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Surface harmonics for pentagonal point groups

K RAMA MOHANA RAO, P HEMAGIRI RAO* and V SATYAVATHI**
Department of Applied Mathematics, Andhra University, Visakhapatnam 530 003, India
*Department of Mathematics, Bapatla Engineering College, Bapatla 522 101, India
**Department of Applied Mathematics, A.U.P.G. Centre, Nuzvid 521 201, India

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Abstract. Surface harmonics for the seven pentagonal point groups $5(C_5)$, $\bar{5}(S_{10})$, $\overline{10}(C_{5h})$, $\overline{10}m2(D_{5h})$, $52(D_5)$, $5m(C_{5v})$ and $\bar{5}2m(D_{5d})$ that represent the symmetries of quasicrystals in two and three dimensions are obtained, employing the projection operator method [11] and the simplified (authors) method. The results obtained are tabulated and are briefly discussed.

Keywords. Pentagonal point groups; quasicrystals; spherical and surface harmonics; Euler angles, induced representations.

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1. Introduction

The discovery of Al–Mn quasicrystal for the first time by Schectman *et al* [1], the subsequent discovery of Al_6–Li_3–Cu icosahedral phase by Dubost *et al* [2], followed by Al–Cu–Fe system and Al–Pd–Mn quasicrystal by Tsai *et al* [3, 4] have initiated a tremendous burst of theoretical and experimental activity in condensed matter physics, for determining the symmetry, structure, neutron and X-ray diffraction of quasicrystals. The study of the properties of these materials have already emerged from their infancy and work on some prominent physical properties such as electrical resistivity, magnetism, elasticity, photoelasticity and transport phenomenon have been undertaken, employing both experimental and group theoretical [5–8] methods. In this work the seven point groups with five-fold rotations namely: the $5(C_5)$, $\bar{5}(S_{10})$, $\overline{10}(C_{5h})$, $\overline{10}m2(D_{5h})$, $52(D_5)$, $5m(C_{5v})$ and $\bar{5}2m(D_{5d})$ are considered and the surface harmonics (symmetrized linear combinations of spherical harmonics) for the seven pentagonal point groups that represent the symmetry groups of a class of quasicrystals in 2-d and 3-d, have been obtained and tabulated.

Evaluation of spherical harmonics with the symmetry of the regular polyhedrons, particularly for electrostatic problems involving polyhedral conductors, created some interest in group theoretical physicists since a long time. Owing to the connection that existed with the structure of some proteins, interest in the icosahedral groups has arisen. Whereas the spherical harmonics up to $l = 21$ for the total symmetric representation of the icosahedral point groups were derived by Laporate [9], expansions in spherical harmonics up to and including $l = 14$ for all the irreducible representations (IRs) of the icosahedral point groups were derived by Cohan [10], employing the projection operator method of Altmann [11]. Following this commonly used method, the spherical harmonics for all the IRs of the 32 crystallographic point groups were obtained and tabulated by Bradley and Cracknell [12]. Similar work for space groups was carried out by Altmann and Cracknell [13], Altmann and Bradley [14].

We contend that considerable simplification can be achieved in the process of obtaining the surface harmonics of point groups by combining the little group technique [15], of inducing the IRs of a finite group G_i from those of the IRs of its little group, with the projection operator method of Altmann [11]. In § 2, the projection operator method of Altmann is briefly discussed and applied succinctly, to illustrate the case of degenerate IRs of the point group 52 (D_5). In § 3, the authors' simple and elegant method is applied to derive (i) the surface harmonics of the point group 52 from those of its normal subgroup 5 by considering the composition series $\overline{10}\,m2 \supset 52 \supset 5 \supset 1$ and in turn obtain (ii) the surface harmonics of the point group $\overline{10}\,m2$ from those of the point group 52. In § 4, the results obtained in this work are briefly summarized. The results obtained in respect of all the seven considered pentagonal point groups are tabulated.

2. Projection operator method

We now briefly summarize the operational technique of the projection operator method given by Altmann [11]. Suppose G is a point group under consideration and let $R, S, \ldots \in G$. Suppose $D^i(R), D^i(S), \ldots$ denote the matrix representation of G. For the generating functions we take the spherical harmonics $Y_l^m(\theta, \phi)$. Then one has to evaluate

$$W_{ts}^i\, Y_l^m(\theta,\phi) = \left\{ d_i/|G| \sum_{R\in G} P_R\, D^i(R)_{ts}^*\, R \right\} Y_l^m(\theta,\phi), \quad -l \leqslant m \leqslant l. \tag{2.1}$$

To proceed with (2.1) one needs an expression for $RY_l^m(\theta,\phi)$. In (2.1), $R\in G$ may be a proper or an improper rotation. If R is a proper rotation, we find its Euler angles (α, β, γ) and evaluate $RY_l^m(\theta,\phi)$ using the equation

$$R(\alpha,\beta,\gamma)\, Y_l^m(\theta,\phi) = \sum_{n=-l}^{l} Y_l^n(\theta,\phi)\, D^l\{R(\alpha,\beta,\gamma)\}_{nm}. \tag{2.2}$$

In equation (2.2)

$$D^l\{R(\alpha,\beta,\gamma)\}_{nm} = C_{nm} \exp(-in\gamma)\, d^l(\beta)_{nm} \exp(-im\alpha) \tag{2.3}$$

with the usual notation of Bradley and Cracknell [12]. On the other hand if R is improper i.e. $R = IQ$, we use the Euler angles (α, β, γ) for proper rotation Q, evaluate $QY_l^m(\theta,\phi)$ by means of eq. (2.2). To complete the evaluation of $RY_l^m(\theta,\phi)$, we use

$$I\, Y_l^m(\theta,\phi) = (-1)^l\, Y_l^m(\theta,\phi) \tag{2.4}$$

for the transform of $IY_l^n(\theta,\phi)$. This simply adds an extra factor $(-1)^l$ if R is an improper rotation. Hence (2.1) in conjunction with (2.2), (2.3) and (2.4) becomes

$$W_{ts}^i\, Y_l^m(\theta,\phi) = d_i/|G| \sum_{R\in G} P_R\, D^i(R)_{ts}^* \times [\exp(-im\alpha) \sum_n C_{nm} \exp(-in\gamma)\, d^l(\beta)_{nm}\, Y_l^n(\theta,\phi)], \tag{2.5}$$

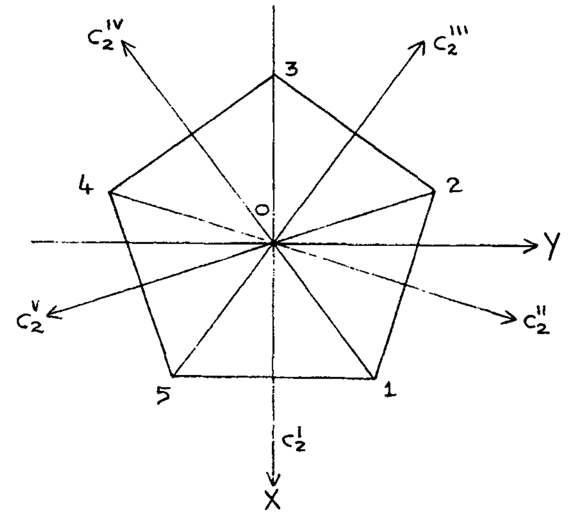

Figure 1. The pentagon depicting the five-fold symmetry. (In figure 1, OZ is taken as the 5-fold axis, which is perpendicular to the plane of the paper.)

Table 1. Euler angles for the elements of the point group $52(D_5)$*.

Symmetry element	α	β	γ
E	0	0	0
C_5	$2\pi/5$	0	0
C_5^2	$4\pi/5$	0	0
C_5^3	$6\pi/5$	0	0
C_5^4	$8\pi/5$	0	0
C_2^{I}	π	π	0
C_2^{II}	$\pi/5$	π	0
C_2^{III}	$7\pi/5$	π	0
C_2^{IV}	$3\pi/5$	π	0
C_2^{V}	$9\pi/5$	π	0

*The symmetry operations listed in table 1 are taken in active convention.

wherein, if R is an improper rotation, we take in the RHS the quantities corres-ponding to the associated proper rotation Q. In eq. (2.5), P_R is taken as unity when R is proper and $(-1)^l$ when R is improper.

We shall now apply this method towards obtaining the surface harmonics for the IRs of the point group 52. For this we consider the following pentagon as a reference figure (figure 1), relative to which the nomenclature of the group elements and their Euler angles (table 1) are specified.

From the character table of the point group 52, it can be seen that (x, Y) transform as the 2-d IR E_1 and $(x^2 - Y^2, xy)$ transform as the IR E_2 of 52. With this information, we calculate the metrics $D^i(R)$ of the degenerate IRs E_1 and E_2 of the point group 52. These matrices obtained for the point group 52 (D_5) are listed in table 2.

In table 2, the symbols a, b, c and d stands for the constants (numbers) $a = \cos\omega$, $b = \sin\omega$, $c = \cos 2\omega$, $d = \sin 2\omega$ with $\omega = 2\pi/5$. Now using (2.1) through (2.5), one can straightaway obtain the surface harmonics having the symmetry of the IRs A_1, A_2, E_1 and E_2 of 52.

Table 2. Matrices for the degenerate representations of the point group 52.

Irreducible representation of 52	Symmetry element g of the group 52	Matrix representative for the element g in the chosen degenerate representation of 52
E_1	E	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
	C_5	$\begin{bmatrix} a & -b \\ b & a \end{bmatrix}$
	C_5^2	$\begin{bmatrix} c & -d \\ d & c \end{bmatrix}$
	C_5^3	$\begin{bmatrix} c & d \\ -d & c \end{bmatrix}$
	C_5^4	$\begin{bmatrix} a & b \\ -b & a \end{bmatrix}$
	C_2^{I}	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
	C_2^{II}	$\begin{bmatrix} c & d \\ d & -c \end{bmatrix}$
	C_2^{III}	$\begin{bmatrix} a & -b \\ -b & a \end{bmatrix}$
	C_2^{IV}	$\begin{bmatrix} a & b \\ b & -a \end{bmatrix}$
	C_2^{V}	$\begin{bmatrix} c & d \\ -d & -c \end{bmatrix}$
E_2	E	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$
	C_5	$\begin{bmatrix} c & -2d \\ d/2 & a \end{bmatrix}$

(*continued*)

Table 2. (*Continued*)

Irreducible representation of 52	Symmetry element g of the group 52	Matrix representative for the element g in the chosen degenerate representation of 52
	C_5^2	$\begin{bmatrix} a & 2b \\ -b/2 & a \end{bmatrix}$
	C_5^3	$\begin{bmatrix} a & -2b \\ b/2 & a \end{bmatrix}$
	C_5^4	$\begin{bmatrix} c & 2d \\ -d/2 & c \end{bmatrix}$
	C_2^{I}	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
	C_2^{II}	$\begin{bmatrix} a & -2d \\ -b/2 & -a \end{bmatrix}$
	C_2^{III}	$\begin{bmatrix} c & -2d \\ -d/2 & -c \end{bmatrix}$
	C_2^{IV}	$\begin{bmatrix} c & 2d \\ d/2 & -c \end{bmatrix}$
	C_2^{V}	$\begin{bmatrix} a & 2b \\ b/2 & -a \end{bmatrix}$

To exemplify, the procedure for the non-degenerate IRs, we consider the IR A_1 of $52(D_5)$.

$$W^{A_1} Y_l^m = 1/10[(1 + e^{-im\omega} + e^{-2im\omega} + e^{-3im\omega} + e^{-4im\omega}) Y_l^m$$

$$+ (-1)^l (e^{-im\pi} + e^{-im\pi/5} + e^{-im7\pi/5} + e^{-im3\pi/5} + e^{-im9\pi/5}) Y_l^{-m}],$$

$$\omega = 2\pi/5$$

$$= 1/10[1 + 2\cos m\omega + 2\cos 2m\omega][Y_l^m + (-1)^{l+m} Y_l^{-m}]. \quad (2.6)$$

It can be seen that the coefficients in the R.H.S of (2.6) is zero for all non-negative values of m excepting $m = 0, 5, 10, 15, \ldots$. Also we find that, when $m = 0$ and l is odd, the function in the curly bracket is zero. Thus for the IR A_1 of 52, the surface harmonics can be taken as

Y_l^0, l even

$1/2\{Y_l^m + (-1)^{l+m} Y_l^{-m}\}$ for any l and for $m = 5, 10, 15, \ldots$

Table 3. Surface harmonics for the irreducible representations of the point group 52.

52	l mod(+ 2)	m mod (+ 5)
A_1	0	0
	5	5
A_2	1	0
	6	5
E_1	1	1
	2	1
	4	4
	5	4
E_2	2	2
	3	2
	3	3
	4	3

The surface harmonics that transform as the other IRs A_2, E_1 and E_2 of the point group 52 are obtained in a similar way and a resumé of the results obtained are provided in table 3. An apparent disadvantage and difficulty in applying (2.1) or (2.6) to the considered degenerate IR Γ_i of a chosen point group G lies in that, one has to construct the matrices $D^i(R)$ for all elements $R \in G$ under consideration. This difficulty is overcome in the authors simplified method, discussed in § 3.

3. The simplified (authors) method

From what has been discussed in § 2, one can see that, in the case of non-degenerate IRs of the point groups, the character of an element $R \in G$ in the considered IR Γ_i is sufficient to obtain the corresponding surface harmonics for Γ_i. One has to construct the matrices for the IR in respect of all the elements of the point group G under consideration, in the case of the degenerate IRs. This is the formidable difficulty that one encounters in the projection operator method discussed in § 2. The authors contend here that this tediousness involved in the calculation of matrices, can be avoided if one combines the projection operator method with (i) the theory of allowable IRs of little groups, (ii) the theory of induced representations and (iii) the idea of composition series that may exist for the generating point groups G, in terms of its maximal normal subgroups G_{i+1}.

It can easily be seen that if G is the symmetry (point) group and H is a properly chosen normal subgroup of G, all the 1-d IRs of G can be obtained from those of the IRs of the factor group G/H, through the process of engendering. Also, the 2-d IRs of G can be seen to be induced from those of the pairs of 1-d complex representations of H since H coincides with the little group L. In short, the proper choice of the normal subgroup H facilitates the process of engendering and inducing the required IRs of G. For example, in the case of the pentagonal point group $G = 52(D_5)$, if $H = 5(C_5)$ is chosen as the normal subgroup, then $G/H = 52/5 \cong 2$ and the IRs Γ_1 and Γ_2 of the factor group

52/5 engender respectively the total symmetric IR A_1 and the alternating IR A_2 of the point group 52. The character table of the factor group 52/5 is given hereunder.

$52/5 \cong 2$	E5	$C_2 5$
Γ_1	1	1
Γ_2	1	-1

It can be readily seen that the pair of 1-d complex representations $^1E'$ and $^1E''$ of the point group 5 induce the 2-d IR E_1 of 52 and the remaining pair of 1-d complex IRs; $^2E'$ and $^2E''$ of 5 together induce the other 2-d IR E_2 of 52. Thus by a proper choice of the maximal normal subgroup G_{i+1} of G_i in the composition series for G, a degenerate IR Γ_i of G_i can be seen to be induced by a 1-d real or complex IR of G_{i+1}.

We now formulate the composition series such that the maximal normal subgroups $G_{i+1} = H$ is a subgroup of index two to the generating point group G_i so that, the surface harmonics transforming according to an IR Γ of G_i can be obtained from those of the surface harmonics transforming as the appropriate IR γ_i of $H = G_{i+1}$ where γ_i induce the IR Γ of G_i.

3.2 Formulation of composition series

It is well known that if $G = G_0$ is a finite group and G_1 is a maximal normal subgroup of G_0 and G_2 is a maximal normal subgroup of G_1, etc., then these groups can be expressed in terms of composition series of the form $G = G_0 \supset G_1 \supset \cdots \supset G_i \supset G_{i+1} \supset \ldots \supset G_s = E$. Since G_0 is of finite order, this process shall ultimately terminate with group G_s consisting of the identity element $\{E\}$ only. Because a maximal normal subgroup G_{i+1} of a group G_i may not be unique, we may write several such composition series for a group G_0 under consideration. However, the factor groups G_i/G_{i+1} are unique but for isomorphism, they need not occur in the same order.

The six composition series expressed in table 4 are just sufficient for the purpose of obtaining the required surface harmonics of the pentagonal point groups. International (Hermann–Maugüin) notation is adopted for denoting the point groups in the various series. From table 4, it can be noted that the seven pentagonal point groups are subgroups of either $\overline{10}m2$ or $\bar{5}2m$.

Table 4. Pentagonal point groups in terms of the chosen composition series.

Chosen composition series			
$\overline{10}m2$	$\supset 52$	$\supset 5$	$\supset 1$
$\overline{10}m2$	$\supset \overline{10}$	$\supset 5$	$\supset 1$
$\overline{10}m2$	$\supset 5m$	$\supset 5$	$\supset 1$
$\bar{5}m2$	$\supset 52$	$\supset 5$	$\supset 1$
$\bar{5}m2$	$\supset 5m$	$\supset 5$	$\supset 1$
$\bar{5}m2$	$\supset \bar{5}$	$\supset 5$	$\supset 1$

To obtain the surface harmonics for the IR Γ of a point group G_i in a considered series using the authors simplified method, consider an IR γ of G_{i+1} such that the IR μ of the little group $L(G_i, G_{i+1}, \gamma)$ induces the IR Γ of G_i. To obtain a basis of the IR Γ of G_i, we first employ the projection operator method [11] and obtain the basis of the IR μ of the little group $L(G, H, \gamma)$. This does not pose much difficulty since this group is usually a group of smallest order in the composition series. On this obtained basis of the IR μ, we apply the generator g that generates G_i from G_{i+1}. The resulting set becomes a basis for the IR Γ of G_i.

3.3 Evaluation of surface harmonics employing the simplified (authors) method

We shall now exemplify the authors method, also with the composition series $\overline{10}\, m2 \supset 52 \supset 5 \supset 1$. Evaluation of the surface harmonics for the point group 1 is trivial. Since the point group 5 contains all 1-d IRs, the surface harmonics for the point group 5 can be obtained using either the projection operator method discussed in § 2 or the simplified method discussed in § 3. The results obtained for the point group 5 are provided in table 5. We shall now proceed to evaluate the surface harmonics for the point group 52 from those of the point group 5.

From the character table of the point gorup 5, it can be easily seen that either of the 1-d complex representations ${}^1E'$ and ${}^1E''$ of 5 induces the 2-d IR E_1 of 52. Also the symmetry element $C_2 \in 52$ can generate the point group 52 from the point group 5. Since the IRs A_1 and A_2 of 52 are 1-d, one can obtain the surface harmonics for these IRs using either the projection operator method or the simplified method. The surface harmonics transforming as the 1-d complex IR ${}^1E'$ of 5 is Y_l^m; $m = 1, 6, 11, \ldots$. To get the basis for the 2-d IR E_1 of D_5 we apply the generator C_2 on this Y_l^m. From table 1, the Euler angles for C_2 is $R(\pi, \pi, 0)$. Hence $C_2\, Y_l^m = (-1)^{l+m}\, Y_l^{-m}$; $m = 1, 6, \ldots$.

Thus $Y_l^m = (-1)^{l+m}\, Y_l^{-m}$; $m = 1, 6, 11 \ldots$, forms a basis of the 2-d IR E_1 of D_5. Similarly the surface harmonics transforming as the 1-d complex IR ${}^1E''$ is Y_l^m; $m = 4, 9, 14, \ldots$. Applying the generator C_2 on this Y_l^m one gets $C_2\, Y_l^m = (-1)^{l+m}\, Y_l^{-m}$; $m = 4, 9, 14, \ldots$, as a basis of 2-d IR E_1 of 52. Combining these two results, we find

$$1/\sqrt{2}\,[\,Y_l^m + (-1)^{l+m}\, Y_l^{-m}]; \quad 1/\sqrt{2}\,[\,Y_l^m - (-1)^{l+m}\, Y_l^{-m}]$$

are the surface harmonics that transform as the IR E_1 of the point group 52. In a similar manner one can evaluate the surface harmonics for the IR E_2 of 52. The results obtained for the point group 52 are listed in table 3.

Table 5. Surface harmonics for the irreducible representation of the point gorup $C_5(5)$.

C_5	m mod (5)
A	0
${}^1E'$	1
${}^1E''$	4
${}^2E'$	2
${}^2E''$	3

Table 6. Surface harmonics for the irreducible representations of the point group $\overline{10}\,m2$.

$\overline{10}\,m2$	l mod $(+2)$	m mod $(+10)$
A'_1	0	0
	5	5
A'_2	5	5
	10	10
A''_1	6	5
	11	10
A''_2	1	0
	6	5
E'_1	1	1
	4	4
	6	6
	9	9
E'_2	2	2
	3	3
	7	7
	8	8
E''_1	2	1
	5	4
	7	6
	10	9
E''_2	3	2
	4	3
	8	7
	9	8

To obtain the surface harmonics that transform as the IRs of the point group $\overline{10}\,m2$ in the considered composition series, we proceed as follows: We know that σ_h is the generator from 52 to $\overline{10}\,m2$ and the Euler angles for symmetry operator σ_h can be taken as $R(0,\pi,0)$. We now obtain the surface harmonics that transform according to the IRs of $\overline{10}\,m2$ as: $\sigma_h\, Y_l^m = R(0,\pi,0)\, Y_l^m = (-1)^{l+m}\, Y_l^m$.

The results obtained in respect of all the IRs of $\overline{10}m2$, are provided in table 6. By proceeding in much the same manner as has been done in the case of the point groups $\overline{10}m2$, 52 and 5 from the considered series, the surface harmonics transforming as those of the IRs of the point groups contained in the rest of the composition series can be evaluated. The results are listed in tables 3, 5–10.

4. Discussion

The elegance of the simplified method, adopted by the authors in this paper lies in the fact that the surface harmonics pertaining to the irreducible representations of various other groups G_i that contain G_{i+1} in the considered series $G_0 \supset G_1 \supset \cdots \supset G_i \supset G_{i+1} \supset \cdots \supset G_s = E$

Table 7. Surface harmonics for the irreducible representations of the point group $\bar{5}$.

$\bar{5}$	l mod (2)	m mod (5)
A_g	0	0
A_u	1	0
${}^1E'_g$	2	1
${}^1E'_u$	1	1
${}^1E''_g$	2	1
${}^1E''_u$	1	−1
${}^2E'_g$	2	2
${}^2E'_u$	3	2
${}^2E''_g$	2	−2
${}^2E''_u$	3	3

Table 8. Surface harmonics for the irreducible representations of the point group $\overline{10}$.

$\overline{10}$	l mod (+2)	m mod (10)
A′	0 5	0 5
A″	1 6	0 5
${}^1E'_1$	1 4	1 4
${}^2E'_1$	1 4	−1 4
${}^1E'_2$	2 3	2 −3
${}^2E'_2$	2 3	−2 3
${}^1E''_1$	2 5	1 −4
${}^2E''_1$	2 5	−1 4
${}^1E''_2$	3 4	2 −3
${}^2E''_2$	3 4	−2 3

can be obtained simultaneously from those of the surface harmonics of the group G_{i+1}. This method of combining the little group technique with the projection operator method avoids the tedious calculations involved in finding the matrices for the elements $g \in G$ (in the case of degenerate IRs Γ) for all the IRs of the group G.

Table 9. Surface harmonics for the irreducible representations of the point group 5 *m*.

5*m*	*l* mod (2)	*m* mod (+ 5)
A_1	0	0
	5	5
A_2	1	0
	5	5
E_1	1	1
	2	1
	4	4
	5	4
E_2	2	2
	3	2
	3	3
	4	3

Table 10. Surface harmonics for the irreducible representations of the point group $\bar{5}$ 2*m*.

$\bar{5}$ 2*m*	*l* mod (+ 2)	*m* mod (+ 5)
A_{1g}	0	0
A_{1u}	5	5
A_{2g}	6	5
A_{2u}	1	0
E_{1g}	2	1
	4	4
E_{1u}	1	1
	5	4
E_{2g}	2	2
	4	3
E_{2u}	2	2
	3	3

Notation: In tables 3–10, *l* mod (5) stands for the succession of values $m = 1, -4, 6, -9, \ldots$ and *l* mod (+ 5) stands for the succession of values $m = 1, 6, 11, 16, 21, 26, \ldots$.

Surface harmonics are found to be of immense utility in many physical situations, for example, when the variational cellular method [16], is applied to investigate the band structure of a metal, one requires expansions that reproduce the symmetry of the group of the *k*-vectors. Also in augmented plane wave method [17] and tight binding method, one requires expansions in spherical harmonics that belong to a given IR of a symmetry group of the physical system.

The seven point groups for which the surface harmonics are calculated, have interesting geometrical and physical applications. As such the results obtained and reported here, we believe, have physical significance.

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