, faces and edges of the regular solid. Then he finds, for $0 \leqq m \leqq \frac{1}{2}g - 1$,

$$d_1^{(m)} = 0, \qquad 2m + 1 \leqq g \sum 1/q$$
$$= 1, \qquad 2m + 1 > g \sum 1/q$$

where summation extends only to those q_i which are not factors of m. Extension to larger values of m follows of course from the periodicity of $\delta^{(m)}$.

TABLE 1

Data on Groups

	q_1	q_2	q_3	g
$\mathcal{A}_4$	3	3	2	12
$\mathcal{S}_4$	4	3	2	24
$\mathcal{A}_5$	5	3	2	60

	$\mathcal{A}_4$				$\mathcal{S}_4$					$\mathcal{A}_5$			
No. of elements	1	3	4	4	1	6	8	3	6	1	15	20	12	12
ψ_k	0	π	$2\pi/3$	$-2\pi/3$	0	$\pi/2$	$\pm 2\pi/3$	π	π	0	π	$2\pi/3$	$2\pi/5$	$4\pi/5$

Tetrahedral Group $\mathcal{A}_4$

m:	0	1	2	3	4	5
$d_1^{(m)}$:	1	0	0	1	1	0

$$d_1^{(m+6)} = d_1^{(m)} + 1.$$

Octahedral Group $\mathcal{S}_4$

m:	0	1	2	3	4	5	6	7	8	9	10	11
$d_1^{(m)}$:	1	0	0	0	1	0	1	0	1	1	1	0

$$d_1^{(m+12)} = d_1^{(m)} + 1$$

Icosahedral Group $\mathcal{A}_5$

$$m = 0, 1, \cdots, 14: \quad d_1^{(m)} = 1 \quad \text{for } m = 0, 6, 10, 12$$
$$= 0 \quad \text{otherwise}$$
$$m = 15, 16, \cdots, 29: \quad d_1^{(m)} = 0 \quad \text{for } m = 17, 19, 23, 29$$
$$= 1 \quad \text{otherwise}$$
$$d_1^{(m+30)} = d_1^{(m)} + 1$$

The ψ_k, q_i and $d_1^{(m)}$ for all three groups appear in Table 1. The C_p may be found simply by counting the $d_1^{(m)}$. However even this exertion may be avoided by the following observation.
Let

$$(2) \qquad\qquad C_p = \frac{1}{g} (p + 1)^2 + \epsilon(p); \qquad\qquad p = 0, 1, 2, \cdots .$$

Then $\epsilon(p) = 0$ when $(p + 1)$ is a multiple of $\frac{1}{2}g$ and $\frac{1}{5} < \epsilon(p) < \frac{6}{5}$ otherwise.

This statement, once proved, *determines the integer C_p exactly.* Direct calculation, using Table 1, shows that the statement is true when $0 \leqq p \leqq \frac{1}{2}g - 1$. We show that it is valid without restriction on p by proving that $\epsilon(p)$ is periodic, with period $\frac{1}{2}g$.

$$\epsilon(p) \equiv C_p - \frac{1}{g} (p + 1)^2 = \sum_{m=0}^{p} \delta^{(m)}.$$

It is convenient to define $C_{-1} = 0$, so that $\epsilon(-1) = 0$ and

$$\epsilon(p + \tfrac{1}{2}g) - \epsilon(p) = \sum_{m=p+1}^{p+1/2g} \delta^{(m)} \qquad (p = -1, 0, 1, 2, \cdots).$$

Now this is independent of p, because $\delta^{(m)}$ has period $\frac{1}{2}g$, so

$$\epsilon(p + \tfrac{1}{2}g) - \epsilon(p) = \sum_{m=0}^{1/2g-1} \delta^{(m)}$$

$$= \sum_{m=0}^{1/2g-1} d_1^{(m)} - \tfrac{1}{4}g$$

$$= 0$$

by inspection of Table 1. Hence $\epsilon(p)$ is periodic, with period $\frac{1}{2}g$.

4. Choice of Invariant Sets. In Figure 1 the spherical triangle $XX'X''$ matches a face of the tetrahedron, octahedron or icosahedron. Y is the centroid and Z is the mid-point of XX'. The invariant sets $\omega(R)$ are in one-one correspondence with the points of the closure of triangle XYZ together with the interior of triangle $X'YZ$. Each has g points, if we exclude the three *special* sets $\omega(X)$, $\omega(Y)$ and $\omega(Z)$ which *together* have only $(g + 2)$ points. So by (2) an arbitrary C_p-tuple provides an invariant integration formula with $(p + 1)^2 + g\epsilon(p)$ points. It is p-adequate (almost certainly), i.e. it is accurate for

$$\sum_{m=0}^{p} (2m + 1) = (p + 1)^2$$

linearly independent functions.

Now compare what happens if the integration formula is based on $(p + 1)^2$ *arbitrary* points, quite unrelated to any rotation group. Take G_0 to be the (un-interesting) group with just one element. Section 1 still applies and we have in this trivial case $d_1^{(m)} = (2m + 1)$ and $C_p = (p + 1)^2$. So the $(p + 1)^2$ arbitrary points form a C_p-tuple of "invariant sets" for G_0 and the Theorem shows that it is almost certainly p-adequate. Hence the use of formulas invariant under (non-trivial) rotation groups G does not, by itself, achieve anything.
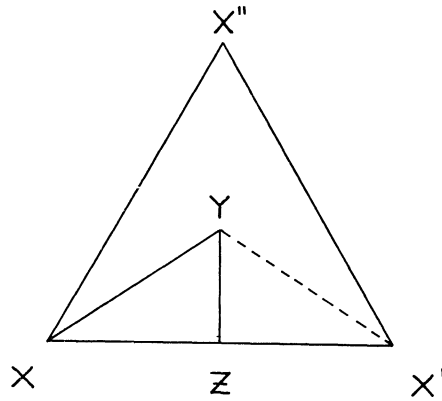
FIG. 1

For the octahedron and icosahedron, invariant sets corresponding to points on the boundary of triangle XYZ are self-antipodal and therefore eliminate odd harmonics automatically, but full use of this property involves restriction to a set of measure zero. Sobolev [13] augments G by reflection in the origin to obtain a group G^* of order $2g$, and considers only sets $\omega^*(R)$ invariant with respect to G^*. These are in one-one correspondence with the points of the closure of triangle XYZ. Unless R is X, Y or Z, $\omega^*(R)$ has g or $2g$ points according as R is or is not on the boundary of triangle XYZ. Sobolev considers two series of formulas, of increasing adequacy, and calculates their efficiency. This depends on the proportion (which tends to zero) of points lying on the boundary of triangle XYZ. So even these are no more efficient, asymptotically, than if the points were chosen at random.

Our theory seems to be useful only where it simplifies the proper choice of invariant sets to obtain efficient formulas. We saw at the beginning of this section that the efficiency of an integration formula based on C_p *arbitrary* invariant sets could not be expected to exceed

$$\frac{(p+1)^2}{3gC_p} = \frac{(p+1)^2}{3[(p+1)^2 + g\epsilon(p)]} \leq \frac{1}{3}.$$

Consider the choice of a formula based on h general invariant sets $\omega(R_i)$ and h' special ones, where h and h' are fixed integers and $0 \leq h' \leq 3$. The R_i vary within a two-dimensional region and so each general set may be said to have two positional degrees of freedom. The weights to be assigned to each set are also (as before) at our disposal so that the formula has altogether

$$2h + (h + h') = 3h + h'$$

degrees of freedom. We hope that each degree of freedom can be used to bring one more independent function within the formula's domain of accuracy. We adopt the *Working Hypothesis*: An invariant integration formula accurate for spherical polynomials of degree not more than p may be found using just h general invariant sets and h' special sets, if

(3) $$3h + h' = C_p.$$

To try and construct the formula seems to be the simplest way of finding out whether, for a particular value of p, the hypothesis is true. Assuming its validity for the moment we shall consider the efficiency

$$E \equiv \frac{(p+1)^2}{3N}$$

of conceivable formulas satisfying (3), where N is the total number of points used. $E \to 1$ as $p \to \infty$, for

$$N = gh + O(1)$$

and so

$$
\begin{aligned}
3N = 3gh + O(1) &= g(C_p - h') + O(1) \\
&= gC_p + O(1) \\
&= (p+1)^2 + O(1).
\end{aligned}
$$

We saw just now that *without* the positional degrees of freedom $3N = 3gC_p = 3(p+1)^2 + O(1)$ so that $E \to \frac{1}{3}$.

In fact $E > 1$ for some finite values of p, as we see below.

1) $h' = 0$: $3h = C_p$ and $N = gh = \frac{1}{3}gC_p$, so $3N = (p+1)^2 + g\epsilon(p) \geqq (p+1)^2$ with equality (i.e. $E = 1$) if and only if $\epsilon(p) = 0$, that is when $(p+1)$ is a multiple of $\frac{1}{2}g$.

2) $h' = 1$: $3h + 1 = C_p$ and $N = gh + g/q_1$ because the smallest special set will be used, of course. So

$$
\begin{aligned}
3N &= g(C_p - 1) + 3g/q_1 \\
&= (p+1)^2 + g(\epsilon(p) - (1 - 3/q_1))
\end{aligned}
$$

3) $h' = 2$: Similar argument gives

$$
\begin{aligned}
3N &= (p+1)^2 + g(\epsilon(p) - (2 - 3/q_1 - 3/q_2)) \\
&= (p+1)^2 + g(\epsilon(p) - (1 - 3/q_1))
\end{aligned}
$$

because $q_2 = 3$ for all three groups.

4) $h' = 3$: $3h + 3 = C_p$. The three special sets have together $(g+2)$ points and would be better replaced by another general set. So E is strictly less than in case 1), that is $E < 1$.

When $\epsilon(p) = 0$, $C_p = \frac{1}{g}(p+1)^2$. Since g is divisible by 3 and C_p is an integer $(p+1)^2$ is divisible by 3. So $(p+1)^2$ is divisible by 3^2. But g is not divisible by 3^2. Hence C_p is a multiple of 3.

So from case 1) every value of p such that $(p+1)$ is a multiple of $\frac{1}{2}g$ gives a formula with $E = 1$. In cases 2) and 3) $E \geqq 1$ if

$$\epsilon(p) \leqq 1 - 3/q_1 = 0, \tfrac{1}{4}, \tfrac{2}{5}$$

for $\mathcal{Q}_4$, $\mathcal{S}_4$ and $\mathcal{Q}_5$ respectively. Now for $\mathcal{S}_4$ $\epsilon(p) \leqq \frac{1}{4}$ only when $\epsilon(p) = 0$. So cases 2) and 3) cannot give $E \geqq 1$, for $\mathcal{Q}_4$ or $\mathcal{S}_4$, because $\epsilon(p) = 0$ implies that C_p is a multiple of 3. For $\mathcal{Q}_5$, $\epsilon(p) = \frac{2}{5}$ when $p + 1 \equiv \pm 6 \pmod{30}$ and $0 < \epsilon(p) < \frac{2}{5}$ when $p + 1 \equiv \pm 10, 15 \pmod{30}$. These give formulas with $E \geqq 1$ only when

C_p is not a multiple of 3. By the periodicity of $\epsilon(p)$

$$C_{p+30} - C_p = \tfrac{1}{60}(p + 1 + 30)^2 - \tfrac{1}{60}(p + 1)^2$$

$$\equiv p + 1 \,(\text{mod } 3).$$

A short calculation shows that cases 2) and 3) give $E \geqq 1$ for $\mathfrak{A}_5$ when

$$p + 1 \equiv \pm 6,\, 15 \,(\text{mod } 30)$$

or

$$p + 1 \equiv \pm 10,\, \pm 20 \,(\text{mod } 90).$$

Combining these results with those of case 1) we list finally those values of p for which the Working Hypothesis (if true) predicts an invariant integration formula of degree p with $E \geqq 1$.

$$p + 1 \equiv 0 \,(\text{mod } 6) \qquad\qquad E = 1$$

$$p + 1 \equiv 15 \,(\text{mod } 30) \qquad\qquad E > 1$$

$$p + 1 \equiv \pm 10 \,(\text{mod } 90)$$

$$p + 1 \equiv \pm 20 \,(\text{mod } 90).$$

In the next section necessary and sufficient conditions are given for a formula to be accurate up to degree p. In section 6 these are used to construct some low-degree formulas. It will then be seen that the Working Hypothesis is frequently valid and that $E > 1$ does occur.

5. Conditions for a pth-Degree Formula. Let $A_1, \cdots, A_t$ be arbitrary points on the unit sphere and let γ_{rs} be the arc-length $A_r A_s$. Let $a_1, \cdots, a_t$ be real weights. Then $\sum_{r=1}^{t} a_r f(A_r)$ vanishes for all surface harmonics $f(\,\cdot\,)$ of degree m if and only if

$$\sum_{r=1}^{t} \sum_{s=1}^{t} a_r a_s P_m(\cos \gamma_{rs}) = 0.$$

This follows from the addition theorem for spherical harmonics

$$\frac{2m + 1}{4\pi} P_m(\cos \gamma_{rs}) = \sum_{n=-m}^{m} T_m{}^n(A_r)(T_m{}^n(A_s))^*$$

where the $T_m{}^n(\,\cdot\,)$ are normalized tesseral harmonics.

Now let $R_1, \cdots, R_k$ be any k-tuple; and define for $i, j = 1, \cdots, k$:

$$\pi_{ij}^{(m)} = \sum_{r=1}^{n_i} \sum_{s=1}^{n_j} P_m(\cos A_r B_s); \qquad\qquad A_r \in \omega(R_i)$$

$$B_s \in \omega(R_j).$$

$n_i = g$ except when $\omega(R_i)$ is one of the special sets. The $k \times k$ matrix

$$\Pi^{(m)} \equiv [\pi_{ij}^{(m)}]$$

is symmetric and non-negative definite (by the addition theorem) and the k in-

variant sets, with vector of weights a, provide a pth degree formula if and only if

$$a'\Pi^{(m)}a = 0; \qquad\qquad m = 1, 2, \cdots, p$$

that is

$$\Pi^{(m)}a = 0; \qquad\qquad m = 1, 2, \cdots, p.$$

In fact $\sum a_i n_i \neq 0$ is also necessary, but it is impossible to overlook the failure of this condition in practice, so we shall not mention it again.

LEMMA. *The rank of $\Pi^{(m)}$ is at most $d_1^{(m)}$.*

Proof. A non-zero vector of weights may be found for any h-tuple of invariant sets, where $h > d_1^{(m)}$, to eliminate the surface harmonics of degree m. This follows from Section 1, since $d_1^{(m)}$ homogeneous equations in $(d_1^{(m)} + 1)$ unknowns have always a non-zero solution. Hence, by the argument of the present Section, all principal minors of $\Pi^{(m)}$ larger than $d_1^{(m)} \times d_1^{(m)}$ vanish. But $\Pi^{(m)}$ is symmetric, so that its rank is at most $d_1^{(m)}$.

In particular when $d_1^{(m)} = 1$

$$\pi_{ij}^{(m)} = \epsilon_i \epsilon_j \sqrt{(\pi_{ii}^{(m)} \pi_{jj}^{(m)})}; \qquad\qquad \epsilon_i = \pm 1.$$

So if $d_1^{(m)} \leqq 1$ $(m = 1, \cdots, p)$ the conditions $a'\Pi^{(m)}a = 0$ for a pth degree formula become

$$\left. \sum_{i=1}^{k} a_i \epsilon_i \sqrt{\pi_{ii}^{(m)}} = 0; \qquad \begin{matrix} 1 \leqq m \leqq p \\ d_1^{(m)} = 1 \end{matrix} \right\}$$

since values of m for which $d_1^{(m)} = 0$ impose no constraint. Returning to the definition we find that $\pi_{ii}^{(m)}$ is a complicated function of the position of R_i. The special set $\omega(X)$ will now play the rôle of a pivot, to simplify the form of the constraints. Define $R_0 \equiv X$, which may or may not be a member of the k-tuple. We have of course

$$\left. \pi_{i0}^{(m)} = \epsilon_i \epsilon_0 \sqrt{(\pi_{ii}^{(m)} \pi_{00}^{(m)})}; \qquad \begin{matrix} i = 1, \cdots, k \\ d_1^{(m)} = 1 \end{matrix} \right\}$$

and so

$$\left. \sum_{i=1}^{k} a_i \pi_{i0}^{(m)} = 0; \qquad \begin{matrix} 1 \leqq m \leqq p \\ d_1^{(m)} = 1 \end{matrix} \right\}.$$

This is sufficient provided $\pi_{00}^{(m)}$ vanishes only when $d_1^{(m)}$ does. It can be shown that, for the tetrahedron $\pi_{00}^{(m)} = 0$ implies $d_1^{(m)} = 0$. We omit a proof because one may be obtained by the methods which are applied below to the other two groups.

For the octahedron and icosahedron, $\pi_{00}^{(m)}$ vanishes for all odd m because $\omega(X)$ is self-antipodal. So if there are odd harmonics to be eliminated they must be treated separately. If m is even and $d_1^{(m)} \geqq 1$ then $\pi_{00}^{(m)}$ could vanish only by accident: we shall show that this never happens.

Group S_4 : The distance between two vertices of the octahedron is either 0, $\pi/2$ or π, and

$$\pi_{00}^{(2r)} = 6 \times 2(1 + 2P_{2r}(0)); \qquad\qquad r = 0, 1, 2, \cdots.$$

The inequality:

$$(\sin \theta)^{1/2} \cdot | P_n(\cos \theta) | < \left(\frac{2}{\pi}\right)^{1/2} n^{-1/2}$$

given in Szegö [14, page 163], shows that $| P_n(0) | < \frac{1}{2}$ when $n \geqq 3$. So $\pi_{00}^{(2r)} \neq 0$, when $r \geqq 2$. But $d_1^{(2)} = 0$.

Group $\mathfrak{C}_5$: The distance between two vertices of the icosahedron is either $0, \alpha, \pi - \alpha$ or π and

$$\pi_{00}^{(2r)} = 12 \times 2(1 + 5P_{2r}(\cos \alpha)); \qquad r = 0, 1, 2, \cdots .$$

Since $d_1^{(2)} = 0$, $\pi_{00}^{(2)} = 0$; so $\cos^2 \alpha = \frac{1}{5}$. The inequality gives $| P_n(1/\sqrt{5}) | < \frac{1}{5}$ when $n \geqq 18$. Thus $\pi_{00}^{(2r)} \neq 0$ when $r \geqq 9$. Since $d_1^{(2)} = d_1^{(4)} = d_1^{(8)} = d_1^{(14)} = 0$, only the cases $2r = 6, 10, 12, 16$ remain.

Now the coefficients of a Legendre polynomial, when multiplied by a suitable power of 2, are integers. So, for $r \geqq 2$, $5P_{2r}(1/\sqrt{5})$ can be an integer only if the coefficient of the leading term of $P_{2r}(\cdot)$ contains a power of 5. If it contains a single factor of 5, then the next coefficient must not contain a power of 5. The leading terms of $P_n(\mu)$ are:

$$\frac{1 \cdot 3 \cdot 5 \cdot \ \cdots \ (2n - 1)}{1 \cdot 2 \cdot 3 \cdot \ \cdots \ n} \left\{ \mu^n - \frac{n(n - 1)}{2(2n - 1)} \mu^{n-2} + \ \cdots \right\}$$

and the first coefficient has no power of 5 for $n = 6, 10, 12$. For $n = 16$ there is a single factor 5, but this is present also in the second coefficient. So $5P_{2r}(1/\sqrt{5})$ is not an integer for $2r = 6, 10, 12, 16$.

Hence $\pi_{00}^{(2r)} \neq 0$ for $2r = 6, 10, 12, 16$.

6. Construction of Formulas. We can now find some formulas whose efficiency is near unity. The tetrahedral group is not considered because every tetrahedral invariant set can be supplemented by another to form an invariant set of an octahedral realization (since two mutually antipodal tetrahedra make a cube). Nor do we look for formulas with more than one general invariant set ($h > 1$), because the calculations become more complex. The results obtained are listed in Table 2.

6.1 Special Sets Only ($h = 0$). Obvious at once are formulas based on a single special set ($h' = 1$). The existence of the others must be proved by calculation and a first step is to find the distances from a point of $\omega(R_0) \equiv \omega(X)$ to the points of $\omega(Y)$ and $\omega(Z)$.

Group $\mathbb{S}_4$: The distance between a vertex of the octahedron and one of the cube is ϕ or $\pi - \phi$ where, since $d_1^{(2)} = 0$, $\pi_{XY}^{(2)} = 0$ (with obvious notation). Thus $P_2(\cos \phi) = 0$, so:

$$\cos^2 \phi = \tfrac{1}{3}.$$

The distance between a vertex of the octahedron and the mid-point of an edge is $\psi, \pi/2$ or $\pi - \psi$ where $\pi_{XZ}^{(2)} = 0$, that is:

$$2P_2(\cos \psi) + P_2(0) = 0,$$

so

$$\cos^2 \psi = \tfrac{1}{2}.$$

Group $\mathfrak{C}_5$: The distance between a vertex of the icosahedron and one of the dodecahedron is $\alpha, \beta, \pi - \beta$ or $\pi - \alpha$ where, since $d_1^{(2)} = d_1^{(4)} = 0$, $\pi_{XY}^{(2)} = \pi_{XY}^{(4)} = 0$.

<div align="center">

TABLE 2

Summary of Formulas

</div>

Tetrahedral Group

The four vertices of the tetrahedron, that is the special set $\omega(X)$, provide a second-degree formula. The group is not exploited any further for the reason given at the beginning of Section 6.

Octahedral Group

p	C_p	N	E	a_X	a_Y	a_Z	a	R	Priority
3	1	6	0.89	1					K S
		8			1				
		12				1			
5	2	14		8	9				K S
		18		1		2			K S
		20			9	-16			
7	3	24	0.89				1	(0.866, 0.423, 0.267)	
		26		40	27	32			K
8	4	30	0.90	16			21	(0.819, 0.517, 0.251)	
11	6	50	0.96	9216	15309	16384	14641	(0.906, 0.302, 0.302)	

Icosahedral Group

p	C_p	N	E	a_X	a_Y	a_Z	a	R	Priority
5	1	12	1.00	1					F S
		20			1				F
		30				1			
9	2	32	1.04	25	27				F S
		42		25		32			S
		50			27	-32			
11	3	62		625	243	512			
14	4	72	1.04	125			143	see Section 6.42	

p: degree of spherical polynomial for which formula is exact.
C_p : number of degrees of freedom of formula.
N: number of points.
E: efficiency (listed only once for each value of p).
a_X, a_Y, a_Z, a: weights assigned to points of $\omega(X)$, $\omega(Y)$, $\omega(Z)$, $\omega(R)$ respectively.
R: Cartesian co-ordinates of generator of $\omega(R)$.

Hence:

$$P_2(\cos\alpha) + P_2(\cos\beta) = P_4(\cos\alpha) + P_4(\cos\beta) = 0,$$

so

$$\cos^2\alpha, \cos^2\beta = \tfrac{1}{15}(5 \pm 2\sqrt{5}).$$

The distance between a vertex of the icosahedron and the mid-point of an edge is γ, δ, $\pi/2$, $\pi - \delta$ or $\pi - \gamma$ where $\pi_{XZ}^{(2)} = \pi_{XZ}^{(4)} = 0$, that is:

$$P_2(\cos\gamma) + P_2(\cos\delta) + P_2(0) = P_4(\cos\gamma) + P_4(\cos\delta) + P_4(0) = 0,$$

so

$$\cos^2\gamma, \qquad \cos^2\delta = \tfrac{1}{10}(5 \pm \sqrt{5}).$$

The three designs for each group that use just two special sets may now be found. So may the designs using three special sets. The calculation is given only for the 11th degree icosahedral design.

We demand:

$$a_X\pi_{XX}^{(m)} + a_Y\pi_{YX}^{(m)} + a_Z\pi_{ZX}^{(m)} = 0; \qquad\qquad m = 6, 10.$$

It is true in any case for $m = 2, 4, 8$. Consider the expansion, when m is even, of $(\cos\theta)^m$ in Legendre polynomials $P_n(\cos\theta)$: the constant term is $\dfrac{1}{m+1}$. It follows that we require for m even and ≤ 10:

$$a_X \sum_{\omega(X)}\sum_{\omega(X)} (\cos\theta_{rs})^m + a_Y \sum_{\omega(X)}\sum_{\omega(Y)} (\cos\theta_{rs})^m + a_Z \sum_{\omega(X)}\sum_{\omega(Z)} (\cos\theta_{rs})^m$$

$$= \frac{1}{m+1}(12^2\cdot a_X + 12.20a_Y + 12.30a_Z)$$

where the angles involved have just been found.

Putting $m = 6, 10$ we obtain

$$a_X/5^2 - a_Y/3^3 - a_Z/2^5 = 0$$
$$7^2 a_X/5^4 - 17a_Y/3^5 - a_Z/2^4 = 0$$

and so

$$a_X:a_Y:a_Z = 5^4:3^5:2^9.$$

6.2 Octahedral Group: $h = 1$. The simplest formula is one with a single, general invariant set but no special sets. The conditions are

$$\pi_{i0}^{(m)} = 0; \qquad\qquad 1 \leq m \leq 7$$

For any $m > 0$, $\pi_{i0}^{(m)}$ vanishes somewhere on the sphere because, regarded as a function of R_i, it is a surface harmonic of degree $m > 0$ so that its integral over the sphere vanishes. Two may or may not vanish together, but there is certainly no reason to expect a simultaneous zero of more than two. So with $g = 24$ points we can hope for a 7th degree formula.

Let $\pm\mu_1$, $\pm\mu_2$, $\pm\mu_3$ be the cosines of the distances from a point of the required

invariant set to the octahedral points. Let $\nu_j \equiv \mu_j{}^2$ $(j = 1, 2, 3)$. Then

$$\pi_{i0}^{(m)} = 0; \qquad\qquad m = 2, 4, 6$$

implies

$$\sum_{j=1}^{3} \nu_j{}^n = \frac{3}{2n + 1}; \qquad\qquad n = 1, 2, 3$$

by the expansion of μ^{2n} in Legendre polynomials. Hence the ν_j are the roots of

$$105\nu^3 - 105\nu^2 + 21\nu - 1 = 0$$

which are, nearly, 0.750, 0.179, 0.071. Since these squares of the direction cosines are real, lie between 0 and 1, and sum to unity, the set exists. In fact there are two mutually antipodal sets. Either gives a 7th degree design.

Two more formulas based on the octahedral group are found. The first is 8th degree with 30 points $(h = 1; h' = 1)$.

$$a_0 \pi_{00}^{(m)} + a \pi_{i0}^{(m)} = 0; \qquad\qquad m = 2, 4, 6, 8.$$

With notation as before and $S_n \equiv \sum_{j=1}^{3} \nu_j{}^n$, then S_4, S_3 and S_2 can be expressed as linear functions of the ratio of weights a/a_0. Since $S_1 = 1$, the cubic whose roots are the ν_j has just two unknown coefficients and S_4, S_3, S_2 have an alternative expression in terms of these. When the unwanted solution $R_i = X$ is rejected the equations can be solved and the cubic is

$$441\nu^3 - 441\nu^2 + 105\nu - 5 = 0$$

with roots 0.670, 0.267, 0.063 approximately, and $a_0{:}a = 16{:}21$. Again there are two equivalent, mutually antipodal formulas.

The case $(h = 1; h' = 2)$ could give a 9th degree formula with (at least) 38 points. We do not investigate this because a 9th degree formula with fewer points has already been found, based on the icosahedral group.

The case $(h = 1; h' = 3)$ is more valuable so we solve it. The only novelty is that an odd harmonic must be eliminated. This is done by confining R_i to the boundary of triangle XYZ (see Figure 1, Section 3). The "even" conditions

$$a_0 \pi_{00}^{(m)} + a_1 \pi_{01}^{(m)} + a_2 \pi_{02}^{(m)} + a \pi_{i0}^{(m)} = 0; \qquad m = 4, 6, 8, 10$$

give, after elimination of the weights, a linear equation in S_5, S_4, S_3, S_2. There are now two possibilities: if R_i is on XZ it is distance $\pi/2$ from X'' and one root of the cubic is zero. This leads only to $R_i = X$ or $R_i = Z$, both of which are unacceptable. So R_i must be tried on XY or YZ, implying that the roots have the form $\nu, \nu, 1-2\nu$. The linear equation in the S_n is now a quintic in ν but after rejection of the solutions corresponding to $R_i = X$, $R_i = Z$ and $R_i = Y$ (twice) only

$$\nu = 1/11$$

remains. The weights $a_0{:}a_1{:}a_2{:}a$ are as $2^{10} \cdot 3^2 {:} 3^7 \cdot 7 {:} 2^{14} {:} 11^4$.

6.3. Icosahedral Group: $h = 1$. An 11th degree formula with one general set alone $(h' = 0)$ is expected. The conditions are

$$\pi_{i0}^{(m)} = 0; \qquad\qquad 1 \leqq m \leqq 11.$$

Let $\pm\mu_j$ $(j = 1, \cdots, 6)$ now be the cosines of the distances from a point of the required invariant set to the vertices of the icosahedron. Let $\nu_j \equiv \mu_j^2$ $(j = 1, \cdots, 6)$. Then

$$\pi_{i0}^{(m)} = 0; \qquad\qquad m = 2, 4, 6, 8, 10$$

implies

$$S_n \equiv \sum_{j=1}^{6} \nu_j^{\,n} = \frac{6}{2n+1}\,; \qquad\qquad n = 1, 2, 3, 4, 5,$$

by the expansion of μ^{2n} in Legendre polynomials. S_6 can be found from the remaining condition $\pi_{i0}^{(14)} = 0$ which is satisfied vacuously, since $d_1^{(14)} = 0$.

The sixth degree polynomial whose roots are the ν_j is now determined, but when it is solved only two of the roots are found to be real. Hence there is no 11th degree formula based on a single invariant set of the icosahedral group.

This instance of failure of the Working Hypothesis of Section 4 is interesting because of its success in all the other cases investigated (those listed in Table 2).

Finally, we solve the case $(h = 1; h' = 1)$ to obtain a 14th degree formula with 72 points. As predicted in Section 3, it is super-efficient $(E > 1)$. The solution is determined by

$$a_0\pi_{00}^{(m)} + a\pi_{i0}^{(m)} = 0; \qquad\qquad m = 2, 4, \cdots, 14,$$

and the calculation, although lengthy, is similar to those already described. After rejecting $R_i = X$ we find

$$a_0:a = 125:143$$

and

$$2556125\nu^6 - 5112250\nu^5 + 3578575\nu^4 - 1043900\nu^3 + 115115\nu^2 - 3562\nu + 9 = 0.$$

This was solved on EDSAC II, with this result:

$$\nu_1 = 0.83186 \qquad \nu_3 = 0.41189 \qquad \nu_5 = 0.044731$$

$$\nu_2 = 0.56075 \qquad \nu_4 = 0.14800 \qquad \nu_6 = 0.0027682$$

We have still to show that these six numbers are the squares of the cosines of the distances from some point R on the sphere to the vertices of the icosahedron. If so then we have a 14th degree formula based on $\omega(X)$ and $\omega(R)$. Now $\cos^{-1}(\nu_1^{1/2})$ is just greater than $24°$ while $\cos^{-1}(\nu_2^{1/2})$ is just greater than $41°$. Thus

$$\cos^{-1}(\nu_1^{1/2}) + \cos^{-1}(\nu_2^{1/2}) > 65°.$$

The distance between two neighboring vertices of the icosahedron is $\cos^{-1}(5^{-1/2})$ which is just less then $64°$ (Section 5). So there is a point R such that ν_1 and ν_2 are the squares of the cosines of the distances from it to *two* vertices of the icosahedron. Now the sixth degree polynomial satisfied by the ν_j $(j = 1, \cdots, 6)$ was constructed so that the sums $S_n \equiv \sum_{j=1}^{6}\nu_j^{\,n}$ satisfied four vacuous conditions, that is conditions satisfied whatever position R_i takes on the sphere. It is shown in the next Section that these conditions ensure that the remaining ν_j $(j = 3, \cdots, 6)$ are the squares of the cosines of the distances of the point R (determined by ν_1 and ν_2) to the remaining vertices of the icosahedron.

So we have found a super-efficient formula accurate for spherical polynomials of degree not more than fourteen. In Section 6.42 we show how to find the co-ordinates of the required points with respect to rectangular axes with origin at the center of the sphere. This will provide also a useful numerical check on the calculation. The co-ordinates are listed in Table 2.

The cases $(h = 1; h' = 2)$ and $(h = 1; h' = 3)$ for the icosahedral group have not been investigated.

6.4. Icosahedral Co-ordinates.

The icosahedral co-ordinates of a point on the sphere are defined to be the squares of the cosines of the distances from that point to the twelve vertices of the icosahedron. Since these vertices are antipodal in pairs a point has just six icosahedral co-ordinates. They are of course the ν_j of the previous Section.

6.41. Existence of a point with given icosahedral co-ordinates.

Remark: Consider a sextic equation with roots ν_j' $(j = 1, \cdots, 6)$ which are real and lie in [0, 1]. Suppose the equation has been constructed as if its roots were the icosahedral co-ordinates of a point on the sphere, that is

$$\pi_{i0}^{(m)} = 0; \qquad m = 2, 4, 8, 14.$$

Suppose further that there is a point on the sphere with icosahedral co-ordinates ν_j'' $(j = 1, \cdots, 6)$ two of which coincide with two of the roots. Say $\nu_1'' = \nu_1'$ and $\nu_2'' = \nu_2'$; then the other icosahedral co-ordinates ν_j'' $(j = 3, \cdots, 6)$ coincide with the other roots ν_j' $(j = 3, \cdots, 6)$.

Outline of Proof: The values $m = 2, 4, 8, 14$ are of course those even ones for which $d_1^{(m)} = 0$. The four conditions $\pi_{i0}^{(m)} = 0$ are linear in the sums

$$S_n' \equiv \sum_{j=1}^{6} \nu_j'^n; \qquad\qquad n = 1, 2, \cdots, 7$$

of the powers of the roots of the sextic equation. The conditions are satisfied also by the same functions

$$S_n'' \equiv \sum_{j=1}^{6} \nu_j''^n; \qquad\qquad n = 1, 2, \cdots, 7$$

of the ν_j'', because the ν_j'' are icosahedral co-ordinates. For the same reason $0 \le \nu_j'' \le 1$; and $0 \le \nu_j' \le 1$ by hypothesis.

We have therefore to show that the solution of the equations

$$\pi_{i0}^{(m)} = 0; \qquad\qquad m = 2, 4, 8, 14$$

in unknowns ν_j $(j = 1, \cdots, 6)$ is unique when ν_1 and ν_2 are given and $0 \le \nu_j \le 1$ $(j = 1, \cdots, 6)$. The quartic whose roots are the ν_j $(j = 3, \cdots, 6)$ is constructed as follows:

$$\pi_{i0}^{(2)} = \pi_{i0}^{(4)} = 0 \quad \text{determines} \quad \sum_{j=3}^{6} \nu_j \quad \text{and} \quad \sum_{j=3}^{6} \nu_j^2$$

and thus two of the coefficients. By use of the relations between the elementary symmetric functions and the sums of the powers of the roots the remaining con-

ditions $\pi_{i0}^{(8)} = \pi_{i0}^{(14)} = 0$ yield one linear and one quadratic equation in the remaining coefficients α and β of the quartic. We find at last that α satisfies a quadratic the sum of whose roots is

$$\sigma \equiv \tfrac{1}{5}(436 - 14f + 40g + 20f^2 - 80fg - 10f^3)$$

where $0 \leqq f \equiv \nu_1 + \nu_2 < 2$ and $0 \leqq g \equiv \nu_1\nu_2 < 1$. By inspection $\sigma > 30$ so that at least one root of the quadratic for α exceeds 15. But $0 \leqq \nu_j \leqq 1$ so

$$|\alpha| \equiv \nu_4\nu_5\nu_6 + \nu_3\nu_5\nu_6 + \nu_3\nu_4\nu_6 + \nu_3\nu_4\nu_5 \leqq 4.$$

Hence α is determined by the quadratic. When α is known β can be found from the linear equation. So all the coefficients of the quartic whose roots are the ν_j $(j = 3, \cdots, 6)$ are determined. In other words, the hypotheses of the Remark ensure that the ν_j' $(j = 1, \cdots, 6)$ are the v_j'' $(j = 1, \cdots, 6)$ in some order.

This result shows that a formal solution obtained by the methods of Section 6.3 will correspond to a real set of points on the sphere if and only if the roots of the sextic are real and lie in $[0, 1]$ and two of the roots are icosahedral co-ordinates of some point. This is what actually happened in the case $(h = h' = 1)$ which we investigated.

6.42. Transformation to Cartesian co-ordinates. The transformation from icosahedral co-ordinates to Cartesian co-ordinates with the center of the sphere as origin is achieved as follows. The 15 diameters of the sphere through mid-points of opposite edges of the icosahedron form 5 sets of 3 mutually perpendicular axes. Choose one set (OA, OB, OC) as axes of co-ordinates (Figure 2).

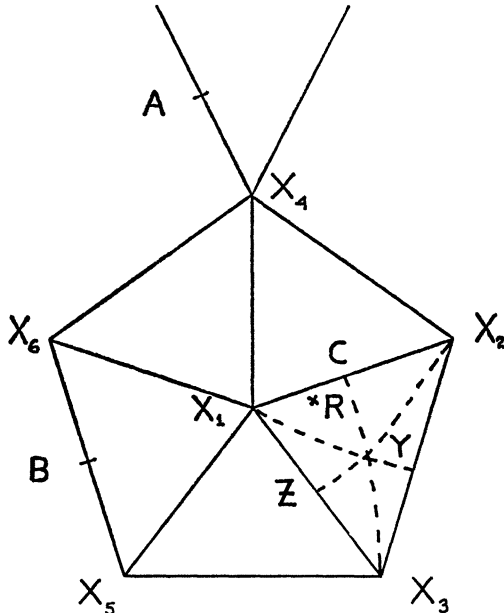Since A, B, C are $(1, 0, 0)$, $(0, 1, 0)$ and $(0, 0, 1)$ respectively then the icosahedral

FIG. 2

vertices X_1, X_2, $\cdots$, X_6 are respectively

$$(0, \lambda, \rho); \quad (0, -\lambda, \rho); \quad (-\rho, 0, \lambda); \quad (\rho, 0, \lambda); \quad (-\lambda, \rho, 0); \quad (\lambda, \rho, 0)$$

where

$$\lambda \equiv \sqrt{\frac{5 - \sqrt{5}}{10}} \quad \text{and} \quad \rho \equiv \sqrt{\frac{5 + \sqrt{5}}{10}}$$

were computed in Section 6.1.

Now consider an arbitrary point $R \equiv (\alpha, \beta, \gamma)$ in triangle X_1YC. It is clear on inspection of Figure 2 that the vertices X_1, X_2, $\cdots$, X_6 are ranked in order of increasing distance from R. So if ν_1, ν_2, $\cdots$, ν_6 are the icosahedral co-ordinates of R in decreasing order of magnitude and $\mu_j \equiv \nu_j^{1/2}$ ($j = 1, \cdots, 6$) then

(4)
$$\left. \begin{array}{lll} \lambda\beta + \rho\gamma = \mu_1; & -\rho\alpha + \lambda\gamma = \mu_3; & -\lambda\alpha + \rho\beta = \mu_5 \\ -\lambda\beta + \rho\gamma = \mu_2; & \rho\alpha + \lambda\gamma = \mu_4; & \lambda\alpha + \rho\beta = \mu_6 \end{array} \right\}$$

So the Cartesian co-ordinates (α, β, γ) of R can be found in terms of the icosahedral co-ordinates.

We have almost immediately the following necessary and sufficient condition for arbitrary positive numbers ν_j' ($j = 1, \cdots, 6$) in decreasing order of magnitude to be the icosahedral co-ordinates of some point on the sphere.

$$\left. \begin{array}{l} \displaystyle\sum_{j=1}^{6} \nu_j' = 2 \\[2mm] \dfrac{\mu_1' + \mu_2'}{\mu_3' + \mu_4'} = \dfrac{\mu_3' - \mu_4'}{\mu_5' - \mu_6'} = \dfrac{\mu_5' + \mu_6'}{\mu_1' - \mu_2'} = \dfrac{\rho}{\lambda} \equiv \tfrac{1}{2}(1 + \sqrt{5}) \end{array} \right\}$$

where as usual $\mu_j' \equiv (\nu_j')^{1/2}$ for $j = 1, \cdots, 6$.

This is an alternative criterion to the Remark of Section 6.41. It differs from the Remark in that in practice it cannot be applied *exactly*, for the roots of a sextic equation can normally be found only approximately. So a very slight deviation of any of the three quotients from $\tfrac{1}{2}(1 + \sqrt{5})$ would pass undetected.

The criterion is useful mainly as a numerical check on the calculations. When it is applied to the roots ν_j' of the sextic equation of Section 5.3, $\sum \nu_j' = 2$ by construction and the three quotients are

$$1.61803, \quad 1.6180, \quad 1.6180$$

where the last digit in each case is doubtful. In fact $\tfrac{1}{2}(1 + \sqrt{5}) = 1.618035 \cdots$.

We saw above how to find the Cartesian co-ordinates of a point R with given icosahedral co-ordinates. All the points of $\omega(R)$, and of the antipodal set, have the same icosahedral co-ordinates. If in Figure 2 we had taken R to be in triangle X_1YZ instead of in triangle X_1YC we would have obtained the antipodal set which would be equivalent.

We show finally how to shorten the calculation of the Cartesian co-ordinates of all the points of $\omega(R)$. The four images of R obtained by rotation about the axis through X_1 are found by permuting suitably the μ_j ($j = 2, \cdots, 6$) of (4). No more calculation is needed, by the following classical property of the regular solids which is described by Ledermann [6].

Five cubes are inscribed in the configuration of the icosahedron-dodecahedron. The rotations of the icosahedral group $\mathcal{Q}_5$ induce just the even permutations of these cubes. The number of rotations of $\mathcal{Q}_5$ that keep a particular cube fixed is thus the number of even permutations of four objects, namely 12. So 12 of the 24 symmetry rotations of this cube are also symmetry rotations of the icosahedron. In fact they are the 12 symmetry rotations of the tetrahedron formed by any four nonadjacent vertices of the cube.

Now consider a general invariant set $\omega(R)$ of the icosahedral rotations. The 60 points of $\omega(R)$ must comprise just five general invariant sets of the tetrahedral rotations. So from any five points of $\omega(R)$ that are mutually inaccessible by these tetrahedral rotations it is possible to generate all the points of $\omega(R)$, simply by applying the tetrahedral substitutions.

The choice of (OA, OB, OC) as axes of co-ordinates (Figure 2) amounts to choosing one of the five cubes. The three directions are perpendicular to its faces. None of the rotations of the icosahedron about the axis through X_1 leave this cube invariant; so R and its four images whose Cartesian co-ordinates have been found by solving equations like (4) are mutually inaccessible by the tetrahedral rotations of this cube. The tetrahedral substitutions appropriate to rectangular axes (OA, OB, OC) are generated by

$$(\alpha, \beta, \gamma) \rightarrow (\beta, \gamma, \alpha)$$

and

$$(\alpha, \beta, \gamma) \rightarrow (\alpha, -\beta, -\gamma).$$

When R and its four images have been identified it is thus simple to write down the Cartesian co-ordinates of all 60 points of $\omega(R)$.

The octahedral substitutions that generate $\omega(R)$ from R when the formula is based on the octahedral group are the 3×3 pseudo-permutation matrices with determinant $+1$.

The tetrahedral substitutions that generate $\omega(R)$ from five suitable representatives when the formula is based on the icosahedral group are those 3×3 pseudo-permutation matrices with determinant $+1$ in which the number of negative elements is either two or none.

Five suitable representatives of $\omega(R)$ for the 14th degree formula are

$$(-0.15111, \quad 0.15524, \quad 0.97626)$$
$$(0.31584, \quad 0.25705, \quad 0.91334)$$
$$(0.34631, \quad 0.66628, \quad 0.66042)$$
$$(-0.10181, \quad 0.81739, \quad 0.56702)$$
$$(-0.40923, \quad 0.50155, \quad 0.76223).$$

7. Review. Some of the formulas have been obtained before by three other writers working independently. They are identified by initial in the last column of Table 2. Finden [2] considers, besides the regular solids, axially symmetric formulas of Cartesian-product type and stereographic images of Simpson's Rule in the plane.

Sobolev [13] employs group characters to investigate some invariant networks of points which reduce in special cases to certain of our formulas. D. G. Kendall [5] has shown how to deduce others from formulas for the solid sphere of the type given by Ditkin [1] and by Hammer and Stroud [3]. Kendall's arguments work in both directions so that formulas for the surface may be combined to obtain formulas for the solid sphere—now the more natural sequence of reasoning.

The formulas listed in Table 2 of the present paper have been constructed to obtain maximum efficiency subject to invariance under the appropriate group of rotations. This invariance seems to be at worst a harmless requirement so that for practical purposes the problem of spherical integration is solved provided the number N of sample points is within the range of Table 2. The existence of larger formulas, of arbitrarily high degree p, that are efficient (E near unity) has not been proved although D. G. Kendall [5] has obtained $E = \frac{2}{3}$ for any odd value of p. This is achieved by means of axially symmetric Cartesian-product formulas which are derived from work of Peirce [9] on the spherical shell. The same idea was applied earlier by Ditkin [1] to the complete solid sphere.

In conclusion two alternative methods of obtaining indefinitely large formulas are suggested.

7.1. The Extremal Property. With the notation of Section 5, let $\sum a_r = \int dS = 4\pi$. The conditions that an integration formula, not necessarily invariant, must satisfy for pth degree accuracy are

$$\sum_{r=1}^{t} \sum_{s=1}^{t} a_r a_s P_m(\cos \gamma_{rs}) = 0; \qquad\qquad m = 1, \cdots, p.$$

Because these expressions are non-negative definite this is equivalent to

$$\sum_{r=1}^{t} \sum_{s=1}^{t} a_r a_s \sum_{m=0}^{p} \lambda_m P_m(\cos \gamma_{rs}) = 16\pi^2 \lambda_0$$

where the $\lambda_m (m = 1, \cdots, p)$ are any positive constants. If

$$L_p(\mu) \equiv \sum_{m=0}^{p} \lambda_m P_m(\mu)$$

then to find a pth degree formula we have simply to arrange that

$$\sum_{r=1}^{t} \sum_{s=1}^{t} a_r a_s L_p(\cos \gamma_{rs})$$

attains its minimum $16\pi^2 \lambda_0$ with respect both to points A_r and to weights a_r. The number of points must be large enough for the required integration formula to exist. $\frac{1}{3}(p + 1)^2$ points may be sufficient while (almost any) $(p + 1)^2$ points are certainly sufficient.

The polynomial $L_p(\mu)$ is highly arbitrary and it may be convenient to use the fact that the coefficients in the expansion of μ^p in Legendre polynomials $P_m(\mu)$ are alternately positive and zero. This follows from the recurrence relation

$$(2m + 1)\mu P_m(\mu) = (m + 1)P_{m+1}(\mu) + m P_{m-1}(\mu)$$

and induction on p.

If the points A_r are accepted only in antipodal pairs, to eliminate the odd harmonics, then the condition for a pth degree integration formula (where p is even) is

$$\sum_{r=1}^{t} \sum_{s=1}^{t} a_r a_s (\cos \gamma_{rs})^p = \frac{16\pi^2}{p+1}$$

with $\sum a_r = 4\pi$.

Instead we may modify the criterion of efficiency, which emphasizes the lower harmonics to the extent of ignoring altogether those whose degree exceeds p. This can be done by choosing a convenient function $L_\infty(\mu)$ with a convergent expansion in Legendre polynomials that has *positive* coefficients, and minimizing

$$\sum_{r=1}^{t} \sum_{s=1}^{t} a_r a_s L_\infty (\cos \gamma_{rs}).$$

In a sequel to this paper the problem of spherical integration is restated in probabilistic terms and shown to lead to an extremal problem of just this form.

7.2. The Reproducing Icosahedron.

In the main part of the paper (Sections 2–6) only integration formulas based on the regular solids were considered and they were judged by the efficiency E. In the preceding Section the notion of efficiency was modified to provide a less artificial criterion and the regular solids played no part at all. In this final Section the idea of efficiency is discarded altogether and appeal is made only to symmetry.

The theory of Section 2, on which we have relied so heavily has two serious limitations. One is its inability to treat more than one regular solid (with its dual) at a time, for it is fundamental that one *fixed* realization of the group G is considered. Finden [2] considers three dodecahedra in a certain mutual orientation but this formula seems to be beyond the scope of Section 2. The second limitation is the lack of further finite subgroups of the rotation group which might provide other regular solids. This apparent shortcoming is a valuable safeguard when icosahedra are reproduced over the sphere in the following manner.

We saw in Section 6.42 that just five cubes could be inscribed in the icosahedral configuration and that they were permuted evenly by its symmetry rotations. The vertices of the cubes coincide in pairs at the centroids of the faces of the icosahedron. The converse property associates with any cube just two icosahedra. They are permuted by the rotations of the cube.

We say two icosahedra are *first neighbors* if there is a cube inscribed in them both in the way just described. Clearly every icosahedron has exactly five first neighbors. We say (inductively) that two icosahedra are *jth neighbors* ($j = 2, 3, \cdots$) if there is an icosahedron that is a first neighbor of one and a $(j - 1)$th neighbor of the other. Two icosahedra are simply *neighbors* if for some $j = 0, 1, 2, \cdots$ they are jth neighbors. Thus "neighborhood" is an equivalence relation.

Let I_0 denote the twelve vertices of a certain icosahedron. Let I_j ($j = 1, 2, \cdots$) denote the set of vertices of all the jth neighbors of I_0. These sets I_j may not be disjoint. We propose equally-weighted integration formulas based on sets of points

of the following form

$$K_M \equiv \bigcup_{j=0}^{M} I_j .$$

Consider the set of points on the sphere

$$K_\infty \equiv \bigcup_{j=0}^{\infty} I_j .$$

It consists of the vertices of all icosahedra that are neighbors of I_0. Let I_0' be any such icosahedron. Because neighborhood is an equivalence relation K_∞ is equally well described as consisting of the vertices of all neighbors of I_0'. So the group G_∞ of rotations of the sphere under which the set K_∞ is invariant includes those rotations that transform I_0 into any one of its neighbors. The ordinary symmetry rotations of I_0 are properly included so G_∞ is too large to be one of the three finite groups associated with regular solids. G_∞ is obviously not cyclic nor dihedral. Hence G_∞ is not finite, by Weyl [15]. Hence K_∞ is not a finite set. It is, of course, countable.

By suitable choice of M the integration formula based on the set K_M has an arbitrarily large number of points. The justification for using the ascending sequence of sets K_M is simply the striking symmetry of their union K_∞, as expressed by invariance under the group G_∞. A high degree of symmetry in the integration formula is a reasonable aim because the integral itself is an invariant of the whole rotation group. The question of whether the points of K_M are asymptotically distributed uniformly over the sphere, and associated matters of convergence are postponed to another occasion.

These formulas have two practical advantages. The sets K_M are nested so that no work is wasted when a crude approximation to the integral is later refined. This applies if the sample points are found explicitly. In fact the second property removes the need for that if a computer is available. All that is necessary is a routine to locate the vertices of the five first neighbors of a given icosahedron. Sequential generation of the sample points should then be possible, followed at once by evaluation there of the integrand.

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Note. Four papers, those of Lyusternik and Ditkin [7], Lyusternik [8], and Sobolev [10, 11] are not mentioned in the text, but appear in this list of references because they are concerned with the approximation of multiple integrals.