

Kaylee Tejada

Candidate

Department of Mathematics and Statistics

Department

This thesis is approved, and it is acceptable in quality and form for publication:

Approved by the Thesis Committee:

Stephen Lau

, Chairperson

Matthew Blair

James Ellison

On Roots of the Macdonald Function

by

Kaylee Robert Tejada

B.S., Pure Mathematics, University of New Mexico, 2003

THESIS

Submitted in Partial Fulfillment of the
Requirements for the Degree of

Master of Science
Mathematics

The University of New Mexico

Albuquerque, New Mexico

July, 2014

©2014, Kaylee Robert Tejada

Dedication

This is for all seekers of the truth, regardless of consequence.

“In the twentieth century it has been understood that all knowledge is dependent upon the question asked; and the relationship of mathematics to nature is one of the profound indicators, I think, that truth can be known. Maybe not ‘the’ truth, but I always think of the positivist philosopher Wittgenstein who was once asked, in a classroom situation about a certain proposition, ‘Is it the truth?’, and he said ‘Well, it’s certainly true enough!’; and that is where we are with our modelling of the world and with our mathematics. It is the truest truth we know. It is true enough.” – Terence McKenna

Acknowledgments

I would like to thank my advisor Stephen Lau for his generous guidance, in addition to all remaining UNM Department of Mathematics and Statistics faculty and staff, particularly Ana Parra Lombard, for their assistance and mentorship over the years. I thank my family, for without them I would not exist. I would also like to thank those who believed in me, for their moral support; as well as those who doubted me, for the inspiration to prove otherwise. Some of this work was supported by NSF grant No. PHY 0855678.

On Roots of the Macdonald Function

by

Kaylee Robert Tejada

B.S., Pure Mathematics, University of New Mexico, 2003

M.S., Mathematics, University of New Mexico, 2014

Abstract

An overview is given for the Dirichlet-to-Neumann map for outgoing solutions to the “radial wave equation” in the context of nonreflecting radiation boundary conditions on a spherical domain. We then consider the Macdonald function $K_{\ell+1/2}(z)$ for $\ell \in \mathbb{Z}_{\geq 0}$, a solution to the half-integer order modified Bessel equation. This function can be expressed as $K_{\ell+1/2}(z) = \sqrt{\frac{\pi}{2z}} e^{-z} z^{-\ell} p_{\ell}(z)$, where $p_{\ell}(z)$ is a degree- ℓ monic polynomial with simple roots in the left-half plane. By exploiting radiation boundary conditions for the “radial wave equation”, we show that the root set of $p_{\ell}(z)$ also obeys ℓ additional polynomial constraints. These constraints are in fact Newton’s identities which relate a polynomial’s coefficients to the power sums of its roots. We follow this with numerical verification up to order $\ell = 20$.

Contents

List of Figures	ix
List of Tables	x
Glossary	xi
1 Introduction	1
2 Radiation boundary conditions and the radial wave equation	2
2.1 Overview	2
2.2 The radial wave equation	3
2.3 Macdonald function as an outgoing solution	5
3 Nonreflecting Boundary Conditions	7
3.1 Proof of Theorem 3.0.1	8
3.2 Alternative proof.	11
4 Newton's Identities	14

Contents

4.1	Main result	14
4.2	Proof of Theorem 4.1.1	16
5	Numerical root evaluation and identity check for several values of ℓ	19
5.1	Root finding and identity verification for $\ell = 20$ to 27 digits of precision . . .	20
6	Conclusion	30
A	Location and count of Macdonald roots	31
A.1	Root count for $K_{\ell+1/2}(z)$	32
A.2	Root count for $K_\nu(z)$	33
	References	36

List of Figures

2.1	Scaled roots of $K_{\ell+1/2}(z)$	6
3.1	Radial axis with support of $\Psi_\ell(0, r)$ and point at $r_B - \epsilon\delta$ (the dashed line).	8
3.2	Retarded time axis and support of profile function f	8
A.1	Keyhole contour with arcs $\Gamma : z = R$ and $\gamma : z = \delta$	34

List of Tables

5.1	Roots of $K_{\ell+1/2}(z)$ for $\ell = 1, \dots, 20$	22
-----	--	----

Glossary

ψ_ℓ	General solution to the radial wave equation
Ψ_ℓ	General solution defined to remove $\frac{1}{r}$ decay
$\widehat{\Psi}_\ell$	Laplace transform of the general non-decaying solution above
Ω_ℓ	Radiation boundary kernel for the radial wave equation
$Y_{\ell m}(\theta, \phi)$	Spherical harmonics
$I_\nu(z), K_\nu(z)$	Modified Bessel functions
$p_\ell(z)$	Bessel polynomial
$b_{\ell n}$	Roots of Bessel polynomial
$\mathcal{W}(r)$	Wronskian
$G(r, \xi; s)$	Green's function

Chapter 1

Introduction

The overall goal of this thesis is to explore a set of identities that arise in the context of outgoing waves and the half-integer order modified Bessel equation. We derive identities for the roots of the Macdonald function, a solution to the modified Bessel equation. These identities prove to be Newton's identities which relate a polynomial's coefficients to the power sums of its roots. Our derivation of these identities exploits the concept of nonreflecting boundary conditions for the wave equation in the presence of a spherical "computational" domain. These identities are then verified numerically using **Mathematica** up to a specified order. The actual code used, along with the tables of roots generated and numerical verification of the identity for each root set are presented in the final chapter. Arguments [2] by Watson concerning the location of the roots of Macdonald's function are presented in the Appendix.

Both subscript style notation ∂_r and ratio notation $\frac{\partial}{\partial r}$ are used interchangeably in this paper to represent the partial derivative with respect to the radial variable r (for example), with the choice of notation based on readability and typesetting. Sometimes we also use, for example, the notation $\Psi_{tt} = \partial_t^2 \Psi$ to denote derivatives.

Chapter 2

Radiation boundary conditions and the radial wave equation

2.1 Overview

In mathematical physics, wave phenomena are typically modelled by hyperbolic partial differential equations on an unbounded domain. Examples include acoustic, electromagnetic, elastic, and gravitational phenomena. In numerical situations, this unbounded domain is usually truncated to produce a computational domain, with “artificial” boundary conditions (BCs) placed at the domain’s boundary, an artificial boundary. One approach for producing BCs which achieve exact domain reduction (i.e. the solution on the computational domain agrees with the restriction thereon of the solution on the unbounded domain) involves the Dirichlet-to-Neumann (DtN) map [3].

Consider the case of the ordinary wave equation on \mathbb{R}^3 ,

$$\Delta\psi - \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} = 0. \tag{2.1}$$

The initial value problem for the wave equation can be solved using spherical coordinates,

chosen for symmetry considerations. We will also assume unit speed $c = 1$ in the rest of this paper for simplicity.

Let $D = \{x \mid |x| \leq r_B\}$ contain the support of the initial data. Then BCs are constructed on the boundary ∂D with the purpose of approximating the exact solution for the whole-space problem restricted to D . We want BCs which are transparent (i.e. nonreflecting). An otherwise approximate BC which does not behave in this manner will generate a spurious reflection, leading to numerical error in the computational domain D . Such BC's are specified in the next chapter. Here we lay some groundwork for their formulation.

2.2 The radial wave equation

In spherical coordinates the Laplace operator has the form

$$\Delta\psi = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \psi + \frac{1}{r^2} \Delta_{S^2} \psi, \quad \Delta_{S^2} = \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2}, \quad (2.2)$$

where Δ_{S^2} is the Laplace operator on the unit sphere.

The general solution to (2.1) can then be expanded in terms of the eigenfunctions $Y_{\ell m}(\theta, \phi)$ of Δ_{S^2} :

$$\psi = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \psi_{\ell m}(t, r) Y_{\ell m}(\theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{\Psi_{\ell m}(t, r)}{r} Y_{\ell m}(\theta, \phi). \quad (2.3)$$

Here the $Y_{\ell m}(\theta, \phi)$ are the standard spherical harmonics which obey

$$\Delta_{S^2} Y_{\ell m}(\theta, \phi) = -\ell(\ell + 1) Y_{\ell m}(\theta, \phi). \quad (2.4)$$

Plugging (2.3) into the wave equation (2.1) we find, using orthogonality, that the multipole coefficients $\psi_{\ell m}$ and $\Psi_{\ell m}$ satisfy

$$-\frac{\partial^2 \psi_{\ell}}{\partial t^2} + \frac{\partial^2 \psi_{\ell}}{\partial r^2} + \frac{2}{r} \frac{\partial \psi_{\ell}}{\partial r} - \frac{\ell(\ell + 1)}{r^2} \psi_{\ell} = 0, \quad (2.5)$$

and

$$-\frac{\partial^2 \Psi_\ell}{\partial t^2} + \frac{\partial^2 \Psi_\ell}{\partial r^2} - \frac{\ell(\ell+1)}{r^2} \Psi_\ell = 0, \quad (2.6)$$

where now we suppress the m indices. Note that (2.6) is similar to the simple 1 + 1 wave equation $-\partial_t^2 \Psi + \partial_r^2 \Psi = 0$ except for the potential term $V = \ell(\ell+1)/r^2$.

The 1 + 1 wave equation has solutions $g(t+r)$, $f(t-r)$ for general profile functions $g(v)$, $f(u)$. In fact, for the radial wave equation (2.6),

$$\Psi_\ell(t, r) = \sum_{k=0}^{\ell} \frac{1}{r^k} c_{\ell k} f^{(\ell-k)}(t-r), \quad c_{\ell k} = \frac{1}{2^k k!} \frac{(\ell+k)!}{(\ell-k)!}, \quad (2.7)$$

is the analog of the outgoing solution $f(t-r)$ to the 1 + 1 wave equation, which we now formulate as a lemma with proof.

Lemma 2.2.1. *Given a sufficiently smooth profile function $f(u)$, the “multipole” $\Psi_\ell(t, r)$ given in (2.7) is a solution to the radial wave equation (2.6).*

Proof. To prove the lemma, note that $f(t-r)$ is clearly a solution to (2.6) for $\ell = 0$, and then proceed by induction on ℓ . First, appealing to the explicit formula (2.7) for $c_{\ell k}$, it can be established that

$$\Psi_\ell = -\left(\frac{\partial}{\partial r} - \frac{\ell}{r}\right) \Psi_{\ell-1}, \quad \Psi_{\ell-1}(t, r) = \sum_{k=0}^{\ell-1} \frac{1}{r^k} c_{\ell-1, k} f^{(\ell-1-k)}(t-r). \quad (2.8)$$

Next, assume that $\Psi_{\ell-1}$ in (2.8) obeys (2.7) with ℓ replaced by $\ell-1$ in the potential:

$$-\frac{\partial^2 \Psi_{\ell-1}}{\partial t^2} + \frac{\partial^2 \Psi_{\ell-1}}{\partial r^2} - \frac{\ell(\ell-1)}{r^2} \Psi_{\ell-1} = 0. \quad (2.9)$$

Finally, apply the raising operator $D_\ell^+ = -\partial_r + \ell/r$ to the last equation, thereby finding

$$-(D_\ell^+ \Psi_{\ell-1})_{tt} + (D_\ell^+ \Psi_{\ell-1})_{rr} - \frac{\ell(\ell+1)}{r^2} D_\ell^+ \Psi_{\ell-1} = 0. \quad (2.10)$$

These steps prove the lemma. □

2.3 Macdonald function as an outgoing solution

The Macdonald function (see p. 374 in [1], also [2]) $K_\nu(z)$ is a solution to the modified Bessel equation

$$z^2 w'' + zw' - (z^2 + \nu^2)w = 0, \quad (2.11)$$

and it plays a prominent role in the representation of outgoing solutions to the ordinary wave equation. As an example, $\Psi_{\ell,s}(t, r) = e^{st} r^{1/2} K_{\ell+1/2}(sr)$ obeys (2.6) and this solution is the one in (2.7) with $f(t-r) = e^{s(t-r)}$ for the underlying profile function. Of course this does not have compact support and is not used in the following.

For half-integer order, we have [1]

$$K_{\ell+1/2}(z) = \sqrt{\frac{\pi}{2z}} e^{-z} W_\ell(z), \quad W_\ell(z) = \sum_{k=0}^{\ell} \frac{c_{\ell k}}{z^k}, \quad c_{\ell k} = \frac{1}{2^k k!} \frac{(\ell+k)!}{(\ell-k)!}, \quad (2.12)$$

and the first few Macdonald functions are (see 10.2.15-17 in [1])

$$\begin{aligned} +K_{3/2}(z) &= \sqrt{\frac{\pi}{2z}} e^{-z} \left(1 + \frac{1}{z}\right) \\ \diamond K_{5/2}(z) &= \sqrt{\frac{\pi}{2z}} e^{-z} \left(1 + \frac{3}{z} + \frac{3}{z^2}\right) \\ \circ K_{7/2}(z) &= \sqrt{\frac{\pi}{2z}} e^{-z} \left(1 + \frac{6}{z} + \frac{15}{z^2} + \frac{15}{z^3}\right) \\ *K_{9/2}(z) &= \sqrt{\frac{\pi}{2z}} e^{-z} \left(1 + \frac{10}{z} + \frac{45}{z^2} + \frac{105}{z^3} + \frac{105}{z^4}\right). \end{aligned} \quad (2.13)$$

The $K_{\ell+1/2}(z)$ can also be expressed as

$$K_{\ell+1/2}(z) = \sqrt{\frac{\pi}{2z}} \frac{e^{-z}}{z^\ell} p_\ell(z), \quad p_\ell(z) = \sum_{k=0}^{\ell} c_{\ell k} z^{\ell-k}, \quad (2.14)$$

where here we refer to the polynomial $p_\ell(z)$ as the *Bessel polynomial*.

Let the roots of $p_\ell(z)$ be denoted by $\{b_{\ell j} : j = 1, \dots, \ell\}$. Watson [2] shows that each $b_{\ell j}$ lies in the left-half plane and is simple. Watson's analysis is presented in the Appendix.

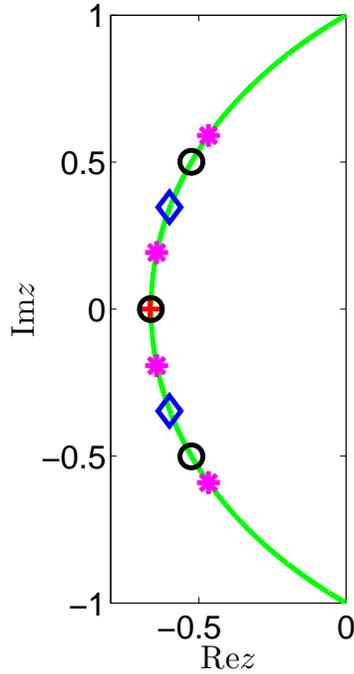


Figure 2.1: Scaled roots of $K_{\ell+1/2}(z)$.

The set $\{b_{\ell j}/(\ell + 1/2) : j = 1, \dots, \ell\}$ is the collection of roots scaled by the Bessel order $\nu = \ell + 1/2$. For $\ell = 1, 2, 3, 4$ the *scaled roots* are depicted in Fig. 2.1 using the symbols $+$, \diamond , \circ , $*$ respectively. Olver [4] showed that for large ℓ the scaled roots tend to lie on the curve given by

$$z(\lambda) = -\sqrt{\lambda^2 - \lambda \tanh \lambda} \pm i\sqrt{\lambda \coth \lambda - \lambda^2}$$

for $\lambda \in [0, \lambda_0]$, where $\lambda_0 \simeq 1.19967864025773$ solves $\tanh \lambda_0 = 1/\lambda_0$. Note that $z(0) = \pm i$, giving the two points at the end of the arc. To the eye the roots are on this curve for even small ℓ , which also illustrates that often asymptotics are good when the parameter is not large.

Chapter 3

Nonreflecting Boundary Conditions

Our goal in this section is to specify an exact transparent BC for the wave equation in the presence of a spherical boundary. Again, we will work “multipole by multipole” and specify a condition obeyed by (2.7). Technically, the analysis will be easier if we work with a spherical annulus centered at $r = 0$, thereby avoiding issues at the origin $r = 0$ which are not relevant for the outer BCs we are considering here. Therefore, we introduce inner r_0 and outer r_B radii (B for “boundary”).

In this chapter we prove the following.

Theorem 3.0.1. *Consider $1 \leq r_0 < r_B$ and the associated interval $D = [-r_B + \delta, -r_0 - \delta]$, where $0 < \delta < (r_B - r_0)/2$. Suppose that $f \in C_0^\infty(D)$, and consider the “wave field”*

$$\Psi_\ell(t, r) = \sum_{k=0}^{\ell} \frac{1}{r^k} c_{\ell k} f^{(\ell-k)}(t - r). \quad (3.1)$$

Then at $r = r_B$ the wave field obeys

$$\Psi_t(t, r_B) + \Psi_r(t, r_B) = \frac{1}{r_B} \int_0^t \Omega_\ell(t - t', r_B) \Psi_\ell(t', r_B) dt', \quad (3.2)$$

where the kernel

$$\Omega_\ell(t, r) = \sum_{n=1}^{\ell} (b_{\ell n}/r) \exp(b_{\ell n} t/r) = \partial_t \sum_{n=1}^{\ell} \exp(b_{\ell n} t/r). \quad (3.3)$$



Figure 3.1: Radial axis with support of $\Psi_\ell(0, r)$ and point at $r_B - \epsilon\delta$ (the dashed line).



Figure 3.2: Retarded time axis and support of profile function f .

We care only about (3.2) at r_B but in fact it holds for $r \geq r_B$.

3.1 Proof of Theorem 3.0.1

Our first proof of the theorem relies on the following lemma.

Lemma 3.1.1. *For $r \in (r_B - \epsilon\delta, \infty)$ with $\epsilon \leq 1$ the Laplace transform $\widehat{\Psi}_\ell(s, r)$ of the expression $\Psi_\ell(t, r)$ given in (3.1) with $f \in C_0^\infty(D)$ has form [cf. Eq. (2.12)]*

$$\widehat{\Psi}_\ell(s, r) = a(s)s^\ell e^{-sr} W_\ell(sr), \quad a(s) = \int_{-r_B + \delta}^{-r_0 - \delta} e^{-su} f(u) du. \quad (3.4)$$

Notice that $a(s)$ is independent of r , and that this holds for any complex number s .

Proof. To obtain (3.4), we proceed as follows. First consider the Laplace transform of $f^{(\ell-k)}(t-r)$ which appears in (3.1). Repeated integration by parts generates $t=0$ boundary terms of the form $f^{(\ell-k-p)}(-r)$ for $1 \leq p \leq \ell-k$; all such terms vanish. Indeed, for $r \in (r_B - \epsilon\delta, \infty)$, we have $-r < -r_B + \delta$ and so $-r \notin D$. Moreover, the profile function f and all of its derivatives vanish on $\mathbb{R} \setminus D$. The repeated integration by parts also generates $t=\infty$ boundary terms which are similarly shown to vanish.

The previous argument establishes that

$$\int_0^\infty e^{-st} f^{(\ell-k)}(t-r) dt = s^{\ell-k} e^{-sr} \int_{-r}^\infty e^{-su} f(u) du. \quad (3.5)$$

Chapter 3. Nonreflecting Boundary Conditions

The lower limit $-r$ of integration can now be replaced with $-r_B + \delta$, because $f(u) = 0$ for $u \in [-r, -r_B + \delta)$ which implies $u \notin D$, and similarly the upper limit by $-r_0 - \delta$. \square

The proof of **Theorem 3.0.1** follows from **Lemma 3.1.1**.

Proof. The explicit expression (3.4) for $\widehat{\Psi}_\ell(s, r)$ determines an exact frequency-domain boundary condition (the Dirichlet-to-Neumann map)

$$s\widehat{\Psi}_\ell(s, r) + \partial_r \widehat{\Psi}_\ell(s, r) = \frac{1}{r} \widehat{\Omega}_\ell(s, r) \widehat{\Psi}_\ell(s, r), \quad (3.6)$$

where the *frequency-domain radiation kernel* $\widehat{\Omega}_\ell(s, r)$ defines the Sommerfeld residual. Indeed, the operator on the left hand of (3.6) corresponds to the Sommerfeld operator $\partial_t + \partial_r$ in the time-domain. If $\ell = 0$, then $s\widehat{\Psi}_\ell(s, r) + \partial_r \widehat{\Psi}_\ell(s, r) = 0$. In (3.6) $\widehat{\Omega}_\ell(s, r)$ is essentially the logarithmic derivative of $W_\ell(sr)$,

$$\widehat{\Omega}_\ell(s, r) \equiv sr \frac{W'_\ell(sr)}{W_\ell(sr)} = \sum_{k=1}^{\ell} \frac{b_{\ell k}/r}{s - b_{\ell k}/r}. \quad (3.7)$$

The last equality arises from the following consideration. We recognize $W_\ell(z)$ as the expression given in (2.12). With this result and (3.6), we get (3.2) - (3.3) upon inverse Laplace transformation. \square

Remark: The proof of **Lemma 3.1.1** shows that **Theorem 3.0.1** actually holds for any $\Psi_\ell(t, r)$ of the form (3.1). That is the $c_{\ell k}$ need not be the special expressions in (2.12). Of course for general $c_{\ell k}$ the $b_{\ell k}$ in **Theorem 3.0.1** must be the corresponding roots of $p_\ell(z) = \sum_{k=1}^{\ell} c_{\ell k} z^{\ell-k}$. Moreover, if the $c_{\ell k}$ are not those given in (2.12), then $\Psi_\ell(t, r)$ will not generally solve the radial wave equation (2.6).

Let us now consider what the boundary kernels for a spherical boundary look like for the cases $\ell = 1$ and $\ell = 2$. For the case $\ell = 1$, we refer to the general radial wave equation (2.6) to get (suppressing the $\ell = 1$ subscript)

$$-s^2 \widehat{\Psi} + \widehat{\Psi}_{rr} - \frac{2}{r^2} \widehat{\Psi} = 0 \quad (3.8)$$

Chapter 3. Nonreflecting Boundary Conditions

for the Laplace-transformed equation. In order to peel off the exponential dependence of the outgoing solution, we let $\widehat{\Psi} = e^{-sr}\widehat{\Phi}$ to obtain

$$\widehat{\Phi}_{rr} - 2s\widehat{\Phi}_r - \frac{2}{r^2}\widehat{\Phi} = 0. \quad (3.9)$$

Letting $z = sr$ gives us

$$\widehat{\Phi}_{zz} - 2\widehat{\Phi}_z - \frac{2}{z^2}\widehat{\Phi} = 0. \quad (3.10)$$

Linearly independent solutions to this equation are

$$W_1(z) = 1 + \frac{1}{z} \quad Z_1(z) = e^{2z}\left(1 - \frac{1}{z}\right). \quad (3.11)$$

The product $\Omega_1(s, r)$ of z and the logarithmic derivative of W_1 for $z = sr$ then takes the form

$$\Omega_1(s, r) = \frac{zW_1'(z)}{W_1(z)} = \frac{z(-\frac{1}{z^2})}{1 + \frac{1}{z}} = -\frac{1}{z + 1}. \quad (3.12)$$

Now, for the case $\ell = 2$, we again refer to the general radial wave equation (2.6) to get (suppressing the $\ell = 2$ subscript)

$$\widehat{\Phi}_{rr} - 2s\widehat{\Phi}_r - \frac{6}{r^2}\widehat{\Phi} = 0 \quad (3.13)$$

for the Laplace-transformed equation. Letting $z = sr$ gives us

$$\widehat{\Phi}_{zz} - 2\widehat{\Phi}_z - \frac{6}{z^2}\widehat{\Phi} = 0. \quad (3.14)$$

The linearly independent solutions to this equation are then

$$W_2(z) = 1 + \frac{3}{z} + \frac{3}{z^2} \quad Z_2(z) = e^{2z}\left(1 - \frac{3}{z} + \frac{3}{z^2}\right), \quad (3.15)$$

and the product $\Omega_2(s, r)$ of z and the logarithmic derivative of W_2 for $z = sr$ then takes the form

$$\Omega_2(s, r) = \frac{zW_2'(z)}{W_2(z)} = \frac{z(-\frac{3}{z^2} - \frac{6}{z^3})}{1 + \frac{3}{z} + \frac{3}{z^2}} = \frac{-3z - 6}{z^2 + 3z + 3}. \quad (3.16)$$

3.2 Alternative proof.

This subsection sketches an outline of a different formal proof of the convolution result (3.2) in **Theorem 3.0.1** by solving (2.6) on (r_0, ∞) as an initial value problem assuming (i) $\Psi(t, r_0) = 0$ and (ii) data of compact support on $[r_0 + \delta, r_B - \delta]$, $0 < \delta < (r_B - r_0)/2$. Unlike the previous proof, this one relies on the wave equation and so assumes ultimately that the $c_{\ell k}$ are those given in (2.12). However, this proof allows for different initial data than that associated with (3.1). In the proof we continue to suppress the ℓ on Ψ .

Proof. The Laplace transform of (2.6) is

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - s^2 \right] \widehat{\Psi}(s, r) = -\dot{\Psi}(0, r) - s\Psi(0, r). \quad (3.17)$$

Since $\Psi(t, r_0) = 0$, we have $\widehat{\Psi}(s, r_0) = 0$. Furthermore, we require $\widehat{\Psi}(s, r) \sim e^{-sr}$ as $r \rightarrow \infty$ (the latter “boundary condition at ∞ ” is the outgoing assumption).

We solve (3.17) subject to the specified boundary conditions via the method of Green’s functions. The following are solutions to the homogeneous equation [i.e. (3.17) with the right-hand side set to zero]:

$$\sqrt{2\pi sr} I_{\ell+1/2}(sr), \quad \sqrt{\frac{2sr}{\pi}} K_{\ell+1/2}(sr), \quad (3.18)$$

where $I_\nu(z)$ is the other modified Bessel function. Choosing linearly independent solutions u, v (for $\text{Re}(s) > 0$) such that $u(r_0) = 0$ and $v(r) \sim e^{-sr}$ we obtain

$$u(r) = I_{\ell+1/2}(r_0 s) \sqrt{\frac{\pi r}{2s}} K_{\ell+1/2}(sr) - K_{\ell+1/2}(r_0 s) \sqrt{\frac{\pi r}{2s}} I_{\ell+1/2}(sr), \quad (3.19)$$

$$v(r) = \sqrt{\frac{2sr}{\pi}} K_{\ell+1/2}(sr), \quad (3.20)$$

where of course these solutions also depend on s . Clearly, $u(r_0) = 0$ and $v(r) \sim e^{-sr}$ as $r \rightarrow \infty$. The Wronskian $\mathcal{W}(r) = u(r)v'(r) - v(r)u'(r)$ is then

$$\begin{aligned} \mathcal{W}(r) &= -sr K_{\ell+1/2}(sr_0) \left[I_{\ell+1/2}(sr) K'_{\ell+1/2}(sr) - K_{\ell+1/2}(sr) I'_{\ell+1/2}(sr) \right] \\ &= -sr K_{\ell+1/2}(sr_0) \left(-\frac{1}{sr} \right) = K_{\ell+1/2}(sr_0), \end{aligned} \quad (3.21)$$

Chapter 3. Nonreflecting Boundary Conditions

where the prime denotes differentiation in the argument. The boundary value problem could be solved using variation of parameters, however we take a Green's function approach.

The Green's function $G(r, \xi; s)$ obeys

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - s^2 \right] G(r, \xi; s) = -\delta(r - \xi), \quad (3.22)$$

as well as the boundary conditions $G(r_0, \xi; s) = 0$ and $G(r, \xi; s) \sim e^{-sr}$ as $r \rightarrow \infty$. The Green's function is then [5]

$$G(r, \xi; s) = \begin{cases} -\frac{u(r)v(\xi)}{K_{\ell+1/2}(sr_0)} & \text{for } r_0 < r \leq \xi \\ -\frac{u(\xi)v(r)}{K_{\ell+1/2}(sr_0)} & \text{for } \xi \leq r < \infty. \end{cases} \quad (3.23)$$

The solution $\widehat{\Psi}(s, r)$ to the boundary problem (3.17) is then the spatial convolution

$$\widehat{\Psi}(s, r) = \int_{r_0+\delta}^{r_B-\delta} G(r, \xi, s) [\dot{\Psi}(0, \xi) + s\Psi(0, \xi)] d\xi. \quad (3.24)$$

For $r > r_B - \delta$, we have

$$\begin{aligned} \widehat{\Psi}(s, r) &= - \int_{r_0+\delta}^{r_B-\delta} \frac{u(\xi)v(r)}{K_{\ell+1/2}(sr_0)} [\dot{\Psi}(0, \xi) + s\Psi(0, \xi)] d\xi \\ &= - \frac{v(r)}{K_{\ell+1/2}(sr_0)} \int_{r_0+\delta}^{r_B-\delta} u(\xi) [\dot{\Psi}(0, \xi) + s\Psi(0, \xi)] d\xi \\ &= - \frac{v(r)}{K_{\ell+1/2}(sr_0)} A(s). \end{aligned} \quad (3.25)$$

Using (2.12) and (3.20) then gives

$$\begin{aligned} \widehat{\Psi}(s, r) &= -A(s) \sqrt{\frac{2sr}{\pi}} \frac{K_{\ell+1/2}(sr)}{K_{\ell+1/2}(sr_0)} \\ &= -A(s) \sqrt{\frac{2sr}{\pi}} \frac{1}{K_{\ell+1/2}(sr_0)} \sqrt{\frac{\pi}{2sr}} e^{-sr} W_\ell(sr) \\ &= b(s) e^{-sr} W_\ell(sr). \end{aligned} \quad (3.26)$$

Chapter 3. Nonreflecting Boundary Conditions

Here

$$b(s) = -\frac{1}{K_{\ell+1/2}(sr_0)} \int_{r_0+\delta}^{r_B-\delta} u(\xi) [\dot{\Psi}(0, \xi) + s\Psi(0, \xi)] d\xi. \quad (3.27)$$

For general compact initial data $b(s)$ cannot be expressed as $s^\ell a(s)$ as in (3.4). From this point the proof follows exactly the steps of the first proof after **Lemma 3.1.1**. \square

Chapter 4

Newton's Identities

4.1 Main result

Our goal is to prove the following result.

Theorem 4.1.1. *The roots $b_{\ell j} : j = 1, \dots, \ell$ of the ℓ th degree polynomial*

$$p_{\ell}(z) = \sum_{k=0}^{\ell} c_{\ell k} z^{\ell-k} \tag{4.1}$$

also obey the following set of ℓ algebraic equations

$$-k c_{\ell k} = \sum_{n=1}^{\ell} b_{\ell n} \sum_{q=1}^k c_{\ell, q-1} (b_{\ell n})^{k-q}, \quad k = 1, \dots, \ell, \tag{4.2}$$

where here we assume $\ell \geq 1$.

Remark: All of the factors in this system (roots $b_{\ell j}$ and coefficients $c_{\ell j}$) carry a lead “name” index ℓ . We now suppress this index, and reorganize the last expressions using $c_{\ell 0} \equiv c_0 = 1$ and the re-indexing $p = q - 1$ to reach

$$-k c_k = \sum_{n=1}^{\ell} (b_n)^k + \sum_{p=1}^{k-1} c_p \sum_{n=1}^{\ell} (b_n)^{k-p}, \quad k = 1, \dots, \ell. \tag{4.3}$$

Chapter 4. Newton's Identities

These formulas involve the power sums $s_k = \sum_{n=1}^{\ell} (b_n)^k$ of the roots. In terms of the s_k and $a_{\ell-k} \equiv c_k$, we then have

$$-ka_{\ell-k} = s_k + \sum_{p=1}^{k-1} a_{\ell-p} s_{k-p}, \quad k = 1, \dots, \ell, \quad (4.4)$$

which we recognize as a subset of Newton's identities [6].

In what remains of this section, we prove **Theorem 4.1.1** assuming **Theorem 3.0.1** which was established in the previous chapter. The idea of the proof is fairly straightforward; using the expressions (3.1) and (3.2), we find the identity

$$-\sum_{k=1}^{\ell} \frac{k}{r_B^{k+1}} c_{\ell k} f^{(\ell-k)}(t-r_B) = \frac{1}{r_B} \int_0^t \Omega_{\ell}(t-t', r_B) \left[\sum_{k=0}^{\ell} \frac{1}{r_B^k} c_{\ell k} f^{(\ell-k)}(t'-r_B) \right] dt', \quad t > 0. \quad (4.5)$$

The proof amounts to a careful comparison of both sides in the last equation.

Lemma 4.1.2. *Let $r = r_B$ and $f \in C_0^{\infty}(D)$ as in **Theorem 3.0.1**, and define*

$$I^{(p)}[b, r, f] = \int_0^t e^{b(t-t')/r} f^{(p)}(t'-r) dt'. \quad (4.6)$$

Then, we have

$$I^{(p)}[b, r, f] = (b/r)^p I^{(0)}[b, r, f] + \sum_{j=1}^p (b/r)^{p-j} f^{(j-1)}(t-r). \quad (4.7)$$

Proof. We prove the lemma by induction, showing that

$$I^{(p)}[b, r, f] = (b/r)^p I^{(0)}[b, r, f] + \sum_{j=1}^p (b/r)^{p-j} [f^{(j-1)}(t-r) - e^{bt/r} f^{(j-1)}(-r)], \quad (4.8)$$

where the second term within the square brackets vanishes since $r = r_B \notin D$. Integration by parts establishes the last formula for $p = 1$. Similarly, integration by parts yields

$$I^{(p)}[b, r, f] = (b/r) I^{(p-1)}[b, r, f] + f^{(p-1)}(t-r) - e^{bt/r} f^{(p-1)}(-r). \quad (4.9)$$

Assuming now that (4.8) holds with p replaced by $p - 1$, we insert the $p - 1$ result into the last equation, thereby recovering (4.8) and verifying the induction step. \square

We now use **Theorem 3.0.1** to prove **Theorem 4.1.1**.

4.2 Proof of Theorem 4.1.1

Proof. First, taking $r = r_B$ and $t > 0$ and then appealing to the formulas (3.1) and (3.3), we get

$$\begin{aligned} \frac{1}{r} \int_0^t \Omega_\ell(t - t', r) \Psi_\ell(t', r) dt' &= \sum_{n=1}^{\ell} (b_{\ell n}/r^2) \int_0^t \exp(b_{\ell n}(t - t')/r) \Psi_\ell(t', r) dt' \\ &= \sum_{n=1}^{\ell} (b_{\ell n}/r^2) \sum_{k=0}^{\ell} r^{-k} c_{\ell k} I^{(\ell-k)}[b_{\ell n}, r, f]. \end{aligned} \quad (4.10)$$

We will now focus on reducing this last expression to a desirable form. Lemma 4.1.2 gives

$$I^{(\ell-k)}[b_{\ell n}, r, f] = (b_{\ell n}/r)^{\ell-k} I^{(0)}[b_{\ell n}, r, f] + \sum_{j=1}^{\ell-k} (b_{\ell n}/r)^{\ell-k-j} f^{(j-1)}(t - r). \quad (4.11)$$

Combination of the last two equations yields

$$\begin{aligned} \frac{1}{r} \int_0^t \Omega_\ell(t - t', r) \Psi_\ell(t', r) dt' &= r^{-(\ell+2)} \sum_{n=1}^{\ell} b_{\ell n} I^{(0)}[b_{\ell n}, r, f] \sum_{k=0}^{\ell} c_{\ell k} (b_{\ell n})^{\ell-k} \\ &\quad + \sum_{n=1}^{\ell} (b_{\ell n}/r^2) \sum_{k=0}^{\ell} r^{-k} c_{\ell k} \sum_{j=1}^{\ell-k} (b_{\ell n}/r)^{\ell-k-j} f^{(j-1)}(t - r). \end{aligned} \quad (4.12)$$

Since $\sum_{k=0}^{\ell} c_{\ell k} (b_{\ell n})^{\ell-k} = p_\ell(b_{\ell n})$ is the Bessel polynomial evaluated at one of its roots, the first term on the right-hand side of the last expression vanishes. Whence, up to now

$$\frac{1}{r} \int_0^t \Omega_\ell(t - t', r) \Psi_\ell(t', r) dt' = \sum_{n=1}^{\ell} (b_{\ell n}/r^2) \sum_{k=0}^{\ell} r^{-k} c_{\ell k} \sum_{j=1}^{\ell-k} (b_{\ell n}/r)^{\ell-k-j} f^{(j-1)}(t - r). \quad (4.13)$$

Chapter 4. Newton's Identities

Within the sum over k , the sum over j is empty when $k = \ell$ (no boundary term is generated by the term in (3.1) corresponding to the undifferentiated profile function f). Therefore, here we may replace $\sum_{k=0}^{\ell}$ by $\sum_{k=0}^{\ell-1}$. This replacement, followed by the re-indexing $q = k + 1$, yields

$$\frac{1}{r} \int_0^t \Omega_{\ell}(t-t', r) \Psi_{\ell}(t', r) dt' = \sum_{n=1}^{\ell} (b_{\ell n}/r^2) \sum_{q=1}^{\ell} r^{-(q-1)} c_{\ell, q-1} \sum_{j=1}^{\ell-q+1} (b_{\ell n}/r)^{\ell-q-j+1} f^{(j-1)}(t-r). \quad (4.14)$$

Now, the double sum $\sum_{q=1}^{\ell} \sum_{j=1}^{\ell-q+1} (\text{terms})_{jq}$ is equivalent to $\sum_{j=1}^{\ell} \sum_{q=1}^{\ell-j+1} (\text{terms})_{jq}$. As a result, we may group the two inner sums and make this exchange, thereby reaching

$$\frac{1}{r} \int_0^t \Omega_{\ell}(t-t', r) \Psi_{\ell}(t', r) dt' = \sum_{n=1}^{\ell} b_{\ell n} \sum_{j=1}^{\ell} r^{j-(\ell+2)} \sum_{q=1}^{\ell-j+1} c_{\ell, q-1} (b_{\ell n})^{\ell-q-j+1} f^{(j-1)}(t-r). \quad (4.15)$$

Finally, re-indexing by $k = \ell - j + 1$ leads to

$$\frac{1}{r} \int_0^t \Omega_{\ell}(t-t', r) \Psi_{\ell}(t', r) dt' = \sum_{n=1}^{\ell} b_{\ell n} \sum_{k=1}^{\ell} r^{-(k+1)} \sum_{q=1}^k c_{\ell, q-1} (b_{\ell n})^{k-q} f^{(\ell-k)}(t-r), \quad (4.16)$$

which is the aforementioned desirable form.

Equation (4.16) can now be used to finish the proof. Recalling that we have set $r = r_B$, with (4.16) the identity (4.5) becomes

$$-\sum_{k=1}^{\ell} k r^{-(k+1)} c_{\ell k} f^{(\ell-k)}(t-r) = \sum_{k=1}^{\ell} r^{-(k+1)} \sum_{n=1}^{\ell} b_{\ell n} \sum_{q=1}^k c_{\ell, q-1} (b_{\ell n})^{k-q} f^{(\ell-k)}(t-r), \quad (4.17)$$

and we may express that last equation as

$$0 = \sum_{k=1}^{\ell} r^{-(k+1)} E_k f^{(\ell-k)}(u), \quad E_k = k c_{\ell k} + \sum_{n=1}^{\ell} b_{\ell n} \sum_{q=1}^k c_{\ell, q-1} (b_{\ell n})^{k-q}. \quad (4.18)$$

Here $u = t - r$ is retarded time.

Introducing the operator $Q \equiv (\partial_t + \partial_r)r^2$, we then use induction to show that

$$Q^p \sum_{k=1}^{\ell} r^{-(k+1)} E_k f^{(\ell-k)}(u) = \sum_{k=p+1}^{\ell} (-1)^p \frac{(k-1)!}{(k-p-1)!} r^{-(k-p+1)} E_k f^{(\ell-k)}(u). \quad (4.19)$$

Chapter 4. Newton's Identities

For $p = \ell - 1$, this identity implies $E_\ell = 0$. Then assuming $E_{p+2} = \cdots = E_\ell = 0$, we find

$$Q^p \sum_{k=1}^{\ell} r^{-(k+1)} E_k f^{(\ell-k)}(u) = (-1)^p \frac{p!}{r^2} E_{p+1} f^{(\ell-p-1)}(u), \quad (4.20)$$

yielding $E_{p+1} = 0$. Therefore, backwards iteration $p = \ell - 1, \ell - 2, \dots, 0$ establishes that $E_k = 0$ for $k = 1, \dots, \ell$. □

Chapter 5

Numerical root evaluation and identity check for several values of ℓ

As a means of verifying the result from the previous chapter, we now proceed to check these identities numerically. One might ask why there is need to check Newton's identities, classical formulas known for centuries. The point is that by checking them for the particular case of the Bessel polynomial we may (i) understand their conditioning in this setting and (ii) further confirm the accuracy of our numerically generated Macdonald roots. Using **Mathematica**, we first generate the roots of the polynomial $p_\ell(z)$ in (2.14) to as much precision as needed for several values of ℓ . These root sets for each value of ℓ are then input into the set of ℓ identities (4.2), specifically by evaluating the expression

$$kc_{\ell k} + \sum_{n=1}^{\ell} b_{\ell n} \sum_{q=1}^k c_{\ell, q-1} (b_{\ell n})^{k-q}, \quad k = 1, \dots, \ell \quad (5.1)$$

to the desired precision. The accuracy with which this expression (5.1) evaluates to zero can be seen as a verification of the identity (4.5). For each ℓ value, this generates a set of ℓ errors for each value of k in (4.2). The maximum absolute error of the identity in this set of ℓ errors is then found as $|Err_{max}| = \max\{|Err_k|\}$, where Err_k is the error in the k^{th} identity for a particular value of ℓ . The accuracy to which this error is known is then output. One

observes that the accuracy of the errors reduces as ℓ grows. The concluding section discusses this observation.

5.1 Root finding and identity verification for $\ell = 20$ to 27 digits of precision

The **Mathematica** code and associated output follow, showing that the identity is indeed verified for these ℓ values at this level of precision. This code can be altered to increase both with satisfying results. Since complex roots appear as conjugate pairs, only the upper conjugate is listed for the sake of brevity.

```
(* set precision of calculations and highest l value *)
```

```
numdigits:=28
```

```
lmax:=20
```

```
$MaxExtraPrecision:=∞
```

```
(*define c_{l,k}*)
```

```
cee[l_,k_]:=1/(2^k * k!) * (l + k)!/(l - k)!
```

```
(* define polynomial to find roots of *)
```

```
polyroots:=NSolve[Sum[cee[l,k] * z^(l - k), {k,0,l}] == 0, z, numdigits]
```

```
(* define identity from main theorem *)
```

```
identity:=k * cee[l,k] + SetPrecision[
```

```
Sum[Part[{z}/.polyroots, n] * Sum[cee[l, q - 1] * Part[{z}/.polyroots, n]^(k - q), {q,1,k}],  
{n,1,l}], numdigits]
```

```
(* loop through each value of l *)
For[l = 1, l < lmax + 1, l++,
Print[]
Print["real and imaginary parts of roots for l=", l]
Print[]

(* print out formatted tables of polynomial roots *)
For[j = 1, j < l + 1, j++,
If[Im[Part[Part[{z}/.polyroots, j - 1], 1]] < 0, ,
Print[ScientificForm[Re[Part[Part[{z}/.polyroots, j - 1], 1]], numdigits - 1,
NumberFormat →
(Row[{#1, E, If[#3 == "", "+000", If[Part[Characters[#3], 1] == "-",
StringJoin["-00", StringDrop[#3, 1]], StringJoin["+00", #3]]]}&)],
" ", ScientificForm[Im[Part[Part[{z}/.polyroots, j - 1], 1]], numdigits - 1,
NumberFormat →
(Row[{#1, E, If[#3 == "", "+000", If[Part[Characters[#3], 1] == "-",
StringJoin["-00", StringDrop[#3, 1]], StringJoin["+00", #3]]]}&)]
]]

(* print error norm of all roots for a given value of l *)
Print[]
Print["identity error accuracy ~ ",
ScientificForm[Max[Abs[Part[Part[Delete[Reap[For[k = 1, k < l + 1, k++, Sow[identity]];
], 1], 1], 1]], numdigits,
NumberFormat →
(Row[{ "1.", E, If[#3 == "", "+000", If[Part[Characters[#3], 1] == "-",
StringJoin["-0", StringDrop[#3, 1]], StringJoin["+0", #3]]]}&)]))]
```


Chapter 5. Numerical root evaluation and identity check for several values of ℓ

real and imaginary parts of roots for $l=4$

-2.89621060282037216839439393E+000 8.67234128934503751818973215E-001
-2.10378939717962783160560607E+000 2.65741804185675271685832210E+000

identity error accuracy $\sim 1.E-025$

real and imaginary parts of roots for $l=5$

-3.64673859532964325973516964E+000 0E+000
-3.35195639915353314301641425E+000 1.74266141618319772272632347E+000
-2.32467430318164522711600093E+000 3.57102292033797640038610261E+000

identity error accuracy $\sim 1.E-024$

real and imaginary parts of roots for $l=6$

-4.24835939586336394493607975E+000 8.67509673231365606386441571E-001
-3.73570835632581466794136197E+000 2.62627231144712564049355159E+000
-2.51593224781082138712255828E+000 4.49267295365394253591824392E+000

identity error accuracy $\sim 1.E-023$

real and imaginary parts of roots for $l=7$

-4.97178685852793567786117785E+000 0E+000
-4.75829052815462894523746281E+000 1.73928606113053654289381190E+000
-4.07013916363813747170592771E+000 3.51717404770975316581518078E+000
-2.68567687894326574412602056E+000 5.42069413071674889584849422E+000

identity error accuracy $\sim 1.E-022$

Chapter 5. Numerical root evaluation and identity check for several values of ℓ

real and imaginary parts of roots for l=8

-5.58788604326308519899909296E+000	8.67614445352786459816302823E-001
-5.20484079063688191825036523E+000	2.61617515264252742873877731E+000
-4.36828921720240240703092253E+000	4.41444250047153908355026146E+000
-2.83898394889763047571961928E+000	6.35391129860487682208469639E+000

identity error accuracy ~ 1.E-020

real and imaginary parts of roots for l=9

-6.29701918171496853775919603E+000	0E+000
-6.12936790427427278778116357E+000	1.73784838348086250370031346E+000
-5.60442181950778141621337163E+000	3.49815691788609357601465626E+000
-4.63843988718039029665812495E+000	5.31727167543565114230342731E+000
-2.97926079818007123046774183E+000	7.29146368834218209076005832E+000

identity error accuracy ~ 1.E-019

real and imaginary parts of roots for l=10

-6.92204490542724611542320812E+000	8.67665195451221438446134323E-001
-6.61529096547687025894515467E+000	2.61156792080008987349400899E+000
-5.96752832858778584036140538E+000	4.38494718894193206818405874E+000
-4.88621956685899957989604215E+000	6.22498548247156710752681539E+000
-3.10891623364909820537418967E+000	8.23269945907358745046141002E+000

identity error accuracy ~ 1.E-018

Chapter 5. Numerical root evaluation and identity check for several values of ℓ

real and imaginary parts of roots for l=11

-7.62233984579642949207664512E+000	0E+000
-7.48422986073193879164098577E+000	1.73710282075340382415004181E+000
-7.05789238766995313732999335E+000	3.48901450355582971973580520E+000
-6.30133745487130838170915958E+000	5.27619174369676828439756131E+000
-5.11564828390827892036268160E+000	7.13702075889336672017633185E+000
-3.22972208992030602291885715E+000	9.17711156870857844433181315E+000

identity error accuracy $\sim 1.E-016$

real and imaginary parts of roots for l=12

-8.25342201141208096388242751E+000	8.67693572009768815999260468E-001
-7.99727059960143416395771680E+000	2.60906653694579815898358031E+000
-7.46557124035177041635434551E+000	4.37016959335456516328553217E+000
-6.61100424995635186370036445E+000	6.17153499303722969677556413E+000
-5.32970859087582917461993816E+000	8.05290686425703263930869928E+000
-3.34302330780253341748520757E+000	1.01242968072408198876735301E+001

identity error accuracy $\sim 1.E-015$

real and imaginary parts of roots for l=13

-8.94770967439179101800795175E+000	0E+000
-8.83025208414490416096754110E+000	1.73666640030763054334032015E+000
-8.47059177147718456305833984E+000	3.48386845066099304960125471E+000
-7.84438027706259622338290970E+000	5.25490340661196188422886280E+000
-6.90037282614665984409350267E+000	7.07064431215294895763843768E+000
-5.53068098334403653612614328E+000	8.97224777515578769951113656E+000
-3.44986722062872316336758754E+000	1.10739285522161970404484911E+001

identity error accuracy $\sim 1.E-013$

```
real and imaginary parts of roots for l=14
```

```
-9.58317139364696666545939559E+000  8.67711028864253165359599786E-001  
-9.36314585160955222518717854E+000  2.60755332438166661179716945E+000  
-8.91100055537504426431713428E+000  4.36160417830244736590463016E+000  
-8.19884696998847462160089744E+000  6.14304107147079673955607766E+000  
-7.17239596217181731547627714E+000  7.97321735418496849451244718E+000  
-5.72035238382751889004599461E+000  9.89470759748915927072561405E+000  
-3.55108688338062601791312240E+000  1.20257380322545244924387964E+001
```

```
identity error accuracy ~ 1.E-012
```

```
real and imaginary parts of roots for l=15
```

```
-1.02731096663224778078893516E+001  0E+000  
-1.01709139964400681778642607E+001  1.73638891945045594842184913E+000  
-9.85956722839627922331631815E+000  3.48067121143276632621161317E+000  
-9.32359932060896942898832732E+000  5.24225889523761694360563458E+000  
-8.53245905229834060184246438E+000  7.03439362551704559270114646E+000  
-7.42939699294215379659889775E+000  8.87898262112151570044737878E+000  
-5.90015171366464763005831176E+000  1.08199991377535732063444092E+001  
-3.64735686248830223738674416E+000  1.29795010707604194609117519E+001
```

```
identity error accuracy ~ 1.E-011
```

Chapter 5. Numerical root evaluation and identity check for several values of ℓ

```
real and imaginary parts of roots for l=16
-1.09118860786775030650439450E+001  8.67722527435720452392272192E-001
-1.07189858189780134799231120E+001  2.60656700725828947911621149E+000
-1.03251196023414622533772726E+001  4.35616338060960859540158749E+000
-9.71232633256350378195566778E+000  6.12576089102176697237096423E+000
-8.84796819650278498065891895E+000  7.92877285588937164588993504E+000
-7.67324079086715998439086145E+000  9.78769743836906830811183539E+000
-6.07124138290869981857329635E+000  1.17478749384808882640804452E+001
-3.73923179716087263607692588E+000  1.39350284758133825846001679E+001

identity error accuracy ~ 1.E-09
```

```
real and imaginary parts of roots for l=17
-1.15985294923395501618999203E+001  0E+000
-1.15080767771397596143175561E+001  1.73620153790806340947249102E+000
-1.12334368172695439283853762E+001  3.47854389076469685688536076E+000
-1.07641341775628432905926096E+001  5.23407490203687631572176595E+000
-1.00802944448577807095976715E+001  7.01200998269376838973610942E+000
-9.14758867760315452597282895E+000  8.82599830149333386118061796E+000
-7.90544959593734230266452814E+000  1.06991450754651671694245213E+001
-6.23458097836041372958967294E+000  1.26781202290665046041369318E+001
-3.82717378509938681792979640E+000  1.48921589246642892796739770E+001

identity error accuracy ~ 1.E-07
```

Chapter 5. Numerical root evaluation and identity check for several values of ℓ

real and imaginary parts of roots for $l=18$

-1.22399021368250294751608712E+001	8.67730500530609374492680708E-001
-1.20681358449367730276078721E+001	2.60588788173345421215154585E+000
-1.17189487956552908233983590E+001	4.35247975429983523855180469E+000
-1.11800390165370403880516547E+001	6.11439409303699536109075213E+000
-1.04300129653021452464250164E+001	7.90089310331303521101324559E+000
-9.43313222080871295101261560E+000	9.72590031412845700845172164E+000
-8.12728394509562492375307106E+000	1.16131317511959929859269619E+001
-6.39097278368397486896633901E+000	1.36105473490914326733665756E+001
-3.91157229115540829562420106E+000	1.58507535969377336782227290E+001

identity error accuracy $\sim 1.E-06$

real and imaginary parts of roots for $l=19$

-1.29239630554237278712291506E+001	0E+000
-1.28428277968952223042629424E+001	1.73606905090273320111409963E+000
-1.25970628096647620973052159E+001	3.47705490010667713280513635E+000
-1.21792312603829384923664555E+001	5.22845054839089777949190898E+000
-1.15756010654031831963984511E+001	6.99707637470125717969882230E+000
-1.07635384400032784129991877E+001	8.79229302167302653136215767E+000
-9.70610240075824858168220378E+000	1.06283211002462878627136475E+001
-8.33980071913673608260638162E+000	1.25294838239446239254763941E+001
-6.54109506216141403075300463E+000	1.45449913030212108164540177E+001
-3.99275891788235286601158213E+000	1.68106920601116228524404469E+001

identity error accuracy $\sim 1.E-04$

```
real and imaginary parts of roots for l=20
```

```
-1.35674242831533132904409805E+001  8.67736254955798277563901221E-001  
-1.34125971436066018984302504E+001  2.60540014717949754240528038E+000  
-1.30988224745771632490213023E+001  4.34986491179146240148265878E+000  
-1.26172813166098517250117887E+001  6.10647987005239646124623649E+000  
-1.19530908024999872535298649E+001  7.88205843424744989157438123E+000  
-1.10825803337311520272082869E+001  9.68609324182857851119637990E+000  
-9.96776247886039112461620511E+000  1.15331147285162466386412696E+001  
-8.54389572685003190873213213E+000  1.34480452734196997247112442E+001  
-6.68552687829519020092395369E+000  1.54813061879236185543330417E+001  
-4.07101856181631732208523537E+000  1.77718690688854561225973949E+001
```

```
identity error accuracy ~ 1.E-03
```

Chapter 6

Conclusion

We conclude with some comments on the significance of the analysis done here as it relates to the larger context. The main result can be viewed from two perspectives regarding Newton's identities (4.2) and their relation to the convolution result (3.2).

Recall that the first proof of **Theorem 3.0.1** does not rely on the particular form of the coefficients $c_{\ell k}$ in (2.12). See **Lemma 3.1.1** and the following remark. Thus, **Chapter 4** may be viewed as a derivation of general Newton's identities (or at least a subset thereof, see [6]), with the derivation assuming the convolution result provided earlier in **Theorem 3.0.1**. Alternatively, by first assuming Newton's identities, the analysis in **Chapter 4** can also be viewed as a time-domain proof of the convolution result in **Theorem 3.0.1** without the need for the Laplace transform.

Newton's identities for the particular case of the roots and coefficients of the Macdonald function appear ill-conditioned. In other words, they seem difficult to verify accurately for large values of ℓ . This is most likely due to the coefficients $c_{\ell k}$ which for a fixed large ℓ ($\ell = 20$ for example) vary over a large range, being factorially defined as they are in (2.12). This combined with the relative proximity of the roots to the origin (see Fig 2.1) leads to a necessity of many digits of precision for accurate numerical verification.

Appendix A

Location and count of Macdonald roots

For any positive $\nu \geq 0$ Watson [2] has shown that the roots of $K_\nu(z)$ are simple and lie in the left-half z plane. This appendix presents some of his analysis, often tailoring it to our specific case $\nu = \ell + 1/2$, that is half-integer order. In what follows we often follow [2] quite closely. Since $K_\nu(z)$ obeys the differential equation (2.11), any root $b \neq 0$ must be simple. Indeed, were $b \neq 0$ a root of multiplicity, then we could conclude that $K_\nu''(b) = K_\nu'(b) = K_\nu(b) = 0$, and by repeated differentiation of (2.11) that $K_\nu^{(p)}(b) = 0$ for all p . Since all nonzero points of the Bessel equation are regular points, this would imply $K_\nu(z) = 0$ in a neighborhood of b . Additionally, the small z asymptotic expansion for $K_\nu(z)$ (see [1]) shows that $z = 0$ is a singular point of $K_\nu(z)$ and not a root.

We begin by noting that the generalization of Bessel's integral (see 9.6.24 [1])

$$K_\nu(z) = \int_0^\infty e^{-z \cosh(t)} \cosh(\nu t) dt, \quad |\arg z| < \frac{\pi}{2}, \quad (\text{A.1})$$

makes it clear that $K_\nu(z)$ has no positive real roots. Watson has extended this result to show that $K_\nu(z)$ has no roots such that $|\arg z| \leq \frac{\pi}{2}$.

Appendix A. Location and count of Macdonald roots

In order to demonstrate this, we must first consider a result of Macdonald (and proven in [2]) which represents the product $K_\nu(Z)K_\nu(z)$ as an integral involving a single function of type K_ν :

$$K_\nu(Z)K_\nu(z) = \frac{1}{2} \int_0^\infty \exp \left[-\frac{v}{2} - \frac{Z^2 + z^2}{2v} \right] K_\nu \left(\frac{Zz}{v} \right) \frac{dv}{v}, \quad (\text{A.2})$$

which is valid for all values of $\nu \geq 0$ when $|\arg Z| \leq \pi$, $|\arg z| \leq \pi$, and $|\arg (Z + z)| \leq \frac{\pi}{4}$. Now, if $z = re^{-i\alpha}$ were such a root ($r > 0$, $-\frac{\pi}{2} < \alpha < \frac{\pi}{2}$), then $Z = re^{i\alpha}$ would be another root by (A.1). However, the integral shows us that

$$\begin{aligned} K_\nu(re^{i\alpha})K_\nu(re^{-i\alpha}) &= \frac{1}{2} \int_0^\infty \exp \left[-\frac{v}{2} - \frac{r^2 \cos(2\alpha)}{v} \right] K_\nu \left(\frac{r^2}{v} \right) \frac{dv}{v} \\ &> 0, \end{aligned} \quad (\text{A.3})$$

which is contrary to the hypothesis that these are roots of $K_\nu(z)$. If $\alpha = \pm\frac{\pi}{2}$, then we have (again, see [2])

$$|K_\nu(re^{\pm\frac{\pi}{2}i})| = \frac{\pi}{2} \sqrt{J_\nu^2(r) + Y_\nu^2(r)}, \quad (\text{A.4})$$

and so $K_\nu(z)$ has no purely imaginary roots, because $J_\nu(r)$ and $Y_\nu(r)$ cannot both vanish simultaneously.

A.1 Root count for $K_{\ell+1/2}(z)$

For $\nu = \ell + 1/2$ (half-integer order) we have formula (2.13). Since $p_\ell(0) = c_{\ell\ell} \neq 0$ and $\sqrt{\pi/2}e^{-z}z^{-(\ell+2)}$ is singular at $z = 0$, then the origin is clearly not a root. This is an explicit check of the general result stated above. Moreover, from (2.14) we conclude that $K_{\ell+1/2}(z)$ has ℓ roots, since $p_\ell(z)$ is degree ℓ . Notice that $p_\ell(z)$ may have a root on the negative real axis, which is technically not in the domain of analyticity of $K_{\ell+1/2}(z)$ due to the branch associated with $z^{-(\ell+2)}$ in the prefactor $\sqrt{\pi/2}e^{-z}z^{-(\ell+2)}$. Nevertheless, we shall consider such a root of $p_\ell(z)$ also as a root of $K_{\ell+1/2}(z)$. With the above analysis, we conclude that $K_{\ell+1/2}(z)$ has ℓ simple roots, each lying in the left-half z plane.

A.2 Root count for $K_\nu(z)$

Now we turn our attention to general $\nu > 0$ and the roots for which $Re(z) < 0$ and with $\frac{\pi}{2} < |\arg z| < \pi$. We show that the number of roots in these two quadrants is the even integer nearest to $\nu - \frac{1}{2}$, unless $\nu - \frac{1}{2}$ itself is an integer, in which case (as seen above) it is also the number of roots.

If $\nu - \frac{1}{2}$ is not an integer, then there are no roots on the negative real axis, where $\arg z = \pm\pi$. This follows from

$$K_\nu(re^{\pm\pi i}) = e^{\mp\nu\pi i} K_\nu(r) \mp \pi i I_\nu(r), \quad (\text{A.5})$$

and for both the real and imaginary parts to vanish, then we must have

$$\cos(\nu\pi)K_\nu(r) = 0, \quad \sin(\nu\pi)K_\nu(r) + \pi I_\nu(r) = 0. \quad (\text{A.6})$$

The Wronskian of the functions on the left of the equations is $\frac{\pi}{r}\cos(\nu\pi)$. Therefore, $K_\nu(r)$ and $I_\nu(r)$ cannot vanish simultaneously unless $\cos(\nu\pi) = 0$. We now use the Argument principle to count the roots in the second and third quadrants.

Now we consider the change in phase of $z^\nu K_\nu(z)$ as z describes a contour consisting of small and large circles terminated by the lines $\arg z = \pm\pi$, together with the parts of these lines terminated by the circular arcs [cf. Fig. A.1]. Let us refer to the circles as Γ and γ , the equations of which are $|z| = R$ and $|z| = \delta$, respectively. It is clear then that the number of roots of $K_\nu(z)$ in the pair of quadrants under consideration is equal to the number of roots of $z^\nu K_\nu(z)$ inside the contour, and therefore is equal to $\frac{1}{2\pi}$ times the change in phase of $z^\nu K_\nu(z)$ as z traverses the contour. The change in phase is now

$$\left[\arg(z^\nu K_\nu(z)) \right]_\Gamma - \left[\arg(z^\nu K_\nu(z)) \right]_\gamma + \left[\arg(z^\nu K_\nu(z)) \right]_{R \exp(\pi i)}^{\delta \exp(\pi i)} + \left[\arg(z^\nu K_\nu(z)) \right]_{\delta \exp(-\pi i)}^{R \exp(-\pi i)}. \quad (\text{A.7})$$

As $R \rightarrow \infty$ and $\delta \rightarrow 0$, the first two terms tend respectively towards $2\pi(\nu - \frac{1}{2})$ and zero. This is evident from the consideration that the following asymptotic expansions are valid

Appendix A. Location and count of Macdonald roots

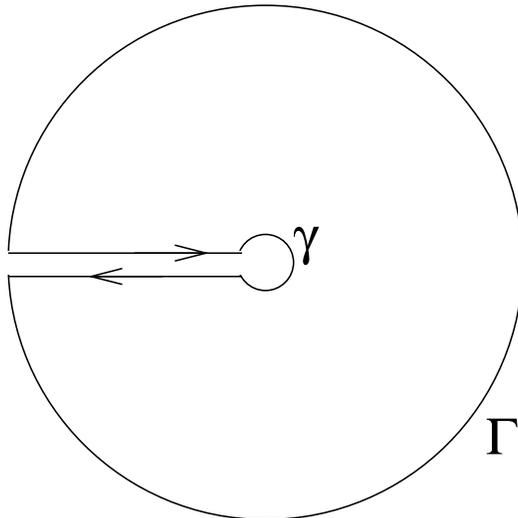


Figure A.1: Keyhole contour with arcs $\Gamma : |z| = R$ and $\gamma : |z| = \delta$

when $|\arg z| < \pi$ [2]. Respectively, when $|z|$ is large or small on the contour,

$$z^\nu K_\nu(z) \sim z^{\nu-\frac{1}{2}} e^{-z} \sqrt{\frac{\pi}{2}}, \quad z^\nu K_\nu(z) \sim 2^{\nu-1} \Gamma(\nu). \quad (\text{A.8})$$

The second expansion requires modification when $\nu = 0$.

Introduce the phase (angle) function $\text{ph}(u, v)$ which is defined as $\text{ph}(u, v) = \arg(w)$, where $w = u + iv$ and \arg is the argument function in (A.6). (In this appendix u, v clearly have a different meaning than in the main text.) The phase function $\text{ph}(u, v) = \arctan(v/u)$ if $u > 0$, but otherwise gives the correct values in the second and third quadrants. Moreover, $-\pi < \text{ph}(u, v) < \pi$ and the expression is undefined for $v = 0, u \leq 0$. Now, above and below the negative real z -axis $z^\nu K_\nu(z)$ can be expressed as

$$(re^{+\pi i})^\nu K(re^{+\pi i}) = r^\nu [K_\nu(r) + \pi \sin(\nu\pi) I_\nu(r)] - ir^\nu \pi \cos(\nu\pi) I_\nu(r) \quad (\text{A.9})$$

$$(re^{-\pi i})^\nu K(re^{-\pi i}) = r^\nu [K_\nu(r) + \pi \sin(\nu\pi) I_\nu(r)] + ir^\nu \pi \cos(\nu\pi) I_\nu(r). \quad (\text{A.10})$$

Therefore, the combination of the last two terms in (A.6) is

$$\lim_{\substack{\delta \rightarrow 0^+ \\ R \rightarrow \infty}} 2 \left[\text{ph}(K_\nu(r) + \pi \sin(\nu\pi) I_\nu(r), \pi \cos(\nu\pi) I_\nu(r)) \right]_\delta^R. \quad (\text{A.11})$$

Appendix A. Location and count of Macdonald roots

Now, $K_\nu(r)$ is a positive decreasing function of r that vanishes at infinity, while $I_\nu(r)$ is a positive increasing function of r that vanishes at $r = 0$. Therefore, $K_\nu(r) + \pi \sin(\nu\pi)I_\nu(r)$ has one root if $\sin(\nu\pi)$ is negative, and no root if $\sin(\nu\pi)$ is non-negative. In the latter case the last expression is

$$\lim_{\substack{\delta \rightarrow 0^+ \\ R \rightarrow \infty}} 2 \left[\arctan \frac{\pi \cos(\nu\pi)I_\nu(r)}{K_\nu(r) + \pi \sin(\nu\pi)I_\nu(r)} \right]_\delta^R. \quad (\text{A.12})$$

Taking the $\delta \rightarrow 0^+$, $R \rightarrow \infty$ limits in (A.11), we then find the phase

$$2 \text{ph}(\sin(\nu\pi), \cos(\nu\pi)) \quad (\text{A.13})$$

for the combination of the last two terms in (A.6). The phase $\text{ph}(\sin(\nu\pi), \cos(\nu\pi))$ has the same sign as $\cos(\nu\pi)$, and, moreover, is less than π in absolute value.

Therefore, by the Argument Principle, the total number of roots of $K_\nu(z)$ in the pair of quadrants for which $\text{Re}(z) < 0$ and $|\arg z| < \pi$ is

$$\begin{aligned} \# \text{ of roots of } K_\nu(z) &= \nu - \frac{1}{2} + \frac{1}{\pi} \text{ph}(\sin(\nu\pi), \cos(\nu\pi)) \\ &= \nu - \frac{1}{2} + \frac{1}{\pi} \text{ph}\left(\cos\left(\frac{\pi}{2} - \nu\pi\right), \sin\left(\frac{\pi}{2} - \nu\pi\right)\right) \\ &= \nu - \frac{1}{2} + \frac{1}{\pi} \left(\frac{\pi}{2} - \nu\pi + 2\pi k\right) \\ &= 2k, \end{aligned} \quad (\text{A.14})$$

where k is chosen so that $2k$ is closest to $\nu - \frac{1}{2}$.

References

- [1] Milton Abramowitz and Irene A. Stegun *Handbook of Mathematical Functions* 1964: National Bureau of Standards.
- [2] G. N. Watson *A Treatise on the Theory of Bessel Functions*, 2nd. ed 1966: Cambridge University Press.
- [3] Marcus J. Grote and Joseph B. Keller “On Nonreflecting Boundary Conditions” *Journal of Computational Physics*, 122, 231 - 243, 1995.
- [4] F. W. J. Olver, *The Asymptotic Expansion of Bessel Functions of Large Order*, Phil. Trans. Roy. Soc. Lond. A 247 (1954) 328-368.
- [5] P. K. Chattopadhyay, *Mathematical Physics*, 1990: New Age International (P) Limited, Publishers.
- [6] D. Kalman, *A Matrix Proof of Newton’s Identities*, Mathematics Magazine, vol. 73, Nov. 4, October 2000.