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THE TRACE PROBLEM FOR TOTALLY POSITIVE ALGEBRAIC INTEGERS

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Abstract

Let α be a totally positive algebraic integer of degree $d \geq 2$ and $\alpha_1 = \alpha, \alpha_2, \ldots, \alpha_d$ be all its conjugates. We use explicit auxiliary functions to improve the known lower bounds of S_k/d, where $S_k = \sum_{i=1}^{d} \alpha_i^k$ and $k = 1, 2, 3$. These improvements have consequences for the search of Salem numbers with negative traces.

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1. Introduction

1.1. The absolute trace of totally positive algebraic integers. Let α be a totally positive algebraic integer of degree $d \geq 2$, that is to say, its conjugates $\alpha_1 = \alpha$, $\alpha_2, \ldots, \alpha_d$ are all positive real numbers, while its minimal polynomial is $P(x) = a_d x^d + a_{d-1}x^{d-1} + \cdots + a_1 x + a_0$, and $a_d = 1$. Let $S_k = \sum_{i=1}^{d} \alpha_i^k$; then S_1 is the trace of α and S_1/d is called the absolute trace of α. The Schur–Siegel–Smyth trace problem (so called by Borwein [4]) is concerned with S_1/d.

PROBLEM 1. Fix $\rho < 2$. Show that all but finitely many totally positive algebraic integers α have $S_1/d > \rho$.

This problem was solved in 1918 by Schur [14] when $\rho = \sqrt{e}$, in 1943 by Siegel [15] when $\rho = 1.737$, in 1984 by Smyth [17] when $\rho = 1.7719$, in 1997 by Flammang *et al.* [6] when $\rho = 1.7735$, in 2004 by McKee and Smyth [11] when $\rho = 1.778\,378\,6$, in 2006 by Aguirre and Peral [1] when $\rho = 1.784\,109$, in 2009 by Flammang [5] when $\rho = 1.787\,02$ and recently by McKee [10] when $\rho = 1.788\,39$.

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In this paper, we improve these results.

THEOREM 1.1. *If α is a totally positive algebraic integer of degree $d \geq 2$, then*

$$\frac{S_1}{d} > 1.791\,93,$$

unless the minimal polynomial of α is one of the following:

$$x^2 - 3x + 1, \quad x^3 - 5x^2 + 6x - 1,$$
$$x^4 - 7x^3 + 13x^2 - 7x + 1, \quad x^4 - 7x^3 + 14x^2 - 8x + 1.$$

1.2. Salem numbers of trace −4, −5. A Salem number is a real algebraic integer greater than 1 whose conjugates all lie in the closed disc $\{z \in \mathbb{C} : |z| \leq 1\}$, with at least one on the unit circle. Its minimal polynomial is a reciprocal polynomial of degree $2d$ with $d \geq 2$.

In 1999, Smyth [19] proved that there are Salem numbers of degree $2d$ and trace -1, for all $d \geq 4$, and the number of such Salem numbers is of larger order than $d/(\log \log d)^2$. In 2004, McKee and Smyth [11] provided several examples of trace -2 and established that the minimal degree for a Salem number of trace -2 is 20; in 2005, they showed [12] that for every negative integer $-T$, there exists a Salem number with trace $-T$, and they gave a bound on the smallest degree. In 2009, Flammang [5] proved that if a Salem number has trace -3, then its degree is at least 30.

Theorem 1.1 has the following corollaries.

COROLLARY 1.2. *If a Salem number has trace -4, then its degree is at least* 40.

In fact, finding all Salem numbers of degree $2d$ and trace -4 is equivalent to finding all totally positive algebraic integers α of degree d and trace $2d - 4$ such that $\alpha > 4$ and all other conjugates of α are in the interval $(0, 4)$. Let

$$P(x) = x^d - (2d - 4)x^{d-1} + \cdots$$

be the minimal polynomial of such a totally positive algebraic integer. The transformation $x = z + 1/z + 2$ produces a reciprocal polynomial

$$Q(z) = z^{2d} + 4z^{2d-1} + \cdots + 4z + 1,$$

which is the minimal polynomial of a Salem number of degree $2d$ and trace -4, because the roots of $P(x)$ in the interval $(0, 4)$ give pairs of roots of $Q(z)$ on the unit circle and the roots of $P(x)$ in the interval $(4, \infty)$ give pairs of reciprocal real positive roots of $Q(z)$.

Corollary 1.2 is an easy consequence of Theorem 1.1. As $1.791\,93 > 34/19$, there exists no totally positive irreducible polynomial of degree 19 and trace 34 corresponding to a Salem number of trace -4. Thus, the possible degree for such a polynomial is 20 and so at least degree 40 for the corresponding Salem number.

Similarly, we get the following result.

COROLLARY 1.3. *If a Salem number has trace -5, then its degree is at least* 50.

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1.3. Other invariants S_k/d of totally positive algebraic integers. In 1984, Smyth [18] studied the set $\mathscr{M}_p$ of all $M_p(\alpha)$, where

$$M_p(\alpha) = \left(\frac{1}{d}\sum_{i=1}^{d} |\alpha_i|^p\right)^{1/p},$$

$p > 0$ is fixed and α varies over the totally real algebraic integers of degree d. He showed that when $p = 4$, the set $\mathscr{M}_p$ consists of seven isolated points in the interval (0, 1.509 80), it is everywhere dense in the interval (1.565 08, ∞), and is undetermined in the interval (1.509 80, 1.565 08). The seven isolated points (called exceptions in this paper) correspond to:

$$x, \quad x-1, \quad x-2, \quad x^2+x-1, \quad x^3+x^2-2x-1,$$
$$x^5+x^4-4x^3-3x^2+3x+1, \quad x^6+x^5-5x^4-4x^3+6x^2+3x-1.$$

It is easy to prove that α^2 is totally positive and $M_p(\alpha^2) = (M_{2p}(\alpha))^2$ if α is totally real. Based on this fact and Smyth's results, we can easily see that if α is a totally positive algebraic integer, then the set S_2/d consists of six isolated points in the interval (0, 5.196 10), is everywhere dense in the interval (5.999 93, ∞) and is undetermined in the interval (5.196 10, 5.999 93). The six isolated points correspond to

$$x-1, x-2, P_1, P_2, P_3, P_4,$$

where

$$\begin{aligned}
P_1 &= x^2 - 3x + 1,\\
P_2 &= x^3 - 5x^2 + 6x - 1,\\
P_3 &= x^5 - 9x^4 + 28x^3 - 35x^2 + 15x - 1,\\
P_4 &= x^6 - 11x^5 + 45x^4 - 84x^3 + 70x^2 - 21x + 1.
\end{aligned}$$

Similarly, when $p = 6$, we see that if α is a totally positive algebraic integer, then the set S_3/d consists of five isolated points in the interval (0, 16.264 81), is everywhere dense in the interval (20.000 08, ∞) and is undetermined in the interval (16.264 81, 20.000 08). The five isolated points correspond to

$$x-1, x-2, P_1, P_2, P_3.$$

In this paper, we use auxiliary functions to study the lower bounds of S_2/d and S_3/d. For S_2/d, we improve the left end point of the interval (5.196 10, 5.999 93), increasing 5.196 10 to 5.319 35, and we find a new exception. For S_3/d, we increase the left end point of the interval (16.264 81, 20.000 08) to 17.567 65, and we find three new exceptions.

THEOREM 1.4. *If α is a totally positive algebraic integer of degree $d \geq 2$, then*

$$\frac{S_2}{d} > 5.319\,35,$$

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unless the minimal polynomial of α *is one of* P_1*,* P_2*,* P_3*,* P_4*, and* P_5*, where*

$$P_5 = x^4 - 7x^3 + 14x^2 - 8x + 1.$$

THEOREM 1.5. *If* α *is a totally positive algebraic integer of degree* $d \geq 2$*, then*

$$\frac{S_3}{d} > 17.567\,65,$$

unless the minimal polynomial of α *is one of* P_1*,* P_2*,* P_3*,* P_4*,* P_6*, and* P_7*, where*

$$\begin{aligned} P_6 &= x^8 - 15x^7 + 91x^6 - 286x^5 + 495x^4 - 462x^3 + 210x^2 - 36x + 1, \\ P_7 &= x^9 - 17x^8 + 120x^7 - 455x^6 + 1001x^5 - 1287x^4 \\ &\quad + 924x^3 - 330x^2 + 45x - 1. \end{aligned}$$

Note that, compared to Smyth's results, the polynomial P_5 in Theorem 1.4 and P_4, P_6 and P_7 in Theorem 1.5 are new exceptions.

This paper is organized as follows: in Section 2, we briefly recall the method; and in Section 3, we describe the numerical results.

2. Principle of the explicit auxiliary functions

2.1. Construction of an explicit auxiliary function. Let α be a totally positive algebraic integer of degree d, with minimal polynomial P, and let $\alpha_1 = \alpha, \alpha_2, \ldots, \alpha_d$ be all its conjugates.

Let $x > 0$, let $\mathbf{e} = (e_1, e_2, \ldots, e_n) \in \mathbb{R}^n$ where $e_i > 0$, and let $Q_i \in \mathbb{Z}[x]$ for $1 \leq i \leq n$. For S_1/d, we consider the explicit auxiliary function

$$f_1(x, \mathbf{e}) = x - \sum_{i=1}^{n} e_i \log |Q_i(x)|.$$

Suppose that $m(\mathbf{e}) = \min_{x>0} f_1(x, \mathbf{e})$. Then

$$\alpha_j - \sum_{i=1}^{n} e_i \log |Q_i(\alpha_j)| \geq m(\mathbf{e}),$$

when $1 \leq j \leq d$, and therefore

$$\sum_{j=1}^{d} \alpha_j - \sum_{i=1}^{n} e_i \log \left| \prod_{j=1}^{d} Q_i(\alpha_j) \right| \geq d \cdot m(\mathbf{e}),$$

$$S_1 - \sum_{i=1}^{n} e_i \log |\mathrm{Res}(P, Q_i)| \geq d \cdot m(\mathbf{e}),$$

where Res is the resultant of the two polynomials. If P does not divide any Q_i, then $\mathrm{Res}(P, Q_i)$ is a nonzero integer, thus

$$\frac{S_1}{d} \geq m(\mathbf{e}).$$

Similarly, to treat S_k/d, let $\mathbf{c}^{(k)} = (c_1^{(k)}, c_2^{(k)}, \ldots, c_{n_k}^{(k)}) \in \mathbb{R}^{n_k}$ where $c_i^{(k)} > 0$, and $P_i^{(k)} \in \mathbb{Z}[x]$; here $1 \leq i \leq n_k$ and $k = 2, 3$. We consider the explicit auxiliary function

$$f_k(x, \mathbf{c}^{(k)}) = x^k - \sum_{i=1}^{n_k} c_i^{(k)} \log |P_i^{(k)}(x)|.$$

If $m_k(\mathbf{c}^{(k)}) = \min_{x>0} f_k(x, \mathbf{c}^{(k)})$ and P does not divide any of the $P_i^{(k)}$, then

$$\frac{S_k}{d} \geq m_k(\mathbf{c}^{(k)}).$$

Clearly, we then have to solve the following optimization problems: determine

$$m = \max_{\mathbf{e}} m(\mathbf{e}) = \max_{(e_i)} \min_{x>0} f_1(x, \mathbf{e})$$

or

$$m = \max_{\mathbf{c}^{(k)}} m_k(\mathbf{c}^{(k)}) = \max_{(c_i^{(k)})} \min_{x>0} f_k(x, \mathbf{c}^{(k)}).$$

Therefore, good e_i, $c_i^{(k)}$ and Q_i, $P_i^{(k)}$ are important for us.

2.2. Explicit auxiliary functions and integer transfinite diameter. We describe the arguments for the Q_i only, as they also apply to the $P_i^{(k)}$.

As can be seen from the last section, to get a good lower bound of S_1/d by the semi-infinite linear programming method, we have to make a good choice of polynomials Q_i in the auxiliary function f_1 so that the value of $m(\mathbf{e})$ is as large as possible.

In fact, if we replace the real numbers e_i in the auxiliary function f_1 by rational numbers, then we may write

$$f_1(x) = x - \frac{t}{h} \log |H(x)|,$$

where H is in $\mathbb{Z}[x]$ of degree h and t is a positive real number. We want a function f_1 whose minimum m in the interval $(0, \infty)$ is as large as possible. Thus we search for a polynomial $H \in \mathbb{Z}[x]$ such that

$$\sup_{x>0} |H(x)|^{t/h} e^{-x} \leq e^{-m}.$$

Now, if we suppose that t is fixed, then it is clear that we need an efficient upper bound for the quantity

$$t_{\mathbb{Z},\phi}((0, \infty)) = \liminf_{\substack{h\geq 1 \\ h\to\infty}} \inf_{\substack{H\in\mathbb{Z}[x] \\ \deg H = h}} \sup_{x>0} |H(x)|^{t/h} \phi(x),$$

in which we use the weight $\phi(x) = e^{-x}$. To get an upper bound for $t_{\mathbb{Z},\phi}((0, \infty))$, it is sufficient to get an explicit polynomial $H \in \mathbb{Z}[x]$ and then to use the sequence of the successive powers of H.

This is a generalization of the integer transfinite diameter in the interval $(0, \infty)$. With the second author's algorithm [20], we compute a polynomial H of degree less than 65 which is small on a set of positive control points and take its irreducible factors as the candidates for the Q_i. As the LLL algorithm (named after A. K. Lenstra, H. W. Lenstra and L. Lovasz) often finds 'smaller' polynomials, it is our main method of finding the candidates for the Q_i. The basic idea is similar to [5, 8, 13], but it is difficult to find the Q_i with higher degrees. So we improve the LLL algorithm, with a view to tackling our problem. These improvements enable us to get more Q_i with higher degrees.

A semi-infinite linear programming method gives good numerical values for the e_i and $c_i^{(k)}$. This method was introduced into number theory by Smyth [18]. More details can be found in [20] or [2].

3. Numerical results

3.1. Computation of the minimum of the explicit auxiliary functions. To ensure that there is only one local minimum between two consecutive real roots of the polynomials Q_i, we prove that the auxiliary functions that we present here are convex functions for $x > 0$. To prove that $f_1''(x)$ is positive, we first factorize all the polynomials Q_i into irreducible real factors. Then $f_1''(x)$ is a sum of a first term which is 0, 2 or $6x$ plus a sum of terms of the form $e_j/(x-\alpha)^2$, where α is a real root of a polynomial Q_j (type 1) and of the form $2e_k((x-\gamma)^2 - \delta^2)/((x-\gamma)^2 + \delta^2)^2$ where $\delta > 0$ and $\gamma + i\delta$ is a complex root of a polynomial Q_k (type 2). We suppose now that all the real roots α are taken in increasing order and that the complex roots $\gamma + i\delta$, where $\delta > 0$, are taken in increasing order of their real parts.

We generalize the algorithm given in [7].

3.2. The algorithm.

Step 1: the general case. Let $\mathcal{S}$ be a sequence of complex roots $\gamma + i\delta$ with increasing real parts. We add all terms of type 2 related to this sequence $\mathcal{S}$. Then we add to this rational function all the terms of type 1, associated with a real root α, from the greatest α less than the smallest δ of the sequence $\mathcal{S}$ to the smallest α greater than the greatest δ of the sequence. Let $F_{\mathcal{S}}$ be the rational function that we obtain. By Sturm's process, we compute the number of real positive zeros of the numerator of the function $F_{\mathcal{S}}$. If, for all sequences $\mathcal{S}$, there is no positive zero then we are done: f_1 is convex. If this is not the case, then we go to Step 2.

Step 2: the exceptional cases. We add to the exceptional functions $F_{\mathcal{S}}$ one or two terms of type 1 associated with real roots α which are close to the real roots already used in $F_{\mathcal{S}}$ such that this new rational function has no positive zeros.

REMARK 3.1. For S_1 there are only five exceptional functions and for S_2 there are four. For S_3 it is sufficient to use the first step.

3.3. Comments on the polynomials which occur in the auxiliary functions. The complete lists of polynomials Q_i and coefficients e_i that occur in the explicit auxiliary function f_1 to obtain Theorem 1.1 are given in Tables 1 and 2.

TABLE 1. The polynomials Q_i. Those with (∗) are exceptions.

i	d	S_1/d	Coefficients of Q_i (from a_0 to a_d)
1	1	0.00000	0 1
2	1	1.00000	−1 1 (∗)
3	1	2.00000	−2 1
4	2	1.50000	1 −3 1 (∗)
5	2	2.00000	1 −4 1
6	2	2.00000	2 −4 1
7	3	1.66667	−1 6 −5 1 (∗)
8	3	2.00000	−1 9 −6 1
9	3	2.00000	−3 9 −6 1
10	3	2.00000	−1 8 −6 1
11	4	1.75000	1 −7 13 −7 1 (∗)
12	4	1.75000	1 −8 14 −7 1 (∗)
13	5	1.80000	−1 11 −29 26 −9 1
14	5	1.80000	−1 12 −31 27 −9 1
15	5	1.80000	−1 13 −32 27 −9 1
16	5	1.80000	−1 15 −35 28 −9 1
17	6	1.83333	1 −15 53 −73 43 −11 1
18	6	1.83333	1 −14 51 −72 43 −11 1
19	6	1.83333	1 −12 45 −67 42 −11 1
20	7	1.85714	−1 18 −89 172 −150 64 −13 1
21	7	1.85714	−1 16 −78 157 −143 63 −13 1
22	8	1.75000	1 −19 111 −277 339 −221 78 −14 1
23	8	1.75000	1 −21 120 −289 345 −222 78 −14 1
24	8	1.87500	3 −40 187 −402 445 −269 89 −15 1
25	8	1.87500	3 −42 200 −428 467 −277 90 −15 1
26	9	1.88889	−3 50 −286 771 −1112 910 −433 118 −17 1
27	9	1.88889	−3 48 −277 759 −1106 909 −433 118 −17 1
28	10	1.80000	3 −53 342 −1096 1973 −2114 1389 −562 136 −18 1
29	10	1.80000	1 −24 194 −743 1526 −1798 1265 −537 134 −18 1
30	10	1.80000	1 −24 200 −766 1560 −1822 1273 −538 134 −18 1
31	10	1.80000	1 −24 206 −813 1662 −1920 1320 −549 135 −18 1
32	10	1.80000	1 −22 183 −722 1508 −1791 1264 −537 134 −18 1

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TABLE 1. Continued.

i	d	S_1/d	Coefficients of Q_i (from a_0 to a_d)
33	12	1.75000	1 −27 277 −1432 4216 −7565 8613 −6373 3090 −971 190 −21 1
34	12	1.75000	1 −27 281 −1470 4336 −7742 8750 −6430 3102 −972 190 −21 1
35	12	1.75000	1 −27 283 −1483 4372 −7789 8780 −6439 3103 −972 190 −21 1
36	12	1.75000	1 −27 280 −1462 4318 −7725 8743 −6429 3102 −972 190 −21 1
37	12	1.75000	1 −25 248 −1278 3808 −6954 8068 −6081 2999 −956 189 −21 1
38	12	1.83333	1 −29 316 −1694 5058 −9075 10250 −7484 3562 −1092 207 −22 1
39	12	1.83333	1 −29 318 −1726 5233 −9481 10709 −7760 3652 −1107 208 −22 1
40	12	1.75000	1 −26 263 −1359 4017 −7242 8291 −6178 3021 −958 189 −21 1
41	13	1.76923	−1 28 −313 1837 −6338 13689 −19217 17929 −11240 4730 −1313 230 −23 1
42	13	1.69231	−1 33 −392 2284 −7514 15183 −19885 17475 −10496 4318 −1196 213 −22 1
43	13	1.76923	−1 32 −392 2372 −8062 16721 −22332 19867 −11975 4895 −1333 231 −23 1
44	13	1.76923	−1 32 −384 2308 −7880 16475 −22157 19800 −11962 4894 −1333 231 −23 1
45	14	1.78571	1 −35 459 −3021 11546 −27859 44569 −48654 36815 −19397 7063 −1736 274 −25 1
46	14	1.78571	1 −33 424 −2816 10964 −26937 43704 −48167 36655 −19369 7061 −1736 274 −25 1
47	14	1.78571	1 −35 460 −3069 11906 −29027 46627 −50813 38215 −19960 7199 −1754 275 −25 1
48	14	1.78571	1 −30 369 −2447 9743 −24658 41129 −46348 35850 −19153 7029 −1734 274 −25 1
49	14	1.78571	1 −32 406 −2701 10625 −26404 43221 −47907 36573 −19355 7060 −1736 274 −25 1
50	14	1.71429	1 −25 270 −1679 6593 −16961 29208 −34227 27620 −15418 5916 −1526 252 −24 1
51	14	1.78571	1 −37 502 −3344 12779 −30594 48328 −51961 38697 −20082 7216 −1755 275 −25 1
52	15	1.86667	−5 147 −1728 10848 −41124 101035 −168255 195583 −161640 95842 −40758 12291 −2559 349 −28 1
53	15	1.80000	−1 32 −424 3079 −13710 39727 −77645 104703 −98793 65693 −30777 10058 −2237 322 −27 1
54	16	1.81250	2 −67 916 −6835 31441 −95254 197940 −289697 303849 −230770 127385 −50911 14533 −2881 376 −29 1
55	16	1.81250	1 −35 514 −4172 20860 −68201 151556 −235052 259051 −205149 117251 −48205 14069 −2835 374 −29 1

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TABLE 1. Continued.

i	d	S_1/d	Coefficients of Q_i (from a_0 to a_d)
56	16	1.75000	1 −37 542 −4272 20579 −64907 139846 −211658 229288 −179856 102629 −42458 12563 −2584 350 −28 1
57	16	1.75000	1 −34 482 −3781 18415 −59232 130638 −202419 223884 −178487 102947 −42815 12677 −2601 351 −28 1
58	16	1.68750	1 −40 634 −5341 27165 −89616 200702 −314602 352281 −285355 168066 −71757 21917 −4656 652 −54 2
59	17	1.88235	−5 164 −2264 17457 −84305 271323 −605133 960549 −1105695 934867 −584793 270975 −92460 22875 −3983 462 −32 1
60	17	1.76471	−1 37 −577 5010 −27083 96981 −239493 419445 −531403 493528 −338436 171512 −63818 17157 −3233 404 −30 1
61	17	1.82353	−3 103 −1469 11605 −57190 187693 −427515 694870 −821490 715331 −461883 221279 −78141 20016 −3608 433 −31 1
62	18	1.72222	1 −42 727 −6907 40541 −157376 422880 −812508 1142885 −1196694 942699 −561334 252284 −84844 20969 −3688 436 −31 1
63	18	1.72222	1 −33 478 −4067 22892 −90195 255672 −529107 806985 −913525 771460 −487085 229460 −80001 20296 −3633 434 −31 1
64	18	1.77778	1 −39 651 −6146 36673 −146885 410245 −820431 1197457 −1292914 1041711 −628749 283862 −95083 23227 −4011 463 −32 1
65	19	1.84211	−1 47 −925 10113 −68943 312586 −982483 2203375 −3601035 4357487 −3950110 2703247 −1401099 548887 −161134 34826 −5369 558 −35 1
66	19	1.71053	−1 46 −885 9487 −63802 287771 −908871 2071144 −3479535 4376867 −4166227 3019357 −1668516 700463 −221143 51515 −8569 961 −65 2
67	19	1.78947	−1 44 −819 8575 −56670 251719 −781936 1746007 −2859126 3485068 −3196547 2221403 −1172621 468992 −140843 31193 −4935 527 −34 1
68	19	1.68421	−1 44 −828 8805 −59197 267778 −848640 1939216 −3263677 4109455 −3914269 2839101 −1571253 661367 −209672 49139 −8241 934 −64 2
69	20	1.75000	1 −48 962 −10769 75934 −360604 1204274 −2915730 5234658 −7087859 7329003 −5836206 3594803 −1712811 628206 −175386 36537 −5492 562 −35 1
70	20	1.75000	1 −46 903 −10004 70208 −333095 1114515 −2709540 4892653 −6670720 6950297 −5578677 3463627 −1663128 614448 −172686 36182 −5464 561 −35 1

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TABLE 1. Continued.

i	d	S_1/d	Coefficients of Q_i (from a_0 to a_d)
71	20	1.75000	1 −50 1045 −12224 90329 −451016 1588164 −4061153 7700259 −10990637 11937184 −9937332 6363821 −3134361 1181511 −337149 71416 −10863 1120 −70 2
72	20	1.75000	1 −44 826 −8812 60123 −280397 932877 −2279025 4170738 −5797043 6176879 −5074124 3220793 −1577448 592638 −168801 35724 −5432 560−35 1
73	21	1.76190	−1 45 −884 10059 −74300 379059 −1389264 3758545 −7655428 11911880 −14312946 13380711 −9775667 5587613 −2492289 861331 −227645 45027 −6435 626 −37 1
74	21	1.80952	−1 51 −1093 13170 −100780 524413 −1938661 5247437 −10626547 16357099 −19360218 17762885 −12694903 7078377 −3072478 1031341 −264374 50677 −7018 662 −38 1
75	21	1.76190	−1 48 −988 11574 −86772 444767 −1626575 4371857 −8822270 13577179 −16117217 14874086 −10720947 6043199 −2657659 905654 −236128 46121 −6520 629 −37 1
76	21	1.80952	−1 49 −1022 12109 −91779 475365 −1755219 4757487 −9668384 14962741 −17834633 16500575 −11903758 6704016 −2939999 996915−258012 49887 −6959 660 −38 1
77	21	1.76190	−1 45 −878 9906 −72717 370329 −1361262 3707186 −7616692 11961174 −14494118 13642521 −10012934 5735638 −2557644 881750 −232062 45656 −6488 628 −37 1
78	21	1.80952	−3 131 −2473 26822 −187631 902307 −3107178 7882931 −15042941 21928842 −24700189 21670417 −14879915 8008289 −3370612 1101992 −276352 52049 −7113 665 −38 1
79	21	1.76190	−1 47 −951 11026 −82341 422456 −1551385 4194537 −8520973 13201104 −15768232 14631953 −10595414 5994942 −2644137 902977 −235774 46093 −6519 629 −37 1
80	21	1.76190	−1 47 −955 11134 −83566 430266 −1582897 4280355 −8685147 13427552 −15997184 14803141 −10690231 6033609 −2655564 905351 −236102 46120 −6520 629 −37 1
81	22	1.68182	1 −46 919 −10614 79739 −416400 1578704 −4481884 9745042 −16494534 21979515 −23223218 19528813 −13079899 6962665 −2930012 965712 −245657 47147 −6587 631 −37 1
82	22	1.77273	1 −51 1125 −14252 116373 −652779 2621343 −7758681 17295813 −29517782 39047517 −40404573 32906078 −21161658 10747996 −4296863 1341779 −322908 58600 −7743 702 −39 1

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TABLE 1. Continued.

i	d	S_1/d	Coefficients of Q_i (from a_0 to a_d)
83	24	1.79167	1 −57 1416 −20408 191731 −1251551 5911985 −20793445 55622727 −115037530 186332598 −238772580 243924711 −199729262 131488158 −69643298 29615965 −10058436 2702879 −566171 90344 −10592 859 −43 1
84	24	1.75000	3 −158 3616 −48105 419588 −2564356 11453393 −38481612 99319618 −200028124 318127194 −403167371 409837747 −335650552 221958772 −118502680 50943798 −17532759 4783780 −1019205 165667 −19812 1641 −84 2
85	26	1.76923	1 −62 1683 −26676 277855 −2030239 10852323 −43703948 135521029 −329029059 633676899 −978044645 1219478349 −1235752896 1022031531 −691564941 383082531 −173463233 63959801 −19074158 4552122 −855646 123684 −13251 990 −46 1

For $k = 2, 3$ the complete lists of polynomials $P_i^{(k)}$ and coefficients $c_i^{(k)}$ that occur in the explicit auxiliary function f_k to obtain Theorems 1.4 and 1.5 are not given in this paper. They can be obtained on request from the authors. For $k = 2$, the list of $P_i^{(2)}$ contains 76 polynomials and the largest degree is 25. Most of them are different from the ones in Table 1. There are 65 polynomials in the list of $P_i^{(3)}$ with the largest degree 24. Most of them are also different from Q_i and $P_i^{(2)}$.

Of the polynomials listed in Table 1 for S_1/d, 57 are new compared to Flammang [5]. Five of these are minimal polynomials of totally positive algebraic integers, while the other 52 polynomials have at least two complex roots. This phenomenon was encountered by Habsieger and Salvy [9] and Flammang [5]. The real parts of the roots of Q_i all lie in $[0, 6.179)$. For S_2/d and S_3/d, most of the $P_i^{(k)}$ have at least two complex roots; a few of them are totally real with higher degrees, but have negative roots. Surprisingly, the real parts of the roots of $P_i^{(2)}$ and $P_i^{(3)}$ are less than 5.065 and 4.342, respectively.

From Flammang's result, we know that there are no other exceptions in the totally positive algebraic integers for degree less than 19 and $S_1/d < 1.8$. From Theorem 1.1, we can see that there are no other exceptions in the totally positive algebraic integers of degree less than 29 such that $S_1/d < 1.8$, because there is no integer a_{d-1} such that $1.791\,93d < a_{d-1} < 1.8d$ when $d \leq 28$.

For the new exceptions, note that $(2\cos(2\pi/13))^2$, $(2\cos(2\pi/60))^2$, $(2\cos(2\pi/17))^2$ and $(2\cos(2\pi/19))^2$ are roots of P_4, P_5, P_6, and P_7, respectively. This phenomenon was encountered by Smyth [18].

TABLE 2. The e_i (when $1 \le i \le 85$).

$e_1 = 0.54667828587271$	$e_2 = 0.47871800200563$	$e_3 = 0.06555339063836$
$e_4 = 0.17687800003332$	$e_5 = 0.00448219377598$	$e_6 = 0.00820674276069$
$e_7 = 0.06668043722377$	$e_8 = 0.00125946611406$	$e_9 = 0.00326334656865$
$e_{10} = 0.00066732703529$	$e_{11} = 0.02219899039435$	$e_{12} = 0.02050231566957$
$e_{13} = 0.00596323763882$	$e_{14} = 0.00680493233212$	$e_{15} = 0.00161758504819$
$e_{16} = 0.00649102555420$	$e_{17} = 0.00126784014151$	$e_{18} = 0.00036740931954$
$e_{19} = 0.00009486044026$	$e_{20} = 0.00107768512029$	$e_{21} = 0.00040808070426$
$e_{22} = 0.00050557086357$	$e_{23} = 0.00068294267031$	$e_{24} = 0.00171765600696$
$e_{25} = 0.00161646860599$	$e_{26} = 0.00000217826900$	$e_{27} = 0.00025053345069$
$e_{28} = 0.00035776659865$	$e_{29} = 0.00258586799662$	$e_{30} = 0.00152524181426$
$e_{31} = 0.00261187979809$	$e_{32} = 0.00009450860731$	$e_{33} = 0.00180760919958$
$e_{34} = 0.00381998708930$	$e_{35} = 0.00292108445484$	$e_{36} = 0.00000923432980$
$e_{37} = 0.00030623185520$	$e_{38} = 0.00069348522644$	$e_{39} = 0.00004317611411$
$e_{40} = 0.00010987249521$	$e_{41} = 0.00024101680608$	$e_{42} = 0.00026920860606$
$e_{43} = 0.00009068781304$	$e_{44} = 0.00032741880442$	$e_{45} = 0.00019139938162$
$e_{46} = 0.00246025331757$	$e_{47} = 0.00022043537382$	$e_{48} = 0.00100870070303$
$e_{49} = 0.00123232114596$	$e_{50} = 0.00028646838749$	$e_{51} = 0.00020015964760$
$e_{52} = 0.00028158653190$	$e_{53} = 0.00005028470678$	$e_{54} = 0.00046725062302$
$e_{55} = 0.00028920824667$	$e_{56} = 0.00033453149956$	$e_{57} = 0.00005504355305$
$e_{58} = 0.00013876361417$	$e_{59} = 0.00016196280403$	$e_{60} = 0.00077617405057$
$e_{61} = 0.00176509412348$	$e_{62} = 0.00006934560638$	$e_{63} = 0.00021949303306$
$e_{64} = 0.00003368631008$	$e_{65} = 0.00069694015272$	$e_{66} = 0.00008453104496$
$e_{67} = 0.00017644422693$	$e_{68} = 0.00002003197599$	$e_{69} = 0.00086131382526$
$e_{70} = 0.00025937930484$	$e_{71} = 0.00043707111183$	$e_{72} = 0.00037001316339$
$e_{73} = 0.00019992139283$	$e_{74} = 0.00007015239147$	$e_{75} = 0.00096360138366$
$e_{76} = 0.00050566472131$	$e_{77} = 0.00102203952795$	$e_{78} = 0.00136209986730$
$e_{79} = 0.00146924699630$	$e_{80} = 0.00030962306340$	$e_{81} = 0.00018949632484$
$e_{82} = 0.00020938118202$	$e_{83} = 0.00084741810993$	$e_{84} = 0.00028969646642$
$e_{85} = 0.00090543409795$		

We conjecture that the next exception of S_2/d is P_6, for which $S_2/d = 5.375\,00$, and the next exception of S_3/d is the polynomial

$$x^9 - 17x^8 + 120x^7 - 456x^6 + 1011x^5 - 1324x^4 + 986x^3 - 376x^2 + 57x - 1,$$

for which $S_3/d = 17.888\,89$, but its root is neither of the form $(2\cos(2\pi/n))^2$ nor of the form β_n^2 for any n. Here β_n is a root of the nth Gorshkov–Wirsing polynomial, defined as in [16].

All the computations in this paper were performed using the Pascal programming language and Pari/GP [3].

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