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ON THE ZEROES OF TWO FAMILIES OF POLYNOMIALS ARISING FROM CERTAIN RATIONAL INTEGRALS

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ABSTRACT. We prove a conjecture of Boros, Moll and Shallit on the location of the zeroes of certain polynomials arising in the evaluation of the rational definite integrals $\int_0^\infty [dx/(x^4+2ax^2+1)^{m+1}]$.

1. Introduction. In a series of recent papers George Boros, Victor Moll, and a number of coauthors have studied patterns in closed form expressions for the rational definite integrals

$$\int_0^\infty \frac{dx}{(x^4+2ax^2+1)^{m+1}}, \quad a > -1. \tag{1}$$

The recent article [**4**] gives some of the interesting background behind this line of investigation and a survey of their results. In this note we will take up a question concerning certain polynomials connected to the integrals (1) introduced in [**1**].

A standard argument shows that (1) is equal to

$$\frac{\pi\binom{2m}{m}}{2^{3m+3/2}(a+1)^{m+1/2}}\ {}_2F_1(-m, m+1;\ 1/2-m;\ (1+a)/2),$$

where ${}_2F_1$ is the usual hypergeometric series. For positive integral m, the hypergeometric series terminates and the authors of [**1**] study the polynomials in the variable a defined by $P_m(a) = \binom{2m}{m}\ {}_2F_1(-m, m+1; 1/2-m; (1+a)/2)$. For each m, $P_m(a)$ is a polynomial all of whose coefficients are positive integers.

Let $d_l(m)$ be the coefficient of a^l in $P_m(a)$. In [**1**], it is shown that

$$d_l(m) = \frac{1}{l!m!2^{m+l}}\left(\alpha_l(m)\prod_{k=1}^{m}(4k-1) - \beta_l(m)\prod_{k=1}^{m}(4k+1)\right),$$

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where the $\alpha_l(m)$ and $\beta_l(m)$ are polynomials in m. For example,

$$\begin{aligned}
\alpha_0(m) &= 1 \\
\alpha_1(m) &= 2m + 1 \\
\alpha_2(m) &= 2(2m^2 + 2m + 1) \\
\alpha_3(m) &= 8(2m^4 + 4m^3 + 26m^2 + 24m + 9)
\end{aligned}$$

and

$$\begin{aligned}
\beta_0(m) &= 0 \\
\beta_1(m) &= 1 \\
\beta_2(m) &= 2(2m + 1) \\
\beta_3(m) &= 12(m^2 + m + 1)
\end{aligned}$$

and so on. It can be seen that all the roots of these polynomials lie on the line $\Re(m) = -1/2$. Numerical calculations on subsequent terms in the α and β families suggest the following conjecture.

Conjecture [**1**]. *For all $l \geq 1$, all roots of $\alpha_l(m) = 0$ lie on the line $\Re(m) = -1/2$ in the complex plane. Similarly, the roots of $\beta_l(m) = 0$ for $l \geq 2$ lie on the line $\Re(m) = -1/2$.*

In this note we will present a proof of this conjecture. The first step, given in Section 2 below, is to rewrite the polynomials $\alpha_l(m)$ and $\beta_l(m)$ as functions of the new variable $s = 2m+1$. When this is done, we will see that α_l is an even function for l even, and an odd function for l odd. Similarly, β_l is an odd function of s for l even and an even function of s if l is odd. We prove these facts by expressing the generating functions of the α_l and β_l sequences in terms of hypergeometric series. In the second step of the proof, Section 3, we will show that as functions of s the α_l and β_l satisfy certain three-term recurrence relations. We then finish the proof in Section 4 by adapting the classical proof of the interlacing roots properties of sequences of orthogonal polynomials via Sturm sequences.

2. Expressing α_l and β_l in terms of $s = 2m + 1$. Introduce the new variable $s = 2m+1$, and write A_l for the polynomial in s obtained by substitution: $A_l(s) = \alpha_l((s-1)/2)$. Similarly, $B_l(s) = \beta_l((s-1)/2)$. In this section we will begin by deriving expressions

$$\sum_{l=0}^{\infty} A_l(s)\,\frac{u^l}{l!} = (1+2u)^{s/2}\,{}_2F_1\left(\frac{s}{2}+\frac{1}{4},\frac{1}{4};\,\frac{1}{2};\,4u^2\right)$$

and

$$\sum_{l=0}^{\infty} B_l(s)\,\frac{u^l}{l!} = u(1+2u)^{s/2}\,{}_2F_1\left(\frac{s}{2}+\frac{3}{4},\frac{3}{4};\,\frac{3}{2};\,4u^2\right).$$

These can certainly also be derived from the hypergeometric formula for the value of (1) given in Section 1, using the power series decomposition

$$f(u) = f_{\mathrm{even}}(u^2) + u f_{\mathrm{odd}}(u^2).$$

However, the method we will present leads to useful expressions for these generating functions with fewer manipulations.

We consider the $\alpha_l(m)$ first. Boros, Moll, and Shallit give the following formula:

$$\alpha_l(m) = \sum_{t=0}^{\lfloor l/2\rfloor} \binom{l}{2t} \prod_{\nu=m+1}^{m+t}(4\nu-1) \prod_{\nu=m-l+2t+1}^{m}(2\nu+1) \prod_{\nu=1}^{t-1}(4\nu+1). \tag{2}$$

Then, for instance,

$$\begin{aligned} A_4 = &\binom{4}{0}(s-6)(s-4)(s-2)s \\ &+ \binom{4}{2}(2s+1)(s-2)s \\ &+ \binom{4}{4}(2s+1)(2s+5)\cdot 5 \end{aligned}$$

and

$$\begin{aligned} A_5 = &\binom{5}{0}(s-8)(s-6)(s-4)(s-2)s \\ &+ \binom{5}{2}(2s+1)(s-4)(s-2)s \\ &+ \binom{5}{4}(2s+1)(2s+5)5s. \end{aligned}$$

To express the A_l in a more useful form, notice first that the products such as $(s-6)(s-4)(s-2)s$ in the first term in α_4 can be written as powers of 2 times (formal) binomial coefficients. For instance $(s-6)(s-4)(s-2)s = 2^4\binom{s/2}{4}$. Let

$$f(s,u) = \sum_{k=0}^{\infty} \binom{s/2}{k} (2u)^k.$$

For $|u| < 1/2$, this binomial series converges to $(1+2u)^{s/2}$. Second, consider the series

$$\begin{aligned} g(s,u) &= 1 + \frac{(2s+1)}{2!}\,u^2 + \frac{(2s+1)(2s+5)\cdot 5}{4!}\,u^4 + \cdots \\ &= \sum_{k=0}^{\infty} \left(\prod_{n=1}^{k} (2s+4n-3) \prod_{n=1}^{k} (4n-3) \right) \frac{u^{2k}}{(2k)!}. \end{aligned} \tag{3}$$

An easy argument shows the following result.

Proposition 1. *For each $l \geq 0$, A_l is equal to $l!$ times the coefficient of u^l in the product $f(s,u)g(s,u)$. In particular, A_l has degree exactly l.*

We know from the above that $f(s,u) = (1+2u)^{s/2}$ for suitable u. We can also recognize the series $g(s,u)$ as a ${}_2F_1$ hypergeometric series using the standard algorithm explained for example in [**5**, Section 3.3].

Proposition 2. *The series for $g(s,u)$ given in* (3) *is the hypergeometric series*

$${}_2F_1\left(\frac{s}{2} + \frac{1}{4}, \frac{1}{4}; \frac{1}{2}; 4u^2\right).$$

We are now ready to prove the following characterization of the form of the A_l.

Proposition 3. *A_l is an even function of s if l is even and an odd function of s if l is odd.*

Proof. Since the hypergeometric series $g(s,u)$ has only even powers of u, A_l for l even equals $l!$ times the coefficient of u^l in

$$h_{\text{even}}(s,u) = \left(\frac{(1+2u)^{s/2}+(1-2u)^{s/2}}{2}\right) {}_2F_1\left(\frac{s}{2}+\frac{1}{4}, \frac{1}{4}; \frac{1}{2}; 4u^2\right).$$

Apply the standard hypergeometric function transformation rule

$${}_2F_1(a,b;c;z) = (1-z)^{c-a-b}{}_2F_1(c-a, c-b; c; z)$$

and some elementary algebra on the first factor in h_{even} to see that

$$\begin{aligned}
&\frac{h_{\text{even}}(s,u)}{h_{\text{even}}(-s,u)} \\
&= \frac{\big([(1+2u)^{s/2}+(1-2u)^{s/2}]/2\big)\, {}_2F_1\big((s/2)+(1/4),(1/4);(1/2);4u^2\big)}{\big([(1+2u)^{-s/2}+(1-2u)^{-s/2}]/2\big)\, {}_2F_1((-s/2)+(1/4),(1/4);(1/2);4u^2)} \\
&= (1-4u^2)^{s/2} \frac{{}_2F_1\left((s/2)+(1/4),(1/4);(1/2);4u^2\right)}{(1-4u^2)^{s/2}{}_2F_1\left((s/2)+(1/4),(1/4);(1/2);4u^2\right)} \\
&= 1
\end{aligned}$$

This says every coefficient of h_{even} is an even polynomial in s.

Similarly, for l odd, A_l is $l!$ times the coefficient of u^l in

$$h_{\text{odd}}(s,u) = \left(\frac{(1+2u)^{s/2}-(1-2u)^{s/2}}{2}\right) {}_2F_1\left(\frac{s}{2}+\frac{1}{4}, \frac{1}{4}; \frac{1}{2}; 4u^2\right).$$

Proceeding as before we get

$$\frac{h_{\text{odd}}(s,u)}{h_{\text{odd}}(-s,u)} = -1,$$

so all the coefficients of h_{odd} are odd polynomials in s. □

The β_l are handled by a directly parallel argument starting from another formula from [**1**]:

(4)

$$\beta_l(m) = \sum_{t=1}^{\lfloor (l+1)/2 \rfloor} \binom{l}{2t-1} \prod_{\nu=m+1}^{m+t-1} (4\nu+1) \prod_{\nu=m-l+2t}^{m} (2\nu+1) \prod_{\nu=1}^{t-1} (4\nu-1).$$

As above we let $s = 2m+1$ and write B_l for the substituted polynomial $B_l(s) = \beta_l((s-1)/2)$.

Proposition 4. *For each $l \geq 0$, B_l is equal to $l!$ times the coefficient of u^l in the product $uf(s,u)G(s,u)$, where $f(s,u)$ is the binomial series expansion of $(1+2u)^{s/2}$ as before, and $G(s,u)$ is the hypergeometric series*

$$G(s,u) = {}_2F_1\left(\frac{s}{2} + \frac{3}{4}, \frac{3}{4}; \frac{3}{2}; 4u^2\right)$$

In particular, B_l has degree $l-1$. B_l is an even function of s if l is odd and an odd function of s if l is even.

The proof of the last claim is very similar to the proof of Proposition 3 and uses the same hypergeometric function transformation, so the details are omitted. The parity reversal is produced by the extra factor of u.

3. The three-term recurrences. In this section we will show that the sequences of polynomials A_l and B_l satisfy the three-term recurrences

$$A_{l+1}(s) = 2sA_l(s) - (s^2 - (2l-1)^2)A_{l-1}(s) \tag{5}$$

and

$$B_{l+1}(s) = 2sB_l(s) - (s^2 - (2l-1)^2)B_{l-1}(s) \tag{6}$$

for all $l \geq 1$. (Note that the A_l and B_l actually satisfy the same recurrence relation, but the initial terms A_0 and A_1 are different from B_0 and B_1, so the sequences of polynomials generated are different.)

Proposition 5. *The $A_l(s)$ satisfy the recurrence* (5) *for all $l \geq 1$.*

Proof. Suppressing the dependence on s, we will now write

$$h(u) = \sum_{l=0}^{\infty} A_l(s)\,\frac{u^l}{l!}$$

for the generating function of the A_l. As we saw in the previous section,

$$h(u) = (1+2u)^{s/2}{}_2F_1\left(\frac{s}{2}+\frac{1}{4}, \frac{1}{4}; \frac{1}{2}; 4u^2\right). \tag{7}$$

The recurrence (5) is satisfied if and only if $h(u)$ solves the following differential equation:

$$h''(u) - 2sh'(u) + s^2h(u) = \sum_{l=0}^{\infty}(2l+1)^2 A_l(s)\,\frac{u^l}{l!}. \tag{8}$$

We can manipulate the series for $h(u)$ as follows to reproduce the right side of (8). Setting $u = v^2$, we have

$$\begin{aligned} vh(v^2) &= \sum_{l=0}^{\infty} A_l(s)\,\frac{v^{2l+1}}{l!} \\ \Rightarrow (vh(v^2))' &= \sum_{l=0}^{\infty}(2l+1)A_l(s)\,\frac{v^{2l}}{l!} \\ \Rightarrow (v(vh(v^2))')' &= \sum_{l=0}^{\infty}(2l+1)^2A_l(s)\,\frac{v^{2l}}{l!} \\ &= \sum_{l=0}^{\infty}(2l+1)^2A_l(s)\,\frac{u^{l}}{l!} \end{aligned}$$

which is what we want. But

$$\begin{aligned} (v(vh(v^2))')' &= h(v^2) + 8v^2h'(v^2) + 4v^4h''(v^2) \\ &= h(u) + 8uh'(u) + 4u^2h''(u). \end{aligned}$$

So, the equation (8) is equivalent to:

$$(1-4u^2)h''(u) - (2s+8u)h'(u) + (s^2-1)h(u) = 0.$$

Direct computation shows that this differential equation is satisfied by the function $h(u)$ from (7). $\square$

The proof of the recurrence (6) for the B_l polynomials is entirely similar.

For future reference, we note the following patterns that follow by induction from the recurrences (5) and (6) and the equations $A_0 = 1$, $A_1 = s$, $B_0 = 0$, and $B_1 = 1$.

Corollary 1. *For all $l \geq 1$, the leading coefficient of A_l is 1 (A_l is monic), and the leading coefficient of B_l is l.*

4. The roots of $\alpha_l(m) = 0$ and $\beta_l(m) = 0$. We now want to use the results of the previous sections to deduce our main result on the roots of $\alpha_l(m) = 0$ and $\beta_l(m) = 0$. Under our first change of variables $s = 2m + 1$, the line $\Re(m) = -1/2$ corresponds to the imaginary axis $\Re(s) = 0$. Thus Boros, Moll, and Shallit's conjecture is equivalent to the statement that the nonzero roots of $A_l(s) = 0$ and $B_l(s) = 0$ are purely imaginary. In order to apply some standard results about location of roots of polynomials in their usual forms, we will next consider the following transformations of our polynomials. Let $s = it$ and

$$C_l(t) = (-i)^l A_l(it), \qquad D_l(t) = (-i)^{l-1} B_l(it). \tag{9}$$

Under this change of variables, the imaginary axis in the s-plane corresponds to the real axis in the t-plane. Boros, Moll, and Shallit's conjecture is now equivalent to the statement that the roots of $C_l(t) = 0$ and $D_l(t) = 0$ are all real. The constant multipliers $(-i)^l$ and $(-i)^{l-1}$ ensure that all the coefficients in C_l and D_l are real and that the leading coefficient of $C_l(t)$ is 1 for all l, while the leading coefficient of $D_l(t)$ is l for all l.

The recurrence relations (5) and (6) from Section 3 are equivalent to the following recurrences for $C_l(t)$ and $D_l(t)$:

$$C_{l+1}(t) = 2tC_l(t) - (t^2 + (2l-1)^2)C_{l-1}(t) \tag{10}$$

and

$$D_{l+1}(t) = 2tD_l(t) - (t^2 + (2l-1)^2)D_{l-1}(t) \tag{11}$$

(note the sign changes in the coefficients of C_{l-1} and D_{l-1} introduced by the powers of $-i$).

To set the stage, we recall that there is a well-known theorem of Favard which states that any sequence p_l of polynomials satisfying a three-term recurrence of the form:

$$p_{l+1}(t) = (a_l t + b_l)p_l(t) - c_l p_{l-1}(t)$$

with constant $a_l > 0, c_l > 0$ for all l is *orthogonal* with respect to some measure on an interval $[a, b]$. Hence all the roots of the polynomials are real and simple.

Because of the t^2 terms in the coefficients of the $C_{l-1}(t)$ and $D_{l-1}(t)$ in (10) and (11), Favard's theorem does not apply. However, it is possible to use the same sort of reasoning as that presented for instance in [**6**, Section 3.3] in the case of orthogonal polynomial sequences. Even though our C_l and D_l are not orthogonal sequences, they still have the same "interlacing roots" properties that orthogonal sequences do. The key step will be to see that the C_l and D_l satisfy the main property of *Sturm sequences*.

For the convenience of the reader, we include a very brief review of Sturm sequences and Sturm's Theorem on counting real roots of polynomials in an interval. See [**2**] or [**3**] for more details and the proof of Sturm's theorem.

A (general) Sturm sequence for a nonconstant polynomial $f \in \mathbf{R}[x]$ on the interval $[a, b]$ is any sequence of polynomials $f = g_l, g_{l-1}, g_{l-2}, \dots, g_1, g_0$ in $\mathbf{R}[x]$ such that

1. $f(a)f(b) \neq 0$
2. g_0 has no roots in $[a, b]$
3. If $a < c < b$ and $g_j(c) = 0$ for $j < l$, then $g_{j+1}(c)g_{j-1}(c) < 0$
4. If $a < c < b$ and $f(c) = 0$, then there is a neighborhood of c on which $f(x)g_{l-1}(x)$ has the same sign as $x - c$.

Sturm's theorem states that the number of real roots of f in the interval $[a, b]$ is equal to the number $V(a) - V(b)$ where $V(x)$ is the number of sign changes in the sequence of values $f(x), g_{l-1}(x), g_{l-2}(x), \dots, g_1(x), g_0(x)$.

Sturm's theorem is often stated (and most often used) in the specific case that the sequence of polynomials is obtained by letting $g_{l-1} = f'$ (the derivative), and the other polynomials are the *negatives* of the remainders on division following the Euclidean algorithm for the gcd. The theorem applies more generally to any sequence as above, though. There is also a criterion for all the roots of a polynomial to be real that is essentially a corollary of the proof of Sturm's theorem.

Corollary of proof of Sturm's theorem. *Let $f = g_l, g_{l-1}, \dots, g_1, g_0$ be a sequence of polynomials in $\mathbf{R}[x]$, satisfying $\deg(g_j) = j$ for all j, and whose leading coefficients are all positive. Assume that*

1. *No two consecutive polynomials in the chain have a common real zero, and*

2. *If $g_j(c) = 0$ for $0 < j < l$, then $g_{j+1}(c)g_{j-1}(c) < 0$.*

Then the polynomial f has $\deg(f)$ distinct real roots.

Proof. This is essentially [**3**, Chapter 5, Exercise 11], but we provide a proof for completeness. The number of sign changes in the sequence $f(x), g_{l-1}(x), \dots, g_0(x)$, denoted $V(x)$, can only change when x is a root of one of the g_j. By the hypotheses, g_0 is a positive constant, hence has no real roots. Moreover, as in the proof of the usual form of Sturm's theorem, if $x = c$ is a root of g_j, $0 < j < l$, V does not change at c because of the hypotheses 1 and 2. Hence V changes only at the roots of f. However, our hypotheses also imply that for very negative x there will be $l = \deg(f)$ sign changes in the sequence of values, while for very positive x there are no sign changes. Hence $V(-\infty) - V(+\infty) = l = deg(g_l)$. Hence $f = g_l$ must have l real roots. $\square$

We are now ready to state and prove the result that completes the proof of the main conjecture.

Theorem 1. *Let $C_l(t)$ and $D_l(t)$ be the polynomials given in* (9). *For each $l \geq 1$, the equation $C_l(t) = 0$ has $l = \deg(C_l)$ distinct real roots and $D_l(t) = 0$ has $l - 1 = \deg(D_l)$ distinct real roots.*

Proof. For each l, we will show that the sequence $C_j(t)$, with j starting from l and decreasing to 0, satisfies the hypotheses of the corollary above, and similarly for the $D_j(t)$, j starting from l and decreasing to 1, after a shift in indexing to satisfy the hypotheses of the corollary.

For condition 1 in the corollary, note that the recurrence relations (10) and (11) imply that if any two consecutive C_j have a common root t_0, then all the C_j have t_0 as a root. But that is not possible since the equation $C_0(t) = 0$ has no roots. Similarly for the D_j. The crucial condition 2 is satisfied because of the recurrence relation as well. For instance if $C_j(c) = 0$, then from (10)

$$C_{j+1}(c) = -(c^2 + (2j-1)^2)C_{j-1}(c)$$

which implies that the signs of $C_{j+1}(c)$ and $C_{j-1}(c)$ are opposite (because the sum of squares is strictly positive). Similarly for the D_j. $\square$

Moreover, it also follows that, between each consecutive pair of roots of C_l, there is precisely one root of C_{l-1}, and similarly for the D_j. In other words, the roots of the C_j and D_j polynomials have the same "interlacing" properties that roots of sequences of orthogonal polynomials have.

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