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BOUNDS FOR QUATERNIONIC LINE SYSTEMS AND REFLECTION GROUPS*

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1. Introduction.

Let F denote R, C or the quaternions H. We are here concerned with bounds on the size of sets X of unit vectors in F which carry a specified set or specified number of angles.

Results in a unified manner for R, C were obtained by Delsarte, Goethals and Seidel [3], using Koornwinder's addition formula in certain spaces of harmonic polynomials [9]. Following a program proposed in [8] we use addition formula results [6] described in section 2 to attack the case $F=\mathsf{H}$, which turns out interestingly different.

Let A denote the set of all values of $|\langle\xi,\eta\rangle|^2$ for pairs $\xi \neq \eta$ in X. Bounds on $v=|X|$ for specified A (*special* bounds) are the subject of section 3. Our results show, for example, that five quaternionic reflection groups of vectors (Conway [2], Cohen [1]) are not only non-extendable, but of maximum size as systems of vectors carrying the given angles.

In section 4 we derive bounds depending not on the specific angles but on their number $|A|$ (*absolute* bounds). One bound is met by J. H. Conway's 165 vectors in H^5 with $A=\{0,\frac{1}{4}\}$.

2. Jacobi polynomials and an addition formula.

Henceforth ε, k will denote non-negative integers and n an integer greater than 1.

For convenience, let $m=2n$ in this section. We need the polynomials derived in [6], namely

$$Q_k^\varepsilon(x) = Q_k^\varepsilon(1)R_k^{m-3,\varepsilon+1}(2x-1),$$

where the right hand side is a Jacobi polynomial [10] suitably normalized, and

$$(2.1)\quad Q_k^\varepsilon(1) = (k+\varepsilon+2)_{m-3}(k+1)_{m-3}(\varepsilon+1)(2k+m+\varepsilon-1)/(m-1)!\,(m-3)!$$

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$$(2.2)\quad Q_k^\varepsilon(x) = \frac{(\varepsilon+1)(2k+m+\varepsilon-1)}{k!\,(m-1)!}\sum_{l=0}^{k}(-1)^{k-l}\binom{k}{l}(l+\varepsilon+2)_{k+m-3}x^l\,,$$

where $(a)_b$ denotes $a(a+1)\ldots(a+b-1)$ for arbitrary a and positive integer b. When working with a fixed ε we will often omit suffix ε. For any ε and polynomial $F(x)$ of degree k we have its expansion $f_0Q_0+\ldots+f_kQ_k$. The coefficients for a polynomial $G(x)$ will be denoted by g_i.

2.3. LEMMA ([6], cf. [3]). *For $k,\varepsilon=0,1,\ldots$ we have*

$$\text{(a)}\quad \frac{\varepsilon+1}{\varepsilon+2}xQ_k^{\varepsilon+1} = \lambda_{k+1}Q_{k+1}^\varepsilon+(1-\lambda_k)Q_k^\varepsilon\,,$$

$$\text{(b)}\quad \frac{\varepsilon+2}{\varepsilon+1}Q_{k+1}^\varepsilon = \mu_{k+1}Q_{k+1}^{\varepsilon+1}+(1-\mu_k)Q_k^{\varepsilon+1}\,,$$

where $\lambda_k=k/(2k+m+\varepsilon-1)$, $\mu_k=(k+\varepsilon+2)/(2k+m+\varepsilon)$.

2.4. LEMMA.

$$Q_iQ_j = \sum_{k=|i-j|}^{i+j} q_k(i,j)Q_k,\qquad \textit{with } q_0(i,i)=Q_i(1)\,.$$

If $\varepsilon\leqq m-4$, then all $q_k\geqq 0$.

2.5. LEMMA. *Let $G(x)=Q_k(x)F(x)/Q_k(1)$, with $\varepsilon\leqq m-4$. Then $g_0=f_k$, and if all $f_i\geqq 0$, then all $g_i\geqq 0$.*

Lemma 2.4 comes from Gaspar [5] and implies 2.5, stated for the polynomials used in the real case in [4].

2.6. *Define*

$$R_k(x) = Q_0(x)+\ldots+Q_k(x)\,.$$

Then if $Q_k(x)=Q_k(m;\,x)$ we compute from [10, p. 71] that

$$(2.7)\qquad R_k(x) = \frac{m}{2k+m+\varepsilon}Q_k(m+1;\,x)$$

$$(2.8)\qquad R_k(1) = \frac{\varepsilon+1}{k+\varepsilon+1}\binom{k+m+\varepsilon-1}{k+\varepsilon}\binom{k+m-2}{k}.$$

2.9. We now come to the reason for introducing these polynomials. To fix notation, we define the innerproduct

$$\langle (a_1, \ldots, a_n), (b_1, \ldots, b_n) \rangle = \sum \bar{a}_i b_i$$

in H^n, writing $\langle \xi, \eta \rangle = z + jw$ $(z, w \in \mathsf{C})$ and $|\langle \xi, \eta \rangle|^2 = r$. Let Ω be the unit sphere in H^n, with volume $|\Omega|$.

For each integer $\varepsilon \geqq 0$ there is a sequence of mutually orthogonal linear spaces $W_0, W_1, \ldots$ of (harmonic) complex functions on Ω, with W_k of dimension $N = Q_k(1)$, such that the following holds [6].

Addition formula for W_k. For any orthogonal basis $S_1, S_2, \ldots, S_N$ of W_k with norm $\|S_t\|^2 = |\Omega|$, and any $\xi, \eta \in \Omega$, we have

$$\sum_{t=1}^{N} S_t(\xi)\overline{S_t(\eta)} = \bar{z}^{\varepsilon} Q_k(r) . \tag{2.10}$$

REMARK. Although this need not concern us here, W_k is the Sp (n)-irreducible subspace of harm $(k+\varepsilon, k)$ with highest weight $(k+\varepsilon, k, \mathbf{0})$. See [6] for further details.

3. Special bounds.

A complete solution for case $n = 2$, $A = \{\alpha\}$, is given by the author in [7]. For the general case we first prove an auxiliary result, for which the notation was established in sections 1, 2.

3.1. THEOREM.

$$\sum_{\xi, \eta \in X} r^{\varepsilon} Q_k(r) \geqq \delta_{k,0}(\varepsilon + 1)v^2 \qquad (\varepsilon, k \geqq 0) .$$

PROOF. Case $k \geqq 1$. We proceed by induction on ε. For $\varepsilon = 0$, let x be the N-vector with tth component $\sum_{\xi \in X} S_t(\xi)$. Then

$$0 \leqq \|x\|^2 = \sum_t \left(\sum_{\xi} \overline{S_t(\xi)} \right) \left(\sum_{\eta} S_t(\eta) \right) = \sum_{\xi, \eta} \left(\sum_t \overline{S_t(\xi)} S_t(\eta) \right) .$$

The last expression is the left hand side of Theorem 3.1 by the addition formula for W_k, so the inequality holds for $\varepsilon = 0$. Now assume the result for some $\varepsilon \geqq 0$. Then 2.3a implies

$$\sum_{\xi, \eta} r^{\varepsilon+1} Q_k^{\varepsilon+1}(r) = \sum_{\xi, \eta} r^{\varepsilon}(A Q_{k+1}^{\varepsilon}(r) + B Q_k^{\varepsilon}(r)) ,$$

where $A, B \geqq 0$. By the induction hypothesis, the last expression is $\geqq 0$.

Case $k = 0$. Again we use induction on ε. The result holds for $\varepsilon = 0$ since

$$\sum_{\xi, \eta} r^0 Q_0^0(r) = \sum_{\xi, \eta} (1) = v^2 .$$

Assume it holds for some $\varepsilon \geqq 0$. To apply this hypothesis we set $k=1$ in the first case, using the formula 2.2 for Q_1^ε to obtain

$$\sum_{\xi,\eta} r^\varepsilon\left(r-\frac{\varepsilon+2}{2n+\varepsilon}\right) \geqq 0,$$

and so

$$\sum_{\xi,\eta} r^{\varepsilon+1}Q_0^{\varepsilon+1} \geqq \sum_{\xi,\eta}\left(Q_0^{\varepsilon+1}\cdot\frac{\varepsilon+2}{2n+\varepsilon}\right)r^\varepsilon \geqq (\varepsilon+2)v^2$$

by the induction hypothesis. This completes the proof of Theorem 3.1.

3.2. Definition. We say $F(x)$ has *property* P_ε if all $f_k \geqq 0$ in its expansion in the polynomials Q_k^ε.

3.3. Theorem. *If $F(x)$ is P_ε and* (*) $x^\varepsilon F(x) \leqq 0$, $\forall x \in A$, *then*

$$v = |X| \leqq F(1)/(\varepsilon+1)f_0 \qquad (\text{provided } f_0>0).$$

Proof. We have

$$\begin{aligned} vF(1) = \sum_{\xi\in X} F(1) &\geqq \sum_{\xi,\eta\in X} r^\varepsilon F(r) \quad \text{by } (*) \\ &= \sum_{k\geqq 0} f_k \sum_{\xi,\eta} r^\varepsilon Q_k^\varepsilon(r) \\ &\geqq v^2(\varepsilon+1)f_0, \quad \text{by } P_\varepsilon \text{ and Theorem 3.1}. \end{aligned}$$

3.4. Remarks. With the factor $\varepsilon+1$, the bound of Theorem 3.3 is best possible in the sense that it is actually attained for certain values of the parameters (3.6–9, 3.14). The corresponding bound for vectors in $\mathbf{R}^n$ or $\mathbf{C}^n$ has the form $F(1)/f_0$, likewise attained [3]. We cannot here use characteristic matrix arguments as in [3] for $\varepsilon \geqq 1$, because the "quaternionic" addition formula 2.10 involves separately the z-part of the quaternion $\langle \xi, \eta\rangle$.

3.5. Definitions. Let $A^* = A \setminus \{0\}$. Theorem 3.3 yields the following table of bounds $v(A)$ if we let

$$F(x) = \prod \frac{x-\alpha}{1-\alpha} \qquad (\alpha \in A^*),$$

the *annihilator* of A, and set $\varepsilon=1$ if $0 \in A$, otherwise $\varepsilon=0$.. Each bound is valid when its denominator is positive and, where appropriate, $\alpha+\beta \leqq L$ (see [3] for the prototypes of tables 1 and 2).

Table 1. *Special bounds.*

A	$v(A)$	L
$\{\alpha\}$	$\dfrac{n(1-\alpha)}{1-n\alpha}$	
$\{\alpha,\beta\}$	$\dfrac{n(2n+1)(1-\alpha)(1-\beta)}{3-(2n+1)(\alpha+\beta)+n(2n+1)\alpha\beta}$	$\dfrac{3}{n+1}$
$\{0,\alpha\}$	$\dfrac{n(2n+1)(1-\alpha)}{3-(2n+1)\alpha}$	
$\{0,\alpha,\beta\}$	$\dfrac{n(n+1)(2n+1)(1-\alpha)(1-\beta)}{6-3(n+1)(\alpha+\beta)+(n+1)(2n+1)\alpha\beta}$	$\dfrac{8}{2n+3}$

We notice the first line is the van Lint–Seidel bound of the real and complex case (cf. [6]); setting $\beta=0$ in the second gives the third. The following three examples realize bounds of the table and so are of greatest possible size for the parameters. They come from reflection groups.

ADDED IN PROOF. Line two of the table is further realized by the 64 diameters of a polytope in H^4 with $A=\{\frac{1}{3},\frac{1}{9}\}$, due to the author.

3.6. EXAMPLE [2]. 63 vectors in H^3 with $A=\{0,\frac{1}{4},\frac{1}{2}\}$.

3.7. EXAMPLE [1, 2]. 36 vectors in H^4 with $A=\{0,\frac{1}{4}\}$.

3.8 EXAMPLE [2]. 165 vectors in H^5 with $A=\{0,\frac{1}{4}\}$.

A fourth reflection group example requires a separate calculation because of its large number of angles.

3.9. EXAMPLE [2]. 315 vectors in H^3 with $A=\{0,\frac{1}{4},\frac{1}{2},(3\pm\sqrt{5})/8\}$.

The annihilator $F(x)=(128x^4-192x^3+96x^2-18x+1)/15$ has non-negative coefficients f_k for $\varepsilon=1$, and so the bound of Theorem 3.3 is $v\leqq 1/(\varepsilon+1)f_0=315$. Hence this also is a maximal set.

At this point the reader may wonder if it is really useful to consider $\varepsilon>1$. One reason is that 3.3 can "almost always" be made to yield a bound, by suitable choice of ε. We have

3.10. THEOREM. *Let $\alpha\leqq\frac{1}{2}$ for all $\alpha\in A$. Then the annihilator of A is P_ε for some* ε (see Definition 3.2).

PROOF. The annihilator (3.5) is a positive multiple of the product of the factors $x-\alpha$, so by Lemma 2.4 it suffices to prove the result for $x-\alpha$, provided we ensure $\varepsilon \leqq 2n-4$. But $Q_1^{2n-4}(x)$ is a positive multiple of $x-\frac{1}{2}$, so

$$x-\alpha = x-\tfrac{1}{2}+\tfrac{1}{2}-\alpha = AQ_1^{2n-4}(x)+BQ_0^{2n-4}(x)$$

with $A, B \geqq 0$, provided $\alpha \leqq \frac{1}{2}$.

3.11. REMARKS. 3.10 is not best possible since A in 3.9 contains $(3+\sqrt{5})/8 > \frac{1}{2}$, whereas the annihilator of A is P_ε for $\varepsilon=1$. If all $f_i \geqq 0$ but $f_0=0$ in Theorem 3.3 (for some F with equality in *), suppose $f_k>0$. Then from 2.5 the polynomial $G(x)=Q_k(x)F(x)/Q_k(1)$ satisfies the hypotheses of 3.3, and $g_0=f_k$. Thus we still have a bound

$$v \leqq G(1)/(\varepsilon+1)g_0 = F(1)/(\varepsilon+1)f_k\,.$$

Now let $(F)_\varepsilon$ denote the expression $F(1)/(\varepsilon+1)f_0$ for any polynomial F with $f_0=f_0^\varepsilon \neq 0$. The following is an easy consequence of Lemma 2.3.

3.12. THEOREM. (a) *If $F(x)$ is P_ε, then $xF(x)$ is $P_{\varepsilon-1}$,*
(b) $(F)_\varepsilon=(xF)_{\varepsilon-1}$,
(c) *If F is P_ε, then it is also $P_{\varepsilon+1}$.*

3.13. REMARKS. Part (b) does *not* depend on coefficients being non-negative. 3.12a, b says that if $F(x)$ gives a bound (3.3) for some ε, then we get the *same* bound by expanding $x^\varepsilon F$ in terms of the Q_k^0. But of course the higher degree polynomial takes much more work to expand. On the other hand, the converse of 3.12a is false. For in the next example xF has non-negative coefficients in the Q_k^0 whilst F has some negative coefficient in the Q_k^1.

3.14. EXAMPLE [1]. A reflection group of 180 vectors in H^4 with $A=\{0,\frac{1}{4},\frac{1}{2}\}$. With $\varepsilon=1$ and $F(x)$ the annihilator we obtain $f_0=1/360$, $f_1=-1/3960$, $f_2=1/1485$. By 3.12b this implies $v \leqq 1/2f_0=180$, and hence that the set is maximal, *provided* we somehow know xF has non-negative coefficients g_k in the polynomials Q_k^0. But we can check this without using a 3rd degree polynomial xF and a new set of Q's, for by relations 2.3a we have

$$\begin{aligned} \tfrac{1}{2}g_3 &= \lambda_3 f_2 & \lambda_3 &= 3/13\\ \tfrac{1}{2}g_2 &= \lambda_2 f_1+(1-\lambda_2)f_2, & \lambda_2 &= 2/11\,,\\ \tfrac{1}{2}g_1 &= \lambda_1 f_0+(1-\lambda_1)f_1 & \lambda_1 &= 1/9\\ \tfrac{1}{2}g_0 &= f_0\,. \end{aligned}$$

Thus all $g_i>0$ and the set is maximal.

4. Absolute bounds.

4.1. THEOREM. *Set* $\varepsilon=1$ *if* $0 \in A$ *and* $\varepsilon=0$ *otherwise. Let* $S=|A^*|$. *Then*

$$v \leqq R_S(1)/(\varepsilon+1)\,.$$

If equality occurs, then the annihilator of A *is* $R_S(x)/v(\varepsilon+1)$.

REMARK. The last part implies that if the bound is met, then the non-zero elements of A are the roots of $R_S(x)$. These all lie in the interval $(0,1)$ as required, from the theory of orthogonal polynomials [10]. We note as in 3.3 the factor $\varepsilon+1$, again distinguishing the quaternionic from the real and complex cases [3].

PROOF OF 4.1. We use an extension of the characteristic matrix methods of [3]. First assume $\varepsilon=1$, $0 \in A$.

In the notation of the addition formula (2.9, 2.10) we define for W_k the $v \times Q_k(1)$ characteristic matrices H_k, V_k by $(H_k)_{\xi,t}=S_t(\xi)$ and $(V_k)_{\eta,t}=S_t(nj)$. Then

$$(H_k\tilde{H}_k)_{\xi,\eta} = \sum_t S_t(\xi)\overline{S_t(\eta)} = \bar{z}Q_k(r)\,,$$

where $\tilde{H}_k$ is the conjugate transpose. With $F(x)$ the annihilator of A, let I_k be the identity matrix of order $Q_k(1)$ and

$$\Delta = f_0I_0\oplus\ldots\oplus f_SI_S\,,$$

of order $R_S(1)$. The compound matrices

$$H = [H_0H_1\ldots H_S], \qquad V = [V_0V_1\ldots V_S]$$

are $v \times R_S(1)$ and satisfy

$$H\Delta\tilde{H} = \sum_k f_kH_k\tilde{H}_k = [\bar{z}F(r)] = I\,,$$

since $zF(r)=0$ for $r \in A$ and $F(1)=1$.

Now $\langle\xi,\eta j\rangle = -\bar{w}+j\bar{z}$, so $H\Delta\tilde{V}=[-wF(r)]=0$. For similar reasons $V\Delta\tilde{H}=0$, $V\Delta\tilde{V}=I$, so that

$$\begin{bmatrix} H \\ V \end{bmatrix}\begin{bmatrix} \Delta & \\ & \Delta \end{bmatrix}\begin{bmatrix} H \\ V \end{bmatrix}^{\sim} = \begin{bmatrix} I & \\ & I \end{bmatrix}. \tag{1}$$

Therefore

$$2v \leqq \operatorname{rank}\begin{bmatrix} H \\ V \end{bmatrix} \leqq R_S(1)\,,$$

establishing the first statement of the theorem, for $\varepsilon=1$.

In case of equality $[{H \atop V}]$ is square, hence non-singular by (1). It follows all $f_k > 0$. Then from 3.3, 3.11, all $f_k \leqq 1/2v$. Thus

$$vF(1) = \sum_{k=0}^{S} vf_kQ_k(1) \leqq \sum_{k=0}^{S} \tfrac{1}{2}Q_k(1) = \tfrac{1}{2}R_S(1) = v\,.$$

Since $F(1)=1$, all these are equal, implying each $f_k = 1/2v$ and hence $F(x) = R_S(x)/2v$ as required for $\varepsilon = 1$.

For $\varepsilon = 0$ we simply use matrix H.

Table 2. *Absolute bounds.*

A	Bound	annihilator (normalized)
$\{\alpha\}$	$\binom{2n}{2}$	$(2n+1)x-2$
$\{\alpha,\beta\}$	$n\binom{2n+1}{3}$	$(n+1)(2n+3)x^2-6(n+1)x+3$
$\{0,\alpha\}$	$\binom{2n+1}{3}$	$2(n+1)x-3$
$\{0,\alpha,\beta\}$	$n\binom{2n+2}{4}$	$(n+2)(2n+3)x^2-4(2n+3)x+6$.

4.2. Example. The third bound is realized by J. H. Conway's reflection group of 165 vectors in H^5 with $A=\{0,\frac{1}{4}\}$ ([2]). Also by the 10 diameters of a polygon in H^2 with $A=\{0,\frac{1}{2}\}$ due to D. W. Crowe [Canad. Math. Bull. 2 (1959), 77–79].

A conjecture.

In our known examples with $0 \in A$, the annihilator works well, giving exactly the right bound. For $0 \notin A$, results can be better with a polynomial multiple of the annihilator. We recall from 3.11 that any non-zero f_k can be used in Theorem 3.3, although so far f_0 has been the best choice.

4.3. Example. $A=\{\frac{1}{3}\}$, $n=4$. Special bounds $F(1)/(\varepsilon+1)f_k$ for some choices of $F(x)$ are shown below, with $G(x)$ the annihilator.

$F(x)$	ε	$k=0$	$k=1$	$k=2$
$G(x)$	0	$(f_0<0)$		
$xG(x)$	0	$(f_0=0)$	90	440
$G(x)$	1	$(f_0=0)$	80	
$G(x)$	2	120	220	
$(15x-4)G(x)$	0	22	0	968/3

The best result is the last line, obtained by optimizing the result for $(x-\alpha)G(x)$. The same bound is given by the formula of [6, Corollary 4.5]. The middle three rows of the table give valid bounds in case $A=\{0,\frac{1}{3}\}$, $n=4$; the best is $v\leqq 80$.

The optimization of $F(x)$ in general seems a complicated question, but further experimentation suggests the following is true.

4.4. CONJECTURE. Let X be of greatest size for given n, A. Then for some ε and some polynomial multiple $F(x)$ of the annihilator, we have strict equality

$$v = |X| = F(1)/(\varepsilon+1)f_0 .$$

REFERENCES

1. A. M. Cohen, *Private communication* (University of Technology, Enschede, The Netherlands).
2. J. H. Conway, *Private communication* (Cambridge University, England).
3. P. Delsarte, J. M. Goethals, and J. J. Seidel, *Bounds for systems of lines, and Jacobi polynomials*, Philips Research Reports 30 (1975), 91–105. Bouwkamp volume.
4. P. Delsarte, J. M. Goethals, and J. J. Seidel, *Spherical codes and designs*, Geometria Dedicata. To appear.
5. G. Gaspar, *Linearization of the product of Jacobi polynomials*, I, Canad. J. Math. 22 (1970), 171–175.
6. S. G. Hoggar, *Zonal functions and the symplectic group*, Preprint, Matematisk Institut, Aarhus Universitet. To appear.
7. S. G. Hoggar, *Quaternionic equi-isoclinic n-planes*, Ars Combinatoria 2 (1976), 11–13.
8. S. G. Hoggar, *Equiangular lines*, Proc. 5th Hungarian Colloq. on Combinatorics, Keszthely, 1976, pp. 599–606, North Holland Publ. co., Amsterdam 1978.
9. T. Koornwinder, *The addition formula for Jacobi polynomials* II, Math. Centrum Amsterdam. Afd. Toegepaste Wisk. Rep. 133 (1972).
10. G. Szegö, *Orthogonal polynomials*, 4th ed. Amer. Math. Soc., Providence, R.I., 1975.

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