Using a computer algebra system to simplify

expressions for Titchmarsh-Weyl m-functions

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by

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Using a computer algebra system to simplify expressions for Titchmarsh-Weyl m-functions associated with the Hydrogen Atom on the half line*

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Abstract

Abstract: In this paper we give simplified formulas for certain polynomials which arise in some new Titchmarsh-Weyl m-functions for the radial part of the separated Hydrogen atom on the half line \((0, \infty)\) and two independent programs for generating them using the symbolic manipulator Mathematica.

1 Introduction

Recently Fulton[1] and Fulton and Langer [2] considered the following Sturm-Liouville problem for the hydrogen atom on the half line, \(x \in (0, \infty)\):

\[
- y'' + \left( -\frac{a}{x} + \frac{\ell(\ell + 1)}{x^2} \right) y = \lambda y, \quad 0 < x < \infty
\]

(1.1)

\[
\lim_{x \to 0} W_x \left( y, x^{\frac{\ell}{2}} J_{2\ell+1}(\sqrt{4ax}) \right) = 0.
\]

(1.2)

In [1] a fundamental system of Frobenius solutions defined at \(x = 0\) was introduced having the forms:

\[
\phi(x, \lambda) = x^{\ell+1} \left[ 1 + \sum_{n=1}^{\infty} a_n(\lambda)x^n \right] = \frac{1}{(-2\sqrt{\lambda})^{\ell+1}} M_{\beta, \ell+\frac{1}{2}}(-2ix\sqrt{\lambda}), \quad \beta := \frac{ia}{2\sqrt{\lambda}}
\]

(1.3)

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and
\[
\theta(x, \lambda) = -\frac{1}{2\ell + 1} \left[ K_\ell(\lambda) \phi(x, \lambda) \ln x + x^{-1} + \sum_{n=1}^\infty d_n(\lambda) x^{-\ell+n} \right]
\] (1.4)

Where \(a_n(\lambda)\) and \(d_n(\lambda)\) are polynomials in \(\lambda\), \(M_{\beta, \ell + \frac{1}{2}}\) is the Whittaker function of first kind and
\[
K_\ell(\lambda) = -\frac{a}{(2\ell + 1)! (2\ell)!} \prod_{j=1}^\ell \left( 4\lambda j^2 + a^2 \right) = \frac{(-2i\sqrt{\lambda})^{2\ell+1}(-\ell - \beta)_{2\ell+1}}{(2\ell)! (2\ell + 1)!}.
\] (1.5)

Then a Titchmarsh-Weyl \(m\)-function was introduced in [1] by the requirement
\[
\theta(x, \lambda) - m_\ell(\lambda) \phi(x, \lambda) \in L_2(0, \infty),
\] (1.6)

which gives \(m_\ell\) as
\[
m_\ell(\lambda) = -ak_\ell(\lambda) \left\{ \log(-2i\sqrt{\lambda}) + \Psi \left( 1 - \frac{ia}{2\sqrt{\lambda}} \right) - H_{2\ell} + 2\gamma \right\} - ak_\ell(\lambda) \left\{ \sum_{j=1}^\ell \left( \frac{1}{j - \frac{ia}{2\sqrt{\lambda}}} \right) \right\} + \left( i\sqrt{\lambda} \right)^{2\ell+1} \frac{(2\ell)!}{(2\ell + 1)!} \left[ \sum_{k=0}^{2\ell} \frac{2^k \left( -\ell - \frac{ia}{2\sqrt{\lambda}} \right)_k}{k! (2\ell + 1 - k)} \right]
\] (1.7)

where \(\Psi(z) = \frac{\Gamma'(z)}{\Gamma(z)}\) is the psi or digamma function, \(H_{2\ell} = \sum_{j=1}^{2\ell} \frac{1}{j}\), \(\gamma = Euler’s constant), and the Pochhammer symbol is defined for any complex \(z\) as \((z)_k = z(z + 1)...(z + k - 1)\). Here \(k_\ell(\lambda)\) is the polynomial of degree \(\ell\) defined by
\[
k_\ell(\lambda) = -\frac{1}{a(2\ell + 1)!} K_\ell(\lambda) = -\frac{1}{(2\ell + 1)!} \prod_{j=1}^\ell \left( 4\lambda j^2 + a^2 \right).
\] (1.8)

For \(\ell = 0\), we define \(k_0(\lambda) = 1\). The function \(m_\ell(\lambda)\) is an analytic function in the half planes \(\text{Im}\ \lambda < 0\) and \(\text{Im}\ \lambda > 0\), has poles on the negative \(x\)-axis at the eigenvalues of the problem (1.1)-(1.2), and a branch cut, corresponding to the continuous spectrum, on the positive real \(\lambda\)-axis. In [2] a Pick-Nevalinna representation of \(m_0(\lambda)\) was obtained for \(\ell = 0\) and for \(\ell \geq 1\) it was shown that \(m_\ell(\lambda)\) has a \(Q\)-function representation which puts it in the class \(N_\kappa\) of generalized Nevalinna functions with \(\kappa = \frac{\ell + \frac{1}{2}}{2}\).

Our purpose in this paper is to show that the last two terms in \(m_\ell(\lambda)\) can be decomposed into real and imaginary parts as
\[
-ak_\ell(\lambda) \left\{ \sum_{j=1}^\ell \left( \frac{1}{j - \frac{ia}{2\sqrt{\lambda}}} \right) \right\} + \left( i\sqrt{\lambda} \right)^{2\ell+1} \frac{(2\ell)!}{(2\ell + 1)!} \left[ \sum_{k=0}^{2\ell} \frac{2^k \left( -\ell - \frac{ia}{2\sqrt{\lambda}} \right)_k}{k! (2\ell + 1 - k)} \right] = i\sqrt{\lambda} k_\ell(\lambda) + \frac{r_\ell(\lambda)}{2\ell + 1},
\] (1.9)

where \(r_\ell(\lambda)\) is a polynomial of degree \(\ell\) in \(\lambda\).

Effectively, the decomposition (1.9) into real and imaginary parts becomes a defining equation for \(r_\ell(\lambda)\). Our first Mathematica program enables the decomposition to be verified. Next, in Section 3 we separate the left hand side of (1.9) into real and imaginary parts by introducing polynomial representations of \((-\ell-t)_k\) in \(t\) and
\[
\prod_{j=1}^\ell \left( \lambda + \frac{a^2}{4j^2} \right) \quad \text{in} \ \lambda,
\]

so that the real part can be represented as a polynomial of degree \(\ell\). This yields a real, somewhat explicit, representation for \(r_\ell/(2\ell+1)\), and using it a second Mathematica program shows that this real representation yields the same result as the first Mathematica program.
2 The First Mathematica program

A simple program in Mathematica can be used to verify that the polynomial \( r_\ell(\lambda) \) in (1.9) is real valued. This makes use of the built-in function \texttt{Pochhammer} \([a, k]\) which executes the multiplications in the Pochhammer symbol \((a)_k\).

Using the second expression in (1.5) for \( K_\ell(\lambda) \), we have using (1.8) that

\[
\begin{aligned}
 b &:= -a k_\ell(\lambda) = \frac{K_\ell(\lambda)}{2\ell + 1} = \frac{(-2i\sqrt{\lambda})^{2\ell+1}(-\ell - \beta)_{2\ell+1}}{(2\ell + 1)!^2}.
\end{aligned}
\]

Accordingly, solving (1.9) for \( r_\ell(\lambda) \), we have

\[
\begin{aligned}
 r_\ell(\lambda) &= \frac{b}{2\ell + 1} \left\{ \sum_{j=1}^{\ell} \frac{1}{j - \beta} \right\} + c + \frac{bi\sqrt{\lambda}}{a}, \quad \text{where } c := \frac{(i\sqrt{\lambda})^{2\ell+1}}{(2\ell + 1)!} \left[ \sum_{k=0}^{2\ell} \frac{2k}{k!(2\ell + 1 - k)} \right].
\end{aligned}
\]  

(2.1)

Following is the Mathematica program which implements equation (2.1). The output for \( r_\ell(\lambda) \) for \( \ell = 1, 2, 3, \) and 4 is shown. The program was executed up to \( \ell = 30 \) showing that \( r_\ell(\lambda) \) remained real-valued. Observe that the constant \( a \) multiplies all terms of \( r_\ell(\lambda) \) which in the Mathematica output is \( \text{ans1} \). This is also proved in (3.7) below.

First Program

Program input: \( \ell \)

\[
\begin{aligned}
\ell &= 4; \\
\text{While}[\ell < 6, \beta = \frac{\sqrt{\lambda} a}{2\sqrt{\lambda}}; \\
b &= \text{Expand}[(-2i\sqrt{\lambda})^{2\ell+1} \text{Pochhammer}[\frac{\ell - \beta, 2\ell + 1}{(2\ell + 1)!^2}; \text{(*This generates } K_\ell/(2\ell + 1). \text{ See (1.5).*)}) \\
c &= \text{Apart}[\text{Simplify}[(i\sqrt{\lambda})^{2\ell+1} \left( \sum_{k=0}^{2\ell} \frac{\text{Pochhammer}[\frac{-\ell - \beta, k]}{k!(2\ell + 1 - k)} \right)]; \\
g &= b \left( -\sum_{j=1}^{2\ell} \frac{1}{j - \beta} \right); \\
e &= b \sum_{j=1}^{\ell} \frac{1}{j - \beta}; \\
f &= \frac{bi\sqrt{\lambda}}{a}; \\
\text{Print}["For } \ell = " , \ell ]; \\
\text{ans1} &= \text{Simplify}[c + e + f]; \\
\text{Print}["ans1 = " , \text{ans1}]; \text{(*This generates the RHS of (2.1).*)} \\
\text{ans2} &= \text{Series}[\text{ans1}, \{\lambda, 0, \ell}\]; \text{Print}[" = " , \text{ans2}]; \\
\text{ans3} &= \text{Simplify}[g + c + e + f]; \text{Print}["ans3 = " , \text{ans3}]; \text{(*This generates the RHS of (2.6).*)} \\
\text{ans4} &= \text{Series}[\text{ans3}, \{\lambda, 0, \ell}\]; \text{Print}[" = " , \text{ans4}]; \\
\ell &= \ell + 1
\end{aligned}
\]

Program output:

For \( \ell = 1 \)

\[
\begin{aligned}
\text{ans1} &= -\frac{a\lambda}{36} \\
\text{ans3} &= \frac{1}{72}(3a^3 + 10a\lambda) = \frac{a^3}{24} + \frac{5a\lambda}{36}
\end{aligned}
\]  

(2.2)
For $\ell = 2$

\[
\begin{align*}
\text{ans}1 & = -\frac{a\lambda(a^2 + 13\lambda)}{7200} = -\frac{a^3\lambda}{7200} = \frac{13a\lambda^2}{7200} \\
\text{ans}3 & = \frac{25a^5 + 476a^3\lambda + 1288a\lambda^2}{172800} = \frac{a^5}{6912} + \frac{119a^3\lambda}{43200} + \frac{161a\lambda^2}{21600}
\end{align*}
\]  

For $\ell = 3$

\[
\begin{align*}
\text{ans}1 & = -\frac{a\lambda(a^4 + 46a^2\lambda + 400\lambda^2)}{8467200} = -\frac{a^5\lambda}{8467200} = \frac{23a^3\lambda^2}{4233600} = \frac{a\lambda^3}{21168} \\
\text{ans}3 & = \frac{49a^7 + 2684a^5\lambda + 35656a^3\lambda^2 + 88896a\lambda^3}{508032000} \\
& = \frac{a^7}{10368000} + \frac{671a^5\lambda}{12700800} + \frac{4457a^3\lambda^2}{6350400} + \frac{463a\lambda^3}{2646000}
\end{align*}
\]  

For $\ell = 4$

\[
\begin{align*}
\text{ans}1 & = -\frac{a\lambda(a^6 + 107a^4\lambda + 3124a^2\lambda^2 + 22548\lambda^3)}{32920473600} \\
& = -\frac{a^7\lambda}{32920473600} + \frac{107a^5\lambda^2}{32920473600} + \frac{781a^3\lambda^3}{8230118400} + \frac{1879a\lambda^4}{2743372800} \\
\text{ans}3 & = \frac{761a^9 + 90200a^7\lambda + 3204208a^5\lambda^2 + 36438400a^3\lambda^3 + 86960256a\lambda^4}{36870930432000} \\
& = \frac{761a^9}{3687093043200} + \frac{451a^7\lambda}{184354652160} + \frac{4087a^5\lambda^2}{11522165760} + \frac{226459a\lambda^3}{96018048000}
\end{align*}
\]  

Output for the polynomials

\[
p_\ell(\lambda) := \frac{r_\ell(\lambda)}{2\ell + 1} + ak_\ell(\lambda)H_{2\ell},
\]

which arise in the representation of the $m_\ell$ function from [1, Equation(8.15)],

\[
m_\ell(\lambda) = k_\ell(\lambda) \left\{-a \log(-2i\sqrt{\lambda}) - a\Psi\left(1 - \frac{ia}{2\sqrt{\lambda}}\right) - 2\gamma a + i\sqrt{\lambda}\right\} + p_\ell(\lambda)
\]

is also given below for $\ell = 1, 2, 3, 4$.

\[
\begin{align*}
p_1 & = \frac{a^3}{24} + \frac{5a\lambda}{36}, \\
p_2 & = \frac{a^5}{6912} + \frac{119a^3\lambda}{43200} + \frac{161a\lambda^2}{21600}, \\
p_3 & = \frac{a^7}{10368000} + \frac{671a^5\lambda}{12700800} + \frac{4457a^3\lambda^2}{6350400} + \frac{463a\lambda^3}{2646000}, \\
p_4 & = \frac{761a^9}{3687093043200} + \frac{451a^7\lambda}{184354652160} + \frac{4087a^5\lambda^2}{47029248000} + \frac{11387a^3\lambda^3}{11522165760} + \frac{226459a\lambda^4}{96018048000}
\end{align*}
\]

Here $p_\ell$ is printed as $\text{ans}3$ in the above program.
3 Explicit Representation for $r_\ell$

In this section we give a method for separating the expression in equation (1.9) into real and imaginary parts, yielding a real representation for the polynomial $r_\ell(\lambda)$. The difficulty arises from the complicated product in the Pochhammer symbol $(\ell - \beta)_k$ where $\beta = \frac{i\alpha}{2\sqrt{\lambda}}$. Replacing $\beta$ by a real variable $t$, we let the coefficients of the polynomial $(-\ell - t)_k$ be defined by

$$g_k(t) := (-\ell - t)_k = \prod_{j=0}^{k-1} (-\ell + j - t) = \sum_{n=0}^{k} \alpha(k, n)t^n = \sum_{j=0}^{k_1} \alpha(k, 2j)t^{2j} + \sum_{j=0}^{k_2} \alpha(k, 2j + 1)t^{2j+1}, \quad (3.1)$$

where $k_1 = \lceil \frac{k}{2} \rceil$ and $k_2 = \lceil \frac{k-1}{2} \rceil$. Here $\alpha(k, n) = \alpha_\ell(k, n)$, and we are interested for fixed $\ell$ to have $\alpha_\ell(k, n)$ available for all $0 \leq k \leq 2\ell$, and all $0 \leq n \leq k$. For $n = 0$, the constant term is $\alpha_\ell(k, 0) = \prod_{j=0}^{k-1} (-\ell + j) = (-\ell)_k$, $k = 0, 1, \cdots 2\ell$. Formulas for larger values of $n$ become increasingly more complicated and are not known in closed form. We can, however, represent the real and the imaginary parts of (1.9) in terms of $\alpha(k, n)$. Putting $t = \beta = \frac{i\alpha}{2\sqrt{\lambda}}$ in (3.1) gives

$$g_k(\beta) = \sum_{n=0}^{k} \alpha(k, n) \left( \frac{a}{2} \right)^n i^n (\lambda^{-\frac{1}{2}})^n$$

$$= \sum_{j=0}^{k_1} (-1)^j \alpha(k, 2j) \left( \frac{a}{2} \right)^{2j} i^n (\lambda^{-\frac{1}{2}})^{2j}$$

$$+ i \sum_{j=0}^{k_2} (-1)^j \alpha(k, 2j + 1) \left( \frac{a}{2} \right)^{2j+1} (\lambda^{-\frac{1}{2}})^{2j+1}. \quad (3.2)$$

Now for the $(i\sqrt{\lambda})^{2\ell+1}$ term in (1.9) we have $(i)^{2\ell+1} = (-1)^\ell i$, $\ell = 0, 1, 2, \ldots$. Thus the second sum in (1.9) may be written as

$$i(-1)^\ell \sum_{k=0}^{2\ell} \frac{2^k}{(2\ell + 1)!k!(2\ell + 1 - k)} g_k(\beta)(\lambda^{\frac{1}{2}})^{2\ell+1}$$

$$= -(-1)^\ell \sum_{k=1}^{2\ell} \frac{2^k}{(2\ell + 1)!k!(2\ell + 1 - k)} \left[ \sum_{j=0}^{k_2} (-1)^j \alpha(k, 2j) \left( \frac{a}{2} \right)^{2j+1} (\lambda^{\frac{1}{2}})^{2\ell+1-(2j+1)} \right]$$

$$+ i(-1)^\ell \sum_{k=0}^{2\ell} \frac{2^k}{(2\ell + 1)!k!(2\ell + 1 - k)} \left[ \sum_{j=0}^{k_1} (-1)^j \alpha(k, 2j + 1) \left( \frac{a}{2} \right)^{2j+1} (\lambda^{\frac{1}{2}})^{2\ell+1-2j} \right]$$

$$= \sum_{k=0}^{2\ell} \frac{2^k A_k}{(2\ell + 1)!k!(2\ell + 1 - k)} + i \sum_{k=0}^{2\ell} \frac{2^k B_k}{(2\ell + 1)!k!(2\ell + 1 - k)} \quad (3.3)$$

where

$$A_k = (-1)^{\ell+1} \sum_{j=0}^{k_2} (-1)^j \alpha(k, 2j + 1) \left( \frac{a}{2} \right)^{2j} \lambda^{\ell-j} \quad (3.4)$$

and

$$B_k = (-1)^{\ell} \sum_{j=0}^{k_1} (-1)^j \alpha(k, 2j) \left( \frac{a}{2} \right)^{2j} \lambda^{\ell-j} \lambda^{\frac{1}{2}} \quad (3.5)$$
Similarly, we may decompose the first term in (1.9) as

\[\sum_{m=1}^{\ell} \frac{1}{m - \frac{ia}{2\sqrt{\lambda}}} = \sum_{m=1}^{\ell} \frac{4\lambda m}{4\lambda m^2 + a^2} + i \sum_{m=1}^{\ell} \frac{2a\lambda^{\frac{1}{2}}}{4\lambda m^2 + a^2}.\]  

(3.6)

Using (1.8) and cancelling one \(4\lambda j^2 + a^2\) factor for each term in the above sums, we find that

\[-a k_\ell(\lambda) \left[ \sum_{m=1}^{\ell} \frac{1}{m - \frac{ia}{2\sqrt{\lambda}}} \right] = -\frac{a}{[(2\ell + 1)]^2} \left[ \sum_{m=1}^{\ell} 4\lambda m \prod_{j=1, j\neq m}^{\ell} (4\lambda j^2 + a^2) \right] + i \left( -\frac{a}{[(2\ell + 1)]^2} \left[ \sum_{m=1}^{\ell} 2a\lambda^{\frac{1}{2}} \prod_{j=1}^{\ell} (4\lambda j^2 + a^2) \right] \right).\]  

(3.7)

Combining (3.3) and (3.7) and taking real and imaginary parts of (1.9), we thus obtain:

\[\sqrt{\lambda} k_\ell(\lambda) = -\frac{2a^2 \sqrt{\lambda}}{[(2\ell + 1)]^2} \left[ \sum_{m=1}^{\ell} \prod_{j=1, j\neq m}^{\ell} (4\lambda j^2 + a^2) \right] + \sum_{k=0}^{2\ell} \frac{2k B_k}{(2\ell + 1)!k!(2\ell + 1 - k)} \]  

(3.8)

and

\[\frac{r_\ell(\lambda)}{2\ell + 1} = -\frac{4\lambda a}{[(2\ell + 1)]^2} \left[ \sum_{m=1}^{\ell} m \prod_{j=1, j\neq m}^{\ell} (4\lambda j^2 + a^2) \right] + \sum_{k=1}^{2\ell} \frac{2k A_k}{(2\ell + 1)!k!(2\ell + 1 - k)}.\]  

(3.9)

Since every \(A_k\) involves \(a\) as a factor, it follows that a factor of \(a\) occurs in both terms on the right hand side of (3.9). Hence \(a = 0\) will give \(r_\ell(\lambda) = 0\).

To bring the expression in (3.9) into a simpler form, we now isolate the coefficients of the powers of \(\lambda\). For the second term in (3.9) we insert the formula (3.4) for \(A_k\) into the sum, change the summation index \((m = \ell - j)\), and then interchange the order of summation:

\[\sum_{k=1}^{2\ell} \frac{2k A_k}{(2\ell + 1)!k!(2\ell + 1 - k)} = \sum_{k=1}^{2\ell} \sum_{j=0}^{k^2} \frac{2^k(-1)^{\ell+1+j} \alpha(k, 2j + 1) \left(\frac{a}{2}\right)^{2j+1} \lambda^{\ell-j}}{(2\ell + 1)!k!(2\ell + 1 - k)} \]  

\[= \sum_{k=1}^{2\ell} \sum_{m=\ell-k^2}^{\ell} \left[ \frac{2^k(-1)^{m+1} \alpha(k, 2(\ell - m) + 1) \left(\frac{a}{2}\right)^{2(\ell-m)+1}}{(2\ell + 1)!k!(2\ell + 1 - k)} \right] \lambda^m \]  

\[= \sum_{m=1}^{\ell} \sum_{k=2(\ell-m)+1}^{2\ell} \left[ \frac{2^k(-1)^{m+1} \alpha(k, 2(\ell - m) + 1) \left(\frac{a}{2}\right)^{2(\ell-m)+1}}{(2\ell + 1)!k!(2\ell + 1 - k)} \right] \lambda^m \]  

\[= \sum_{j=1}^{d_j \lambda^j} \]  

(3.10)

where
\[ d_j := \frac{a}{2} \sum_{k=2(\ell-j)+1}^{2\ell} \left[ \frac{2^k(-1)^{m+1}(\frac{a}{4})^{2(\ell-j)}}{(2\ell+1)!k!(2\ell+1-k)} \right]. \tag{3.11} \]

Similarly, to isolate the powers of \( \lambda \) in the first term in (3.7) we first define the coefficients \( \gamma(m, n) \) of the \( \ell - 1 \) degree polynomial,

\[ \prod_{j=1, j \neq m}^{\ell} \left( \lambda + \frac{a^2}{4j^2} \right) = \sum_{n=0}^{\ell-1} \gamma(m, n) \lambda^n. \tag{3.12} \]

Insertion of this into the first term in (3.9), changing the summation index \( (j = n+1) \), and interchanging the order of summation then yields:

\[
\begin{align*}
&\frac{-4a\lambda}{[(2\ell+1)!]^2} \left[ \sum_{m=1}^{\ell} m \prod_{j=1, j \neq m}^{\ell} (4\lambda j^2 + a^2) \right] \\
&= \frac{-a4^{\ell}(\ell)!^2}{[(2\ell+1)!]^2} \left[ \sum_{n=1}^{\ell} \sum_{n=0}^{\ell-1} \left[ \frac{\gamma(m, n)}{m} \right] \lambda^{n+1} \right] \\
&= \frac{-a4^{\ell}(\ell)!^2}{[(2\ell+1)!]^2} \left[ \sum_{m=1}^{\ell} \sum_{j=1}^{\ell} \left[ \frac{\gamma(m, j-1)}{m} \right] \lambda^j \right] \\
&= \frac{-a4^{\ell}(\ell)!^2}{[(2\ell+1)!]^2} \left[ \sum_{j=1}^{\ell} \sum_{m=1}^{\ell} \left[ \frac{\gamma(m, j-1)}{m} \right] \lambda^j \right] \\
&= \sum_{j=1}^{\ell} c_j \lambda^j 
\end{align*}
\tag{3.13} \]

where

\[ c_j := -\frac{a4^{\ell}(\ell)!^2}{[(2\ell+1)!]^2} \sum_{m=1}^{\ell} \left( \frac{\gamma(m, j-1)}{m} \right). \tag{3.14} \]

Putting (3.10) and (3.13) in (3.9) we thus have for the polynomial \( r_\ell(\lambda)/(2\ell+1) \) the representation,

\[ \frac{r_\ell(\lambda)}{2\ell+1} = \sum_{j=1}^{\ell} (c_j + d_j) \lambda^j. \tag{3.15} \]

Here it is clear that \( a \) is a common factor in \( c_j \) and \( d_j \) for all \( j \), and hence for the case \( a = 0, r_\ell \equiv 0 \). The expression (3.15) is somewhat more explicit than the expression (2.11) and (3.9) since the coefficients of the powers of \( \lambda \) are isolated, and there are no complex terms present. On the other hand, further simplifications are certainly desirable; however, this requires closed form formulas for \( \alpha(k, n) \) and \( \gamma(m, n) \) which remain elusive. However, the formulas for \( c_j \) and \( d_j \) are easily implemented using a symbolic manipulator.

4 The Second Mathematica Program

As an independent check on the first Mathematica program we implemented the formulas (3.11) and (3.14) for \( d_j \) and \( c_j \) and computed the polynomial of degree \( \ell \) in (3.15). This required computing and storing the
coefficient $\alpha(k, n)$ and $\gamma(m, n)$ in (3.11) and (3.12). Following is the Mathematica program that does this to compute $r_\ell(\lambda)/(2\ell + 1)$. The output for $\ell = 1, 2, 3$ and 4 is shown. The program was executed up to $\ell = 30$ and gave exact agreement with the first Mathematica program.

Second Program

Program input: $\ell$

\[
\ell = 4; k = 0; \\
\text{While}[k \leq 2\ell, \\
\quad p[t_] = \text{Expand}[\text{Pochhammer}[-\ell - t, k]]; n = k; i = 0; \\
\quad \text{While}[i \leq n, \\
\quad \quad \alpha[k, i] = p[0]; \\
\quad \quad p[t_] = \text{Simplify}[\text{Expand}[(p[t] - \alpha[k, i])/t]]; \\
\quad \quad i++ \\
\quad k++] \\
\text{Clear}[k]; j = 1; \\
\text{While}[j \leq \ell, \\
\quad d[j] = \sum_{k=2(\ell-j)+1}^{2\ell} \frac{2^k(-1)^{k-1}\alpha[k,2\ell-2j-1](\frac{a}{4})^{2\ell-2j+1}}{(2\ell+1)k!(2\ell+1-k)}; j++] \\
\text{Clear}[j]; m = 1; \\
\text{While}[m \leq \ell, \\
\quad q[t_] = \left(\prod_{j=1}^{\ell} \left(t + \frac{a^2}{4j^2}\right)\right) / \left(t + \frac{a^2}{4m^2}\right); n = \ell - 1; i = 0; \\
\quad \text{While}[i \leq n, \\
\quad \quad \gamma[m, i] = q[0]; \\
\quad \quad q[t_] = \text{Simplify}[\text{Expand}[(q[t] - \gamma[m, i])/t]]; \\
\quad \quad i++ \\
\quad m++] \\
\text{Clear}[i]; j = 1; \\
\text{While}[j \leq \ell, \\
\quad c[j] = \frac{-a^{\ell}(\ell)!^2}{(2\ell+1)!^2} \sum_{m=1}^{\ell} \frac{\gamma[m, j-1]}{m}; j++] \\
\text{Print}[\sum_{j=1}^{\ell} (c[j] + d[j])t^j]
\]

Output of second program

For $\ell = 1$:

\[
\frac{r_\ell}{(2\ell + 1)} = -\frac{at}{36}
\]

For $\ell = 2$:

\[
\frac{r_\ell}{(2\ell + 1)} = -\frac{a^3t}{7200} - \frac{13at^2}{7200}
\]

For $\ell = 3$:

\[
\frac{r_\ell}{(2\ell + 1)} = -\frac{a^5t}{8467200} - \frac{23a^3t^2}{4233600} - \frac{at^3}{21168}
\]

For $\ell = 4$:

\[
\frac{r_\ell}{(2\ell + 1)} = -\frac{a^7t}{32920473600} - \frac{107a^5t^2}{32920473600} - \frac{781a^3t^3}{8230118400} - \frac{1879at^4}{2743372800}
\]

This output is in agreement with the output of the first program, and was also checked up to $\ell = 30$. The two Mathematica programs verify that the imaginary part of the expression (2.11) for $r_\ell(\lambda)/(2\ell + 1)$ is zero.
for all values of $\ell$ for which the programs were executed. A general proof that this is true for all $\ell$, that is, a proof of (3.8) (or, equivalently, a proof of (3.9)) requires that the $\alpha(k, n)$ and $\gamma(m, n)$ coefficients be obtained in a simplified form, and this appears to be a formidable task. It is quite difficult to perform induction on $\ell$ to prove (3.8) or (3.9) because of the complicated manner in which $\alpha(k, n) = \alpha_{\ell}(k, n)$ and $\gamma(m, n) = \gamma_{\ell}(m, n)$ change with $\ell$. Nevertheless, it may be possible to construct rigorous proofs by making use of some combinatorial analysis. For example, there are general forms for the coefficients of a polynomial having $k$ known roots $x_i$, $i = 1, 2, ..., k$. Sen and Krishnamurthy [3], for example, show that

$$q_k(x) := \prod_{j=1}^{k} (x - x_j) = x^k + \sum_{m=1}^{k} a_m x^{k-m}$$

(4.1)

with

$$a_m := (-1)^m S_m := (-1)^m \sum x_1 x_2 ... x_m,$$

(4.2)

where the sum is taken over all the products of $x_i$ taken $m$ at a time. Thus, for the polynomial $g_k(t)$ of (3.1) we have

$$g_k(t) = (-1)^k \prod_{j=0}^{k-1} [t - (j - \ell)] = (-1)^k \prod_{j=1}^{k} [t - (j - 1 - \ell)] = (-1)^k \left( t^k + \sum_{m=1}^{k} a_m t^{k-m} \right),$$

(4.3)

with

$$a_m = a_{\ell}(k, m) = (-1)^m \sum t_1 t_2 ... t_m$$

(4.4)

where the sum is taken over all the products of $t_j := j - 1 - \ell$ taken $m$ at a time. But, a general solution for $a_m$ as a function of $k$ and $\ell$, valid for all $\ell$ and all $0 \leq k \leq 2\ell$, remains elusive. Another idea would be to establish (3.8) or (3.9) by induction on $\ell$, but it unfortunately appears difficult to employ the induction hypothesis. So, an analytic proof of (3.8) or (3.9) valid for all $\ell \geq 1$ remains an open problem.

5 Conclusion

The simplification of $a_{\ell}(k, n)$ and a rigorous proof of (3.8) and/or (3.9) remain as open problems. We have, however, given in this note two Mathematica programs which implicitly establish both of these results.

References

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[3] E.V. Krishnamurthy and S.K. Sen, Numerical Algorithms: Computations in Science and Engineering, Affiliated East West Press, New Delhi, 2001.