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On Polynomials Related With Hermite–Padé Approximations to the Exponential Function

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ABSTRACT

We investigate the polynomials P_n , Q_m and R_s , having degrees n , m and s respectively, with P_n monic, that solve the approximation problem

$$E_{nms}(x) := P_n(x)e^{-2x} + Q_m(x)e^{-x} + R_s(x) = O(x^{n+m+s+2}) \quad \text{as } x \rightarrow 0.$$

We give a connection between the coefficients of each of the polynomials P_n , Q_m and R_s and certain hypergeometric functions, which leads to a simple expression for Q_m in the case $n = s$. The approximate location of the zeros of Q_m , when $n \gg m$ and $n = s$, are deduced from the zeros of the classical Hermite polynomial. Contour integral representations of P_n , Q_m , R_s and E_{nms} are given and, using saddle point methods, we derive the exact asymptotics of P_n , Q_m and R_s as n , m and s tend to infinity through certain ray sequences. We also discuss aspects of the more complicated uniform asymptotic methods for obtaining insight into the zero distribution of the polynomials, and we give an example showing the zeros of the polynomials P_n , Q_m and R_s for the case $n = s = 40$, $m = 45$.

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1. Introduction

Hermite–Padé approximation to the exponential function was introduced by HERMITE (1883) who considered expressions of the form

$$p_k(x)e^{s_k x} + p_{k-1}(x)e^{s_{k-1} x} + \dots + p_1(x)e^{s_1 x} = \mathcal{O}(x^h) \quad \text{as } x \rightarrow 0, \quad (1.1)$$

where p_1, \dots, p_k are polynomials of specified degrees, chosen so that h is as large as possible. Hermite's investigation of expressions of type (1.1) were motivated by problems arising in number theory and led to his proof of the transcendence of e . The formal theory of the two types of Hermite–Padé polynomials that arise from expressions of type (1.1) was developed by Mahler (cf. MAHLER (1967)) and has yielded many successful applications to number theory on the one hand and approximation theory on the other. Excellent historical surveys on the development and applications of Hermite–Padé polynomial theory and further references can be found in APTEKAREV & STAHL (1992) and DE BRUIN (1990).

Included in expressions of the type (1.1) is the ordinary Padé approximation problem for the exponential function, namely, given any positive integers m and n , find polynomials \hat{P}_n and \hat{Q}_m with $\deg(\hat{P}_n) \leq n$, $\deg(\hat{Q}_m) \leq m$, $\hat{Q}_m \neq 0$, such that

$$\hat{E}_{mn}(x) := \hat{Q}_m(x)e^{-x} + \hat{P}_n(x) = \mathcal{O}(x^{m+n+1}) \quad \text{as } x \rightarrow 0. \quad (1.2)$$

A solution to this problem always exists and the polynomials \hat{P}_n and \hat{Q}_m (which are unique, up to normalization) have been thoroughly investigated by SAFF & VARGA (1978), who obtained, inter alia, the distribution of the zeros of \hat{P}_n and \hat{Q}_m , as well as those of the remainder term \hat{E}_{mn} .

In this paper, we investigate a number of properties of the polynomials P_n , Q_m and R_s that arise from the solution of the quadratic Hermite–Padé Type I approximation problem, which may be formulated as follows. Given arbitrary positive integers n , m and s , find polynomials P_n , Q_m and R_s , with P_n monic, such that

$$E_{nms}(x) := P_n(x)e^{-2x} + Q_m(x)e^{-x} + R_s(x) = \mathcal{O}(x^{n+m+s+2}) \quad \text{as } x \rightarrow 0. \quad (1.3)$$

The explicit formulae for these (unique) polynomials are known; in the super-diagonal case $n = m = s$, they were obtained by BORWEIN (1986) and for arbitrary n , m and $s \in \mathbb{N}$, they can be found in DRIVER (1995).

We organize the paper as follows. In Section 2, we prove and exploit a connection between the coefficients of the polynomials P_n , Q_m and R_s and certain hypergeometric functions. For the case $n = s$, $m \in \mathbb{N}$ arbitrary, a simple closed form for Q_m is given, as well as the approximate location of the zeros of Q_m when $n = s$ and $n \gg m$. Section 3 contains contour integral representations of P_n , Q_m and R_s and we apply saddle point methods to obtain the asymptotic behaviour as $n \rightarrow \infty$ of P_n , Q_m and R_s where $m \sim \alpha n$ and $s \sim \beta n$. In Section 4, we discuss aspects of the more complicated uniform asymptotic methods for obtaining insight into the zero distribution of the polynomials P_n , Q_m and R_s . In addition, we present more details on this point by showing a picture of the zero distribution of the polynomials for the case $n = s = 40$, $m = 45$.

At several places we use properties of special functions and orthogonal polynomials for which we refer to TEMME (1996); all information of this kind can also be found in, for instance, ABRAMOWITZ & STEGUN (1964).

2. The polynomials P_n , Q_m and R_s

The polynomials P_n , Q_m and R_s with $\deg(P_n) = n$, $\deg(Q_m) = m$, $\deg(R_s) = s$, P_n monic, that satisfy (1.3) are given by (cf. DRIVER (1995, eqns. (2.9), (2.12), (2.19))

$$P_n(x) = n! \sum_{j=0}^n \frac{p_j x^j}{j!}, \quad (2.1)$$

where

$$p_j = \sum_{k=0}^{n-j} \binom{m+n-k-j}{m} \binom{s+k}{s} 2^{-k} \quad \text{for } j = 0, \dots, n. \quad (2.2)$$

$$Q_m(x) = -2^{s+1} n! \sum_{j=0}^m \frac{q_j x^j}{j!}, \quad (2.3)$$

where

$$q_j = \sum_{k=0}^{m-j} (-1)^{k+j} \binom{m+n-k-j}{n} \binom{s+k}{s} 2^{-k} \quad \text{for } j = 0, \dots, m. \quad (2.4)$$

$$R_s(x) = 2^{s-n} n! (-1)^m \sum_{j=0}^s \frac{r_j x^j}{j!}, \quad (2.5)$$

where

$$r_j = \sum_{k=0}^{s-j} (-1)^j \binom{m+s-k-j}{m} \binom{n+k}{n} 2^{-k} \quad \text{for } j = 0, \dots, s. \quad (2.6)$$

We observe that each of the polynomials P_n , Q_m and R_s depends on all three positive integers n , m and s and the subscript merely denotes the degree of the polynomial in each case. Writing $P_n(x) = P(n, m, s; x)$, $Q_m(x) = Q(n, m, s; x)$ and $R_s(x) = R(n, m, s; x)$, the following symmetries follow immediately from (2.1) — (2.6).

$$P(s, m, n; -x) = \frac{(-1)^m 2^{n-s} s!}{n!} R(n, m, s; x) \quad (2.7)$$

and

$$Q(s, m, n; -x) = \frac{(-1)^m 2^{n-s} s!}{n!} Q(n, m, s; x). \quad (2.8)$$

It is evident from (2.7) that any information regarding the polynomial P_n immediately yields corresponding results about the polynomial R_s , whereas (2.8) tells us that when $n = s$, Q_m is an even (odd) polynomial in x when m is even (odd).

Our first result establishes a connection between the coefficients of P_n , Q_m and R_s and certain ${}_2F_1$ hypergeometric functions. We recall the definition of the Gauss function

$${}_2F_1(a, b; c; z) := \sum_{k=0}^{\infty} \frac{(a)_k (b)_k z^k}{(c)_k k!}, \quad (2.9)$$

where

$$(\alpha)_k := \begin{cases} \alpha(\alpha+1)\dots(\alpha+k-1) = \Gamma(\alpha+k)/\Gamma(\alpha), & \text{if } k \geq 1, \\ 1, & \text{if } \alpha \neq 0, k = 0. \end{cases} \quad (2.10)$$

If $t \in \mathbb{N}$, it follows immediately from (2.10) that

$$(-t)_k = \begin{cases} (-1)^k t! / (t-k)! & \text{for } 0 \leq k \leq t, \\ 0 & \text{for } k > t. \end{cases} \quad (2.11)$$

Therefore, the hypergeometric series ${}_2F_1(-t, b; c; z)$, $t \in \mathbb{N}$, is a polynomial of degree t in z and, from (2.10) and (2.11), we have for $b, c \in \mathbb{N}$,

$${}_2F_1(-t, b+1; c+1; z) = \sum_{k=0}^t \binom{t}{k} \frac{(b+k)! c!}{b! (c+k)!} (-z)^k. \quad (2.12)$$

Theorem 2.1. *Let p_j , q_j and r_j be given by (2.2), (2.4) and (2.6) respectively. Then*

$$p_j = \binom{n+m-j}{m} {}_2F_1\left(j-n, s+1; j-n-m; \frac{1}{2}\right), \quad j = 0, 1, \dots, n, \quad (2.13a)$$

$$q_j = (-1)^j \binom{n+m-j}{n} {}_2F_1\left(j-m, s+1; j-n-m; -1\right), \quad j = 0, 1, \dots, m, \quad (2.14a)$$

$$r_j = (-1)^j \binom{s+m-j}{m} {}_2F_1\left(j-s, n+1; j-s-m; \frac{1}{2}\right), \quad j = 0, 1, \dots, s, \quad (2.15a)$$

Another way of writing is:

$$p_j = \binom{n+m+s+1-j}{n-j} {}_2F_1\left(j-n, s+1; m+s+2; \frac{1}{2}\right), \quad j = 0, 1, \dots, n, \quad (2.13b)$$

$$q_j = (-1)^j \binom{n+m+s+1-j}{m-j} {}_2F_1\left(j-m, s+1; n+s+2; 2\right), \quad j = 0, 1, \dots, m, \quad (2.14b)$$

$$r_j = (-1)^j \binom{n+m+s+1-j}{s-j} {}_2F_1\left(j-s, n+1; n+m+2; \frac{1}{2}\right), \quad j = 0, 1, \dots, s, \quad (2.15b)$$

As an immediate consequence of Theorem 2.1, we can express the coefficients p_j , q_j and r_j as the constant terms in appropriate Jacobi polynomials.

Corollary 2.1. *For any $n, m, s \in \mathbb{N}$, if $\mathcal{P}_k^{(\alpha, \beta)}$ denotes the Jacobi polynomial of degree k with parameters α and β , then*

$$p_j = \mathcal{P}_{n-j}^{(m+s+1, j-m-n-1)}(0), \quad (2.16)$$

$$q_j = 2^{m-j} (-1)^m \mathcal{P}_{m-j}^{(j-m-n-1, j-m-s-1)}(0), \quad (2.17)$$

$$r_j = (-1)^j \mathcal{P}_{s-j}^{(m+n+1, j-m-s-1)}(0). \quad (2.18)$$

Unfortunately, the value of the constant term in the Jacobi polynomial $\mathcal{P}_k^{(\alpha, \beta)}(x)$ is not known in general. However, when $n = s$, the coefficients q_j , and therefore the polynomial Q_m , can be expressed in a simple form.

Theorem 2.2. *Let q_j and Q_m be given by (2.14a) and (2.3) respectively. Suppose that*

$$n = s \in \mathbb{N} \quad \text{and} \quad m \in \mathbb{N} \quad \text{is arbitrary.} \quad (2.19)$$

(a) For $j = 0, \dots, m$, we have

$$q_j = \begin{cases} 0 & \text{for } m - j \text{ odd,} \\ (-1)^j \binom{n+(m-j)/2}{n} & \text{for } m - j \text{ even} \end{cases}. \quad (2.20)$$

(b) We have

$$Q_m(x) = (-1)^{m+1} 2^{n+1} \sum_{k=0}^{\lfloor m/2 \rfloor} \frac{(n+k)!}{k!} \frac{x^{m-2k}}{(m-2k)!}, \quad (2.21)$$

where $\lfloor p \rfloor$ is the integer satisfying $\lfloor p \rfloor \leq p < \lfloor p \rfloor + 1$, with $p \in \mathbb{R}$.

(c) For m even, $m = 2p$, $p \in \mathbb{N}$, we have

$$Q_m(x) = Q_{2p}(x) = -2^{n+1} \frac{(n+p)!}{p!} {}_1F_2 \left(-p; -n-p, \frac{1}{2}; \frac{x^2}{4} \right), \quad (2.22)$$

while, for m odd, $m = 2p+1$, $p \in \mathbb{N}$, we have

$$Q_m(x) = Q_{2p+1}(x) = 2^{n+1} \frac{(n+p)!}{p!} x {}_1F_2 \left(-p; -n-p, \frac{3}{2}; \frac{x^2}{4} \right). \quad (2.23)$$

Remarks 2.1.

[1] The hypergeometric function ${}_1F_2(a; b, c; z)$ that occurs in (2.22) and (2.23) is defined by

$${}_1F_2(a; b, c; z) := \sum_{k=0}^{\infty} \frac{(a)_k z^k}{(b)_k (c)_k k!}, \quad (2.24)$$

where $(\alpha)_k$ is defined in (2.10). Using (2.11), we see that the F -functions in (2.22) and (2.23) are each polynomials of degree p in the variable $x^2/4$. The even (odd) nature of $Q_m(x)$ when m is even (odd) and $n = s$ observed in (2.8) is therefore also apparent from (2.22) and (2.23).

[2] The assumption (2.19) that $n = s$ is restrictive. However, it can be shown that, for general $n, m, s \in \mathbb{N}$, alternate coefficients of Q_m involve a factor $(n-s)$ and are zero only when (2.19) holds. No simple closed form of Q_m seems possible in the general case.

zeros of Q_{10}	approximations	relative errors
3.44274827 i	3.06700270 i	0.12
10.32157031 i	9.27172912 i	0.11
17.17259049 i	15.71225622 i	0.09
23.93313689 i	22.65344077 i	0.06
30.06525844 i	30.73394148 i	0.02

Table 2.1. Zeros on the positive imaginary axis of Q_{10} , with $n = s = 20$, compared with the approximations obtained from (2.26).

Some information regarding the approximate location of the zeros of the polynomial $Q_m(x)$ when n is much larger than m and $n = s$, can be obtained from (2.21) by comparing $Q_m(x)$ with the Hermite polynomial

$$H_m(x) = m! \sum_{k=0}^{\lfloor m/2 \rfloor} \frac{(-1)^k (2x)^{m-2k}}{k! (m-2k)!}. \quad (2.25)$$

We have the following corollary.

Corollary 2.2. *With the assumptions of Theorem 2.2, when $n \gg m$,*

$$Q_m(x) = -2^{n+1} \frac{n!}{m!} i^m n^{m/2} \left[H_m \left(\frac{1}{2} i x / \sqrt{n} \right) + \mathcal{O}(1/n) \right], \quad (2.26)$$

and hence the zeros of $Q_m(x)$ lie approximately in the interval $(-2i\sqrt{n(m+1)}, 2i\sqrt{n(m+1)})$ on the imaginary axis.

Table 2.1 shows the zeros of Q_{10} on the positive imaginary axis with $n = s = 20$, compared with the approximations obtained from the zeros of the Hermite polynomial.

The connection between the coefficients of the polynomials P_n (and R_s) and the hypergeometric functions given by (2.13a) (and (2.15a)), does not seem to provide the same degree of simplification obtained for the coefficients of Q_m , perhaps because the p_j 's are intrinsically more complicated. However, it is possible to obtain exact closed expressions for the first two coefficients p_0 and p_1 , as well as the recurrence relation satisfied by the p_j 's. We have the following result:

Theorem 2.3. Suppose that p_j is given by (2.13a) for $j = 0, \dots, n$ and that $n = s$ while $m \in \mathbb{N}$ is arbitrary. For any $m, n \in \mathbb{N}$, let

$$D(m, n) := (m + 2n)(m + 2n - 2) \dots (m + 2). \quad (2.27)$$

Then

$$p_0 = D(m, n)/n!, \quad (2.28)$$

$$p_1 = [D(m, n) - D(m - 1, n)]/n!, \quad (2.29)$$

and for $j = 2, \dots, n$, we have

$$p_j = \frac{2}{(2n + m - j + 2)} \left\{ \left(2n + m + 3 - \frac{3j}{2} \right) p_{j-1} - (n - j - 2) p_{j-2} \right\}. \quad (2.30)$$

Remarks 2.2.

- (1) When $m = n = s$, we see from (2.28) that $p_0 = 3m(3m - 2) \dots (m + 2)/m!$ for all $m \in \mathbb{N}$. This gives an exact expression in place of the asymptotic $p_0 \sim 3m(3m - 2) \dots (m + 2)/m!$ obtained in BORWEIN (1986), in particular Proposition 3(a) with $x = 0$.
- (2) For m even, say $m = 2p$, we have from (2.27) and (2.28) that

$$p_0 = 2^n \binom{n + p}{n}.$$

2.1. Proofs of the theorems and corollaries

Proof of Theorem 2.1. From (2.2) with $n - j = t$, (2.11) and (2.24) we have, for $0 \leq t \leq n$,

$$p_j = \sum_{k=0}^t \frac{(m + t - k)! (s + k)!}{m! s! k! (t - k)!} 2^{-k} = \frac{(m + t)!}{m! t!} \sum_{k=0}^t \frac{(-t)_k (s + 1)_k}{(-m - t)_k k!} 2^{-k}, \quad (2.31)$$

from which (2.13a) immediately follows. The identities (2.14a) and (2.15a) follow from the same method. In general the function ${}_2F_1(a, b; c; z)$ is not defined if $c = 0, -1, -2, \dots$, but in (2.13a) - (2.15a) the a -parameter equals also a non-positive integer value, with $|a| \leq |c|$. In that case the F -function is well-defined. We use a well-known transformation of the F -function to obtain (2.13b) - (2.15b), where the c -parameter is a positive integer and which are more convenient representations. We use (cf. TEMME (1996, page 113))

$${}_2F_1(a, b; c; z) = \frac{\Gamma(c) \Gamma(c - a - b)}{\Gamma(c - a) \Gamma(c - b)} {}_2F_1(a, b; a + b - c + 1; 1 - z), \quad a = 0, -1, -2, \dots \quad (2.32)$$

Applying this formula to (2.13a) - (2.15a) we observe that all arguments in the gamma functions in front of the F -function in (2.32) become equal to non-positive integers. Hence,

some care is needed in applying the transformation. To verify (2.13a) \rightarrow (2.13b) we use the property

$$\frac{\Gamma(z)}{\Gamma(z-k)} = (-1)^k \frac{\Gamma(1-z)}{\Gamma(k+1-z)}, \quad k = 0, 1, 2, \dots$$

and introduce a small parameter ε . That is, we write using $a = j - n, b = s + 1, c = j - n - m$,

$$\frac{\Gamma(c) \Gamma(c - a - b)}{\Gamma(c - a) \Gamma(c - b)} = \lim_{\varepsilon \rightarrow 0} \frac{\Gamma(c + \varepsilon) \Gamma(c + \varepsilon - a - b)}{\Gamma(c + \varepsilon - a) \Gamma(c + \varepsilon - b)} = \frac{\Gamma(m + 1) \Gamma(n + m + s - j + 1)}{\Gamma(n + m - j + 1) \Gamma(m + s + 2)}.$$

This gives the result in (2.13b). The results for q_j and r_j follow in a similar way. \blacksquare

Proof of Corollary 2.1. We have (cf. TEMME (1996, page 151))

$$\mathcal{P}_n^{(\alpha, \beta)}(x) = \binom{n + \alpha}{n} {}_2F_1 \left(-n, \alpha + \beta + n + 1; \alpha + 1; \frac{1 - x}{2} \right). \quad (2.33)$$

It follows from (2.13b) and (2.33) with $\alpha = m + s + 1, \beta = j - m - n - 1$, and $x = \frac{1}{2}$, that

$$p_j = \mathcal{P}_{n-j}^{(m+s+1, j-m-n-1)}(0),$$

Then (2.16) follows in the same manner. The relation for q_j follows from applying (cf. TEMME (1996, page 110))

$${}_2F_1(a, b; c; z) = (1 - z)^{-a} {}_2F_1 \left(a, c - b; c; \frac{z}{z - 1} \right), \quad (2.34)$$

which transforms the F -function with argument -1 into one with argument $\frac{1}{2}$. A few manipulations with binomial coefficients and gamma functions (again with negative integer arguments) give the proof of (2.17). \blacksquare

Proof of Theorem 2.2.

(a) From (2.17) with $n = s$, we have, for $j = 0, \dots, m$,

$$q_j = (-1)^m 2^{m-j} \mathcal{P}_{m-j}^{(j-m-s-1, j-m-s-1)}(0),$$

The parameters in the Jacobi polynomial are equal, and hence the Jacobi polynomial reduces to a Gegenbauer polynomial (cf. TEMME (1996, page 152)):

$$C_k^\gamma(x) = \frac{(2\gamma)_k}{(\gamma + \frac{1}{2})_k} \mathcal{P}_k^{(\gamma - \frac{1}{2}, \gamma - \frac{1}{2})}(x),$$

which vanishes at $x = 0$ when k is odd. For $(m - j)$ even, say $m - j = 2k$, we use

$$C_{2k}^\gamma(0) = \frac{(-1)^k}{\Gamma(\gamma)} \frac{\Gamma(k + \gamma)}{k!},$$

which gives with $\gamma = -n - 2k - \frac{1}{2}$, after using standard properties of the gamma function,

$$q_j = (-1)^j \binom{n+k}{n}.$$

In particular we have used (2.11) and the duplication formula

$$\sqrt{\pi} \Gamma(2z) = 2^{2z-1} \Gamma(z) \Gamma\left(z + \frac{1}{2}\right). \quad (2.35)$$

(b) From (2.3) with $n = s$, and (2.20), we have

$$Q_m(x) = -2^{n+1} n! \sum_{j=0}^m \frac{q_j x^j}{j!},$$

where

$$q_j = \begin{cases} 0 & \text{for } m-j \text{ odd,} \\ (-1)^j \binom{n+(m-j)/2}{n} & \text{for } m-j \text{ even.} \end{cases}$$

Therefore, for m even, say $m = 2p$, it follows that

$$\begin{aligned} Q_m(x) &= Q_{2p}(x) = -2^{n+1} n! \sum_{k=0}^p \binom{n+p-k}{n} \frac{x^{2k}}{(2k)!} \\ &= -2^{n+1} \sum_{k=0}^p \frac{(n+p-k)!}{(p-k)!} \frac{x^{2k}}{(2k)!}. \end{aligned}$$

Reversing the order of summation yields that, for m even,

$$Q_m(x) = -2^{n+1} \sum_{k=0}^{m/2} \frac{(n+k)!}{k!} \frac{x^{m-2k}}{(m-2k)!}. \quad (2.36)$$

Similarly, for m odd,

$$Q_m(x) = 2^{n+1} \sum_{k=0}^{(m-1)/2} \frac{(n+k)!}{k!} \frac{x^{m-2k}}{(m-2k)!}, \quad (2.37)$$

and combining (2.36) and (2.37), we obtain (2.21).

(c) From the definition (2.24), we have

$${}_1F_2\left(-p; -n-p, \frac{1}{2}; \frac{x^2}{4}\right) = \sum_{k=0}^{\infty} \frac{(-p)_k}{(-n-p)_k \left(\frac{1}{2}\right)_k} \frac{x^{2k}}{k! 2^{2k}}. \quad (2.38)$$

Using (2.10) and (2.11), a simple calculation shows that

$$\frac{(-p)_k}{(-n-p)_k \left(\frac{1}{2}\right)_k k! 2^{2k}} = \begin{cases} \frac{p! (n+p-k)!}{(n+p)! (p-k)! (2k)!}, & 0 \leq k \leq p, \\ 0, & k > p. \end{cases} \quad (2.39)$$

Therefore, from (2.38) and (2.39), we obtain

$${}_1F_2 \left(-p; -n-p, \frac{1}{2}; \frac{x^2}{4} \right) = \frac{p!}{(n+p)!} \sum_{k=0}^p \frac{(n+p-k)! x^{2k}}{(p-k)! (2k)!}, \quad (2.40)$$

and (2.22) follows from (2.43) and (2.40). Similarly,

$${}_1F_2 \left(-p; -n-p, \frac{3}{2}; \frac{x^2}{4} \right) = \frac{p!}{(n+p)!} \sum_{k=0}^p \frac{(n+p-k)!}{(p-k)!} \frac{x^{2k}}{(2k+1)!}, \quad (2.41)$$

and (2.23) follows from (2.45) and (2.41). ■

Proof of Corollary 2.2. For each k , $k = 0, \dots, \lfloor m/2 \rfloor$, if n is large compared with m , we have (cf. TEMME (1996, page 67))

$$\frac{(n+k)!}{n!} = n^k \left[1 + \frac{k(k+1)}{2n} + \mathcal{O}(n^{-2}) \right].$$

Therefore, for $n \gg m$, it follows from (2.21) that

$$Q_m(x) = (-1)^{m+1} 2^{n+1} n! n^{m/2} \left[\sum_{k=0}^{\lfloor m/2 \rfloor} \frac{n^{k-m/2} x^{m-2k}}{k! (m-2k)!} + \mathcal{O}(1/n) \right]. \quad (2.42)$$

Comparing (2.42) with the Hermite polynomial $H_m(x)$ given in (2.25), we see that, for $n \gg m$,

$$Q_m(x) = -2^{n+1} \frac{n!}{m!} i^m n^{m/2} [H_m(\frac{1}{2}ix/\sqrt{n}) + \mathcal{O}(1/n)]. \quad (2.43)$$

Since it is well known (cf. TEMME (1996, page 168)) that the zeros of the Hermite polynomial $H_m(x)$ lie in the real interval $(-\sqrt{2m+1}, \sqrt{2m+1})$, we deduce from (2.43) that the zeros of $Q_m(x)$ for $n \gg m$ lie approximately in the interval $(-2\sqrt{n(m+1)}i, 2\sqrt{n(m+1)}i)$ on the imaginary axis. ■

Proof of Theorem 2.3. Putting $n = s$ and $j = 0$ in (2.13b) we have

$$p_0 = \binom{m+2n+1}{n} {}_2F_1 \left(-n, n+1; m+n+2; \frac{1}{2} \right). \quad (2.44)$$

Applying (2.34), we obtain

$$p_0 = \binom{m+2n+1}{n} 2^{-n} {}_2F_1 \left(-n, m+1; m+n+2; -1 \right).$$

Now, (cf. TEMME (1996, page 129)),

$${}_2F_1(a, b; b - a + 1; -1) = \sqrt{\pi} \frac{2^{-b} \Gamma(b - a + 1)}{\Gamma(1 + \frac{1}{2}b - a) \Gamma(\frac{1}{2} + \frac{1}{2}b)}. \quad (2.45)$$

Therefore, from (2.44) and (2.45) with $a = -n$, $b = m + 1$, and from the duplication formula (2.35), it follows that

$$p_0 = \frac{2^n \Gamma(n + \frac{1}{2}m + 1)}{n! \Gamma(\frac{1}{2}m + 1)} = \frac{1}{n!} D(m, n).$$

This yields (2.28). Next, putting $n = s$ and $j = 1$ in (2.13a), we obtain

$$p_1 = \frac{(m + 2n)!}{(m + n + 1)! (n - 1)!} {}_2F_1(-n + 1, n + 1; m + n + 2; \frac{1}{2}). \quad (2.46)$$

Denoting ${}_2F_1(a, b; c; z)$ by ${}_2F_1$; ${}_2F_1(a + 1, b; c; z)$ by ${}_2F_1(a+)$ and so on, we have the contiguous hypergeometric function relation (cf. TEMME (1996, page 122))

$$(b - a)(1 - z) {}_2F_1 = (c - a) {}_2F_1(a-) - (c - b) {}_2F_1(b-). \quad (2.47)$$

With $a = -n + 1$, $b = n + 1$, $c = m + n + 2$, $z = \frac{1}{2}$, (2.47) becomes

$$\begin{aligned} n {}_2F_1(-n + 1, n + 1; m + n + 2; \frac{1}{2}) &= \\ &= (m + 2n + 1) {}_2F_1(-n, n + 1; m + n + 2; \frac{1}{2}) \\ &- (m + 1) {}_2F_1(-n + 1, n; m + n + 2; \frac{1}{2}). \end{aligned} \quad (2.48)$$

Applying (2.34) on the final F -function in (2.48) and (2.45) we obtain

$${}_2F_1(-n + 1, n; m + n + 2; \frac{1}{2}) = \frac{(m + n + 1)!}{(m + 1)! D(m, n)}. \quad (2.49)$$

From (2.46), (2.48), (2.49) and (2.44), it follows that

$$\frac{n! (m + n + 1)!}{(m + 2n)!} p_1 = \frac{n! (m + n + 1)!}{(m + 2n)!} p_0 - \frac{(m + n + 1)!}{m! D(m, n)},$$

whence we obtain (2.29). Finally, from (2.13a) with $n = s$, we have for $j = 0, \dots, n$,

$$p_j = \frac{(m + 2n - j + 1)!}{(m + n + 1)! (n - j)!} {}_2F_1(-n + j, n + 1; m + n + 2; \frac{1}{2}).$$

Therefore, using the contiguous function relation (cf. TEMME (1996, page 122))

$$a(1 - z) {}_2F_1(a+) = [2a - c + (b - a)z] {}_2F_1 + (c - a) {}_2F_1(a-),$$

we obtain (2.30). ■

3. Contour integral representations and asymptotics

The polynomials P_n , Q_m and R_s that satisfy (1.3), and are given by (2.1) — (2.6), admit simple contour integral representations. In the super-diagonal case $n = m = s$, these representations were already known to Mahler (cf. MAHLER (1967)).

Theorem 3.1. *Let n , m and s be arbitrary positive integers and let C be a circle, centre the origin, radius $r \in (0, 1)$. Let $P_n(x)$, $Q_m(x)$ and $R_s(x)$ be the polynomials given by (2.1), (2.3) and (2.5) respectively. Then*

$$P_n(x) = \frac{2^{s+1}(-1)^n n!}{2\pi i} \oint_C \frac{e^{-xv}}{v^{n+1}(v+1)^{m+1}(v+2)^{s+1}} dv, \quad (3.1)$$

$$Q_m(x) = \frac{2^{s+1}(-1)^{m+1} n!}{2\pi i} \oint_C \frac{e^{xv}}{v^{m+1}(v+1)^{n+1}(1-v)^{s+1}} dv, \quad (3.2)$$

$$R_s(x) = \frac{2^{s+1}(-1)^{m+s} n!}{2\pi i} \oint_C \frac{e^{xv}}{v^{s+1}(v+1)^{m+1}(v+2)^{n+1}} dv. \quad (3.3)$$

Proof. Expanding $e^{\pm xv}$ in its Maclaurin series and using Cauchy's integral theorem and Leibniz' rule, a comparison of the coefficients of powers of x on the right hand sides of (3.1), (3.2) and (3.3) with (2.2), (2.4) and (2.6) respectively, proves the result. ■

In order to analyse the asymptotic behaviour of the polynomials $P_n(x)$, $Q_m(x)$ and $R_s(x)$ given by (3.1), (3.2) and (3.3) respectively, we let

$$N = n + 1, \quad M = m + 1, \quad S = s + 1, \quad (3.4)$$

and assume that all these parameters are large. We write

$$M = \alpha N \quad \text{and} \quad S = \beta N, \quad (3.5)$$

where α and β are real, positive constants. We write (3.1) in the form:

$$P_n(x) = \frac{2^{s+1}(-1)^n n!}{2\pi i} \oint_C e^{-N\widehat{p}(v)} e^{-xv} dv, \quad (3.6)$$

where

$$\widehat{p}(v) := \ln[v(v+1)^\alpha(v+2)^\beta]. \quad (3.7)$$

Applying the saddle point method (cf. OLIVER (1974, §7.3, Theorem 7.1)) to the integral in (3.6), a simple calculation shows that for all real, positive values of α and β , $\widehat{p}(v)$ has derivative equal to zero at a point, say v_0 , lying in $(-1, 0)$, and at another point to the left

of -1 . The contour C can be chosen to run through v_0 . Moreover, $\hat{p}''(v_0) \neq 0$ and, in fact, $\hat{p}''(v_0)$ is real and negative for all $\alpha, \beta > 0$. Therefore, as $N \rightarrow \infty$, we deduce from (3.6) that (cf. OLVER (1974, Theorem 7.1)),

$$P_n(x) \sim \frac{2^{s+1}(-1)^n n!}{2\pi i} 2e^{-N\hat{p}(v_0)} \sqrt{\frac{\pi}{N}} \frac{e^{-xv_0}}{(2\hat{p}''(v_0))^{1/2}}, \quad (3.8)$$

where if $\hat{p}''(v_0) = -k_0^2$ say, $k_0 > 0$, we choose the branch of $(2\hat{p}''(v_0))^{1/2} = i\sqrt{2}k_0$, in accordance with (cf. OLVER (1974, eqn. 7.07)). In Theorem 3.2 more details are given for a special case.

Similarly, for $Q_m(x)$, we have from (3.2)

$$Q_m(x) = \frac{2^{s+1}(-1)^{m+1} n!}{2\pi i} \oint_C e^{-N\hat{q}(v)} e^{xv} dv, \quad (3.9)$$

where

$$\hat{q}(v) := \ln[v^\alpha(v+1)(1-v)^\beta]. \quad (3.10)$$

In this case we can choose C to run through two saddle points: $\hat{q}(v)$ has derivative equal to zero at two distinct points, $v_1 \in (-1, 0)$ and $v_2 \in (0, 1)$ for all $\alpha, \beta > 0$.

The asymptotic formulae for P_n , Q_m and R_s are rather cumbersome arithmetically for arbitrary $\alpha, \beta > 0$. We shall, therefore, restrict ourselves to the (rather natural) case when $\beta = 1$ in (3.5), although the method works for all $\alpha, \beta > 0$.

Theorem 3.2. *Let $P_n(x)$, $Q_m(x)$ and $R_s(x)$ be given by (3.1), (3.2) and (3.3) respectively, and assume that (3.5) holds with $\beta = 1$. Set*

$$\begin{aligned} \rho &:= \sqrt{\frac{\alpha}{\alpha+2}}, \\ D_{n,\alpha} &:= \rho^{1-\alpha} (2n + \alpha n)(2n + \alpha n - 2) \dots (\alpha n + 2). \end{aligned} \quad (3.11)$$

Then, as $n \rightarrow \infty$, we have

$$P_n(x) \sim D_{n,\alpha} e^{x(1-\rho)}, \quad (3.12)$$

$$Q_m(x) \sim (-1)^{m+1} D_{n,\alpha} [e^{x\rho} + (-1)^m e^{-x\rho}], \quad (3.13)$$

$$R_s(x) \sim (-1)^m D_{n,\alpha} e^{-x(1-\rho)}. \quad (3.14)$$

The asymptotics are uniform with respect to x on compact subsets of \mathbb{C} .

Remark 3.1. When $\alpha = 1$, we see from (3.11) that $D_{n,1} = 3n(3n-2) \dots (n+2)$, while $\rho = \frac{1}{\sqrt{3}}$. The asymptotics (3.12), (3.13) and (3.14) then agree exactly with the asymptotics

for the polynomials in the diagonal case (cf. BORWEIN (1986, Proposition 3)), obtained by a different method.

Proof. Putting $\beta = 1$ in (3.7) and differentiating with respect to v , we see that

$$\widehat{p}'(v) = 0 \quad \text{when} \quad v = -1 \pm \rho.$$

Setting

$$v_0 := -1 + \rho, \tag{3.15}$$

it follows from (3.7) that

$$\exp[-N\widehat{p}(v_0)] = (-1)^N \left(\frac{\alpha+2}{2}\right)^N \left(\frac{\alpha+2}{\alpha}\right)^{M/2} \tag{3.16}$$

and

$$2\widehat{p}''(v_0) = -2(\alpha+2)^2. \tag{3.17}$$

Therefore, from (3.8), as $N \rightarrow \infty$, recalling that $N = n+1$, we have by (3.16) and (3.17) that

$$\begin{aligned} P_n(x) &\sim \frac{2^{n+1}(-1)^n n! 2(-1)^{n+1}(\alpha+2)^{n+1}}{2\pi i 2^{n+1} i \sqrt{2}(\alpha+2)} \rho^{-\alpha(n+1)} \sqrt{\frac{\pi}{n+1}} e^{x(1-\rho)} \\ &= \frac{n!}{\sqrt{2\pi}} \frac{(\alpha+2)^n}{\sqrt{n+1}} \rho^{-\alpha(n+1)} e^{x(1-\rho)}. \end{aligned} \tag{3.18}$$

Now, from (3.11), we have

$$D_{n,\alpha} = \rho^{1-\alpha} \frac{2^n \Gamma(n + \alpha/2 + 1)}{\Gamma(\alpha/2 + 1)},$$

and applying Stirling's formula, it follows that as $n \rightarrow \infty$,

$$D_{n,\alpha} \sim \frac{n!}{\sqrt{2\pi}} \frac{(\alpha+2)^n}{\sqrt{n+1}} \rho^{-\alpha(n+1)}. \tag{3.19}$$

We deduce (3.12) from (3.18) and (3.19). Turning to the polynomial $Q_m(x)$, with $\beta = 1$, set

$$\widehat{q}(v) := \ln[v^\alpha(1-v^2)]. \tag{3.20}$$

Then $\widehat{q}'(v) = 0$ when $v = \pm\rho$, so that the integral in (3.9) has two (simple) saddle points inside C at the points on the real axis given by

$$v_1 := \rho, \quad v_2 := -\rho. \tag{3.21}$$

Moreover, from (3.20), we have

$$\hat{q}''(v_j) = -(\alpha + 2)^2, \quad j = 1, 2,$$

while

$$\exp(-N\hat{q}(v_1)) = \left(\frac{\alpha + 2}{\alpha}\right)^{M/2} \left(\frac{\alpha + 2}{2}\right)^N \quad (3.23)$$

and

$$\exp(-N\hat{q}(v_2)) = (-1)^M \left(\frac{\alpha + 2}{\alpha}\right)^{M/2} \left(\frac{\alpha + 2}{2}\right)^N. \quad (3.24)$$

We must choose the branches of $(2\hat{q}''(v))^{1/2}$ at $v = v_1$ and $v = v_2$ in accordance with equation (7.07) of OLVER (1974), namely,

$$(2\hat{q}''(v_1))^{1/2} = -i\sqrt{2}(\alpha + 2), \quad (3.25)$$

$$(2\hat{q}''(v_2))^{1/2} = i\sqrt{2}(\alpha + 2). \quad (3.26)$$

Then, from (3.9) together with (3.23), (3.24), (3.25) and (3.26), we deduce that as N (or n) $\rightarrow \infty$,

$$\begin{aligned} Q_m(x) &\sim \frac{(-1)^M n! (\alpha + 2)^n \rho^{-M}}{\sqrt{2\pi(n+1)}} \{e^{x\rho} + (-1)^m e^{-x\rho}\} \\ &\sim (-1)^m D_{n,\alpha} \{e^{x\rho} + (-1)^m e^{-x\rho}\}, \end{aligned} \quad (3.27)$$

where, in the last line, we have used (3.19). This proves (3.13). Noting that when $\beta = 1$, $R_s(x) \sim (-1)^m P_n(-x)$, the asymptotic (3.14) follows from (3.12). The results hold uniformly with respect to x on compact subsets of \mathbb{C} , because we assume that x is independent of the large parameter n (cf. Olver's theorem mentioned in connection with (3.8)). ■

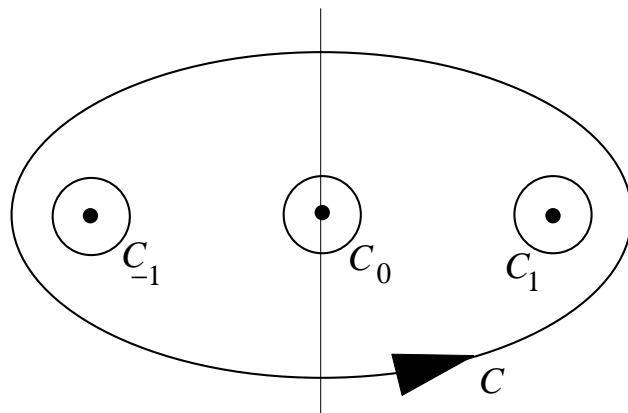


Figure 3.1. The contours for P_n, Q_m, R_s, E_{nms} for (3.28) – (3.31).

The contour integrals for the polynomials P_n , Q_m , R_s and E_{nms} can be written in the following form:

$$P_n(x) = -\frac{2^{s+1}n!e^x}{2\pi i} \oint_{C_1} \frac{e^{-xw}}{(1-w)^{n+1}w^{m+1}(1+w)^{s+1}} dw, \quad (3.28)$$

$$Q_m(x) = -\frac{2^{s+1}n!}{2\pi i} \oint_{C_0} \frac{e^{-xw}}{(1-w)^{n+1}w^{m+1}(1+w)^{s+1}} dw, \quad (3.29)$$

$$R_s(x) = -\frac{2^{s+1}n!e^{-x}}{2\pi i} \oint_{C_{-1}} \frac{e^{-xw}}{(1-w)^{n+1}w^{m+1}(1+w)^{s+1}} dw, \quad (3.30)$$

$$E_{nms}(x) = -\frac{2^{s+1}n!e^{-x}}{2\pi i} \oint_C \frac{e^{-xw}}{(1-w)^{n+1}w^{m+1}(1+w)^{s+1}} dw, \quad (3.31)$$

where C_j is a circle, centre at $w = j$, radius $r \in (0, 1)$, and C is a circle, centre at the origin, radius $r > 1$. The result for the remainder $E_{nms}(x)$ defined in (1.3) follows from adding up the results in (3.28) – (3.30). So, in fact, we have the same integral representation for the quantities P_n , Q_m , R_s and E_{nms} , but with different contours of integration; see Figure 3.1. Of course, all contours can be deformed without crossing the poles.

To obtain the asymptotic behaviour of the remainder, we cannot simply use the results in (3.12) – (3.14). Adding up these results gives

$$E_{nms}(x) = P_n(x)e^{-2x} + Q_m(x)e^{-x} + R_s(x) \sim 0,$$

which does not give useful information, but is in agreement with the approximating property of the Hermite–Padé method. A better estimate for E_{nms} follows from (3.31), by taking into account the exponential function when computing the saddle point.

Theorem 3.3. *Let $E_{nms}(x)$ be defined by (3.31); assume that n, m and s tend to ∞ and $x = o(n + m + s)$. Then*

$$E_{nms}(x) = \frac{(-1)^{m+s} 2^{s+1} n! e^{-x} x^{n+m+s+2}}{(n + m + s + 2)!} [1 + o(1)]. \quad (3.32)$$

Proof. We write (3.31) in the form

$$E_{nms}(x) = \frac{(-1)^n 2^{s+1} n! e^{-x}}{2\pi i} \int_C \frac{e^{-xw}}{w^{n+m+s+3}} q(w) dw, \quad (3.33)$$

where

$$q(w) = \frac{1}{(1 - 1/w)^{n+1} (1 + 1/w)^{s+1}}.$$

The function $e^{-xw}/w^{n+m+s+3}$ has a saddle point at $w_0 = -(n + m + s + 3)/x$, which tends to infinity, and $q(w) = 1 + (n - s)/w + \dots = 1 + o(1)$ in a neighborhood of the saddle point, and in fact on a circle with radius $|w_0|$. This proves the theorem. \blacksquare

4. Further asymptotic aspects and zero distribution

The asymptotic estimates given in (3.11) — (3.14) and (3.32) cannot be used to obtain detailed information on the zeros, because the zeros occur outside compact sets as the orders n, m, s tend to infinity. A first insight on this phenomena can be obtained from Corollary 2.2; it follows (under the conditions given there) that the zeros of Q_m are at least $\mathcal{O}(\sqrt{n})$ and at most $\mathcal{O}(\sqrt{nm})$. From the estimate in (3.13) of Theorem 3.2 we infer that zeros can be expected (again, under the conditions given there) if x is near the points $ik\pi/\rho, k = \pm 1, \pm 2, \dots$ if m is odd, or near $i(k + \frac{1}{2})\pi/\rho, k = \pm 1, \pm 2, \dots$ if m is even. When $n = s$, (2.26) and Table 2.1 suggest that the zeros of Q_m are indeed purely imaginary. This is not true, in general, as we discovered for the case $n = s = 15, m = 14$. In this case Q_m has ten zeros on the imaginary axis and four in the complex plane at the points $\pm 1.684078371 \pm 29.25218473i$, these four being the large zeros. See also the example in §4.2 and Figure 4.2 later in this section.

4.1. Some aspects of uniform asymptotic methods

As explained at the end of the previous section, the four quantities P_n, Q_m, R_s , and E_{nms} all have the same integral representation

$$\int e^{-\phi(w)} \frac{dw}{w(1-w^2)}, \quad (4.1)$$

with different contours and with

$$\phi(w) = zw + n \ln(1-w) + m \ln w + s \ln(1+w), \quad (4.2)$$

where we now write z instead of x , to underline that the argument is complex. The saddle points of the integrand are the zeros of the derivative of ϕ . There are three saddle points defined by the cubic equation

$$zw^3 + (m+n+s)w^2 + (n-s-z)w - m = 0 \quad (4.3)$$

and the saddle points are real when z is real. When $z > 0$ the saddle points occur in $(-\infty, -1)$, $(-1, 0)$, and $(0, 1)$; the saddle point contours have the shape of a parabola, with the real w -axis as axis of symmetry, with summits through the saddle points and with openings at $\Re w = +\infty$. For P_n and E_{nms} one single "parabola" can be used, through the positive saddle and the saddle point at the left of $w = -1$, respectively. For Q_m two parabolas are needed to encircle the pole at $w = 0$. One parabola runs through the saddle point between 0 and 1, and the other one through the saddle point between -1 and 0; the parabolas are joined at $\Re w = +\infty$ to close the loop. A similar contour can be used for R_s . When $z < 0$ the saddle point contours have the same pattern but with parabolas with openings at $\Re w = -\infty$.

A first idea about the location of the saddle points when z is complex can be obtained by considering rather large and rather small values of $|z|$ ("small" and "large" mean compared with $n+m+s$). When z moves along a large circle in the complex plane, the saddle points describe small circuits around the three poles at $w = -1, 0, 1$. When $|z|$ is small, one saddle

point describes a large circuit around the three poles, and the other two saddles describes small circuits around, say, $w = \pm\frac{1}{2}$. In Figure 4.1 we show the paths of the saddle points when z describes a semi-circle in the upper half plane.

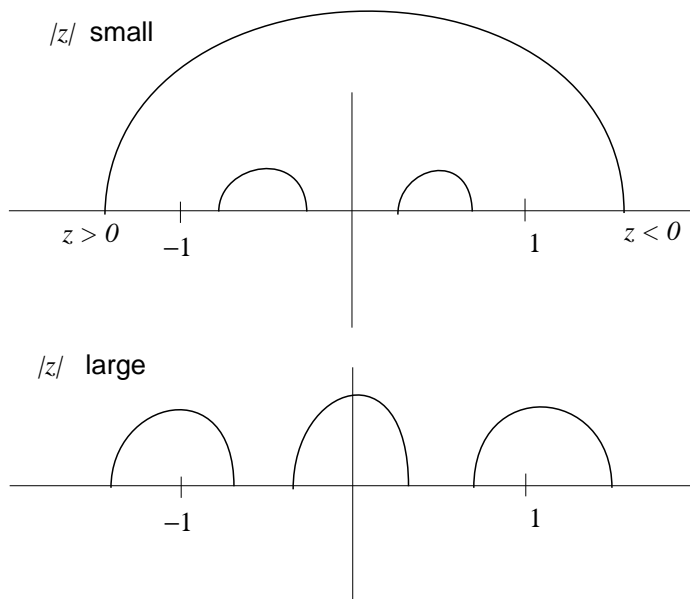


Figure 4.1. Trajectories of the saddle points when z describes a circular arc in the upper half plane.

For certain complex values of z two or three saddle points may coincide. It is known from uniform asymptotics (cf. OLVER (1974) or WONG (1989)), that Airy functions can describe the asymptotic behaviour of the integrals when two saddle points coincide. It is also known that in the z -plane strings of zeros arise near z -values that make the saddle points coalesce.

When $n = s$ two saddle points coincide when z solves the equation

$$z^4 + (n^2 + 10nm - 2m^2)z^2 + m(m + 2n)^3 = 0. \quad (4.4)$$

When $n = s = 4m$ and

$$z^2 = -27m^2 \quad (4.5)$$

three saddle points coincide at

$$w = \pm i/\sqrt{3}. \quad (4.6)$$

It is possible to describe all this by replacing the phase function $\phi(w)$ with a quartic polynomial:

$$\phi(w) = \frac{1}{4}\zeta^4 + \frac{1}{2}\alpha\zeta^2 + \beta\zeta + \gamma, \quad (4.7)$$

which in fact is a conformal mapping of the w -plane to the ζ -plane, where the three parameters α, β, γ follow from substituting the values of the three w -saddles and at the same time the three values of the three corresponding ζ -saddles, which are the zeros of

$$\zeta^3 + \alpha\zeta + \beta = 0. \quad (4.8)$$

When we follow this procedure we need to investigate the Painlevé-type functions

$$F_j(\alpha, \beta) = \frac{1}{2\pi i} \int_{C_j} e^{-(\frac{1}{4}\zeta^4 + \frac{1}{2}\alpha\zeta^2 + \beta\zeta + \gamma)} f(\zeta) d\zeta \quad (4.9)$$

along certain contours C_j in the complex plane, where α, β are complex constants, and (in our problem) depend on the complex parameter z and the non-negative integers n, m, s , and f contains the derivative $dw/d\zeta$ that arises when we transform (4.1) into (4.9) by using the mapping (4.7).

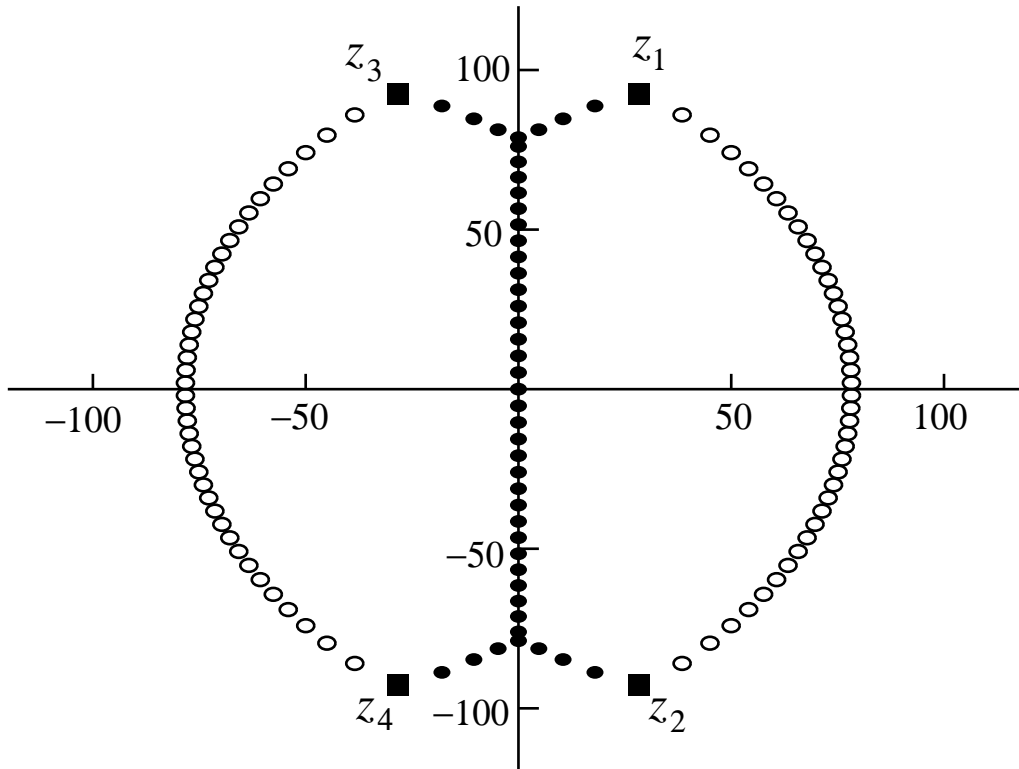


Figure 4.2. The zeros of P_n, Q_m, R_s with $n = s = 40, m = 45$. The black dots indicate the Q -zeros, the open dots those of P_n (left-hand plane) and R_s (right-hand plane); for an explanation of the role of the points z_k we refer to the text of §4.2.

4.2. An example for the zero distribution

In Figure 4.2 we give the zeros of the polynomials P_n, Q_m, R_s with $n = s = 40, m = 25$. The open dots indicate the zeros of the polynomials P_n and R_s . Those in the left-hand plane are the zeros of P_n , the zeros of R_s occur in the right-hand plane. The zeros of Q_m are given by black dots; 33 zeros occur on the imaginary axis, the remaining 12 zeros occur in the neighborhood of the black squares indicated by $z_k, k = 1, 2, 3, 4$.

The four values z_k solve equation (4.4) for the chosen values of n, m, s . For these values of z two saddle points of $\phi(w)$ defined in (4.2) coincide, and Airy-type asymptotic approximations can be derived for all integrals (3.28) – (3.31). As follows from the picture, and as remarked earlier, near z_k the zeros of the polynomials and the remainder arise. The zeros of $E_{n,m,s}$ are not shown, because at present not enough numerical details are available for high degree cases. The zeros of the remainder are located along curves that start near the four points z_k and run to $\pm i\infty$.

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