

On Roots of the Macdonald Function

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Setting

- Outgoing solutions to the “radial wave equation”
- Transparent radiation boundary conditions on spherical domain
- Dirichlet-to-Neumann map, Macdonald function

Outline

- Radial wave equation and the Macdonald function
- Non-reflecting boundary conditions
- Identities for roots of the Macdonald function
- Other work

Radial Wave Equation

Radial Wave Equation

Overview

- Ordinary wave equation on \mathbb{R}^3 , ($c = 1$ here): $\Delta\psi - \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} = 0$
- Laplace operator in spherical coordinates:

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

- Generic solution in terms of $Y_{\ell m}(\theta, \phi)$ of Δ_{S^2} , where

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

is:

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

Radial Wave Equation

Overview

- "multipole" solution $\psi(t, r \sin \theta \cos \phi, r \sin \theta \sin \phi, r \cos \theta)$:

$$\psi_{\ell m}(t, r) Y_{\ell m}(\theta, \phi) = r^{-1} \Psi_{\ell m}(t, r) Y_{\ell m}(\theta, \phi)$$

- Eliminating angular dependence, multipole coefficients $\psi_{\ell m}$ and $\Psi_{\ell m}$ satisfy:

$$-\partial_t^2 \psi_{\ell m} + \partial_r^2 \psi_{\ell m} + \frac{2}{r} \partial_r \psi_{\ell m} - \frac{\ell(\ell+1)}{r^2} \psi_{\ell m} = 0,$$

$$-\partial_t^2 \Psi_{\ell m} + \partial_r^2 \Psi_{\ell m} - \frac{\ell(\ell+1)}{r^2} \Psi_{\ell m} = 0.$$

Radial Wave Equation

Overview

- The Macdonald function $K_\nu(z)$ is a solution to the modified Bessel equation:

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

- For half-integer order,

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

- $K_{\ell+1/2}(z)$ can also be expressed using the monic *Bessel polynomial* $p_\ell(z)$:

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

Radial Wave Equation

Overview

- The set $\{b_{\ell j}/(\ell + 1/2) : j = 1, \dots, \ell\}$ is the collection of roots scaled by the Bessel order $\nu = \ell + 1/2$.
- These roots accumulate on a fixed transcendental curve in the left-half plane, a parametrization of which is 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 $\tanh \lambda_0 = 1/\lambda_0$.

Radial Wave Equation

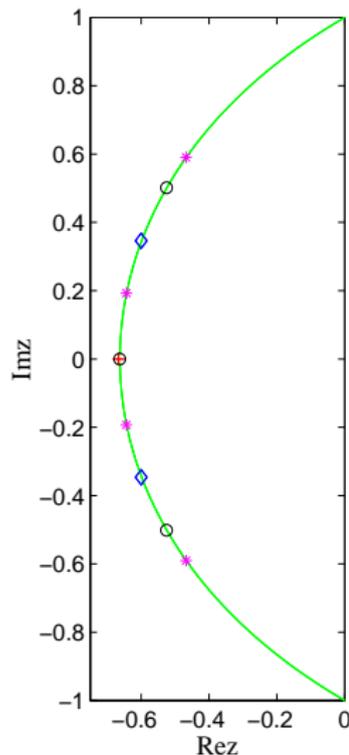
Scaled zeros $\frac{b_{\ell j}}{(\ell + 1/2)}$ of $K_{\ell+1/2}(z)$ and $W_{\ell}(z)$:

$$+ K_{3/2}(z) = \sqrt{\frac{\pi}{2z}} e^{-z} \left(1 + \frac{1}{z}\right)$$

$$\diamond K_{5/2}(z) = \sqrt{\frac{\pi}{2z}} e^{-z} \left(1 + \frac{3}{z} + \frac{3}{z^2}\right)$$

$$\circ K_{7/2}(z) = \sqrt{\frac{\pi}{2z}} e^{-z} \left(1 + \frac{6}{z} + \frac{15}{z^2} + \frac{15}{z^3}\right)$$

$$* K_{9/2}(z) = \sqrt{\frac{\pi}{2z}} e^{-z} \left(1 + \frac{10}{z} + \frac{45}{z^2} + \frac{105}{z^3} + \frac{105}{z^4}\right)$$



Radial Wave Equation

- Radial Wave Equation:

$$-\partial_t^2 \psi_\ell + \partial_r^2 \psi_\ell - \frac{\ell(\ell+1)}{r^2} \psi_\ell = 0$$

- For $\ell = 0$, generic solutions from factoring wave equation:

$$\underbrace{f(t-r)}_{\leftarrow}, \quad \underbrace{g(t+r)}_{\rightarrow}$$

Lemma

For $\ell > 0$, generic outgoing solution:

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

Radial Wave Equation

By induction,

$$\psi_\ell = -\left(\frac{\partial}{\partial r} - \frac{\ell}{r}\right)\psi_{\ell-1}, \quad D_\ell^+ = -\left(\frac{\partial}{\partial r} - \frac{\ell}{r}\right)$$

If

$$-\partial_t^2 \psi_{\ell-1} + \partial_r^2 \psi_{\ell-1} - \frac{\ell(\ell-1)}{r^2} \psi_{\ell-1} = 0,$$

Then

$$-\partial_t^2 (D_\ell^+ \psi_{\ell-1}) + \partial_r^2 (D_\ell^+ \psi_{\ell-1}) - \frac{\ell(\ell+1)}{r^2} D_\ell^+ \psi_{\ell-1} = 0.$$

Non-reflecting Boundary Conditions

Lemma [needed to compute LT of $\Psi_\ell(t, r)$]



Figure: D and open region $r > r_B - \delta$

Assume $f(u)$ supported on $[-r_B + \delta, -r_0 - \delta] = D$, $f \in C_0^\infty(D)$.

For $r > r_B - \delta$, Fourier-Laplace transform of $f^{(\ell-k)}(t-r)$ is

$$s^{\ell-k} e^{-sr} a(s), \quad a(s) = \int_{-r_B+\delta}^{-r_0-\delta} e^{-su} f(u) du.$$

proof

$$\begin{aligned} \int_0^\infty e^{-st} f^{(\ell-k)}(t-r) dt &= e^{-sr} \int_{-r}^\infty e^{-su} f^{(\ell-k)}(u) du \\ &= e^{-sr} \int_{-r_B+\delta}^{-r_0-\delta} e^{-su} f^{(\ell-k)}(u) du, \quad -r < -r_B + \delta \end{aligned}$$

Laplace Transform of $\Psi_\ell(t, r)$

Therefore, for $r = r_B$,

$$\widehat{\Psi}_\ell(s, r) = \sum_{k=0}^{\ell} \frac{C_{\ell k}}{r^k} (s^{\ell-k} e^{-sr} a(s))$$

$$= a(s) s^\ell e^{-sr} W_\ell(sr), \quad W_\ell(sr) = \sum_{k=0}^{\ell} \frac{C_{\ell k}}{z^k}$$

$$s\widehat{\Psi}_\ell(s, r) + \partial_r \widehat{\Psi}_\ell(s, r) = \frac{1}{r} (sr) \frac{W'_\ell(s, r)}{W_\ell(s, r)} \widehat{\Psi}_\ell = \frac{1}{r} \sum_{j=1}^{\ell} \frac{b_{\ell j}/r}{s - b_{\ell j}/r} \widehat{\Psi}_\ell,$$

Laplace Convolution Theorem:

$$\partial_t \Psi_\ell(t, r) + \partial_r \Psi_\ell(t, r) = \frac{1}{r} \int_0^t \Omega_\ell(t-t', r) \Psi_\ell(t', r) dt', \quad \Omega_\ell(t, r) = \sum_{k=1}^{\ell} \frac{b_{\ell k}}{r} e^{\frac{b_{\ell k}}{r} t}$$

Identities for Roots of Macdonald function

Sketch of Main Results

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

$$\partial_t \Psi_\ell(t, r) + \partial_r \Psi_\ell(t, r) = \sum_{n=1}^{\ell} \frac{b_{\ell n}}{r^2} \int_0^t e^{\frac{b_{\ell n}}{r}(t-t')} \Psi_\ell(t', r) dt'$$

- Result:

$$-\sum_{k=1}^{\ell} \frac{k}{r^{k+1}} c_{\ell k} f^{(\ell-k)}(t-r) = \sum_{n=1}^{\ell} \frac{b_{\ell n}}{r^2} \sum_{k=0}^{\ell} \frac{1}{r^k} c_{\ell k} I^{(\ell-k)}[b_{\ell n}, r, f]$$

- Here $I^{(p)}[b, r, f] \equiv \int_0^t e^{\frac{b}{r}(t-t')} f^{(p)}(t'-r) dt'$
- Work into form (argument sketched later...integration by parts)

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

Sketch of Main Results

- Starting with (last line of last slide)

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

isolate terms $E_k f^{(\ell-k)}(u)$ with operator $Q = (\partial_t + \partial_r)r^2$.

- Example ($\ell = 3$):

$$Q\left[\frac{1}{r^2} E_1 f''(u) + \frac{1}{r^3} E_2 f'(u) + \frac{1}{r^4} E_3 f(u)\right] = -\frac{1}{r^2} E_2 f'(u) - \frac{2}{r^3} E_3 f(u)$$
$$Q^2\left[\frac{1}{r^2} E_1 f''(u) + \frac{1}{r^3} E_2 f'(u) + \frac{1}{r^4} E_3 f(u)\right] = \frac{6}{r^2} E_3 f(u)$$

- Profile f arbitrary $\implies E_3 = 0 \implies E_2 = 0 \implies E_1 = 0$.

Technical Lemma (History Integrals)

Lemma

Let $r = r_B$ and $f \in C_0^\infty(D)$, and define

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

Then, we have

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

Technical Lemma (History Integrals)

Proof by induction

We show:

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

The second term within the square brackets vanishes since $r = r_B \notin D$. Note there are no boundary terms at $t' = 0$, only $t' = t$. Integration by parts establishes the last formula for $p = 1$. Similarly,

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

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

Main Result

Theorem

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

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

also obey the following set of ℓ algebraic equations: (Newton's identities!)

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

Here we assume $\ell \geq 1$.

Main Result: careful proof (1)

proof

Taking $r = r_B$ and $t > 0$, we get

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

Previous lemma gives

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

Main Result: careful proof continued...(2)

Combination of the last two equations yields

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

Main Result: careful proof continued...(3)

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

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

Main Result: careful proof continued...(4)

Within the sum over k , the sum over j is empty when $k = \ell$. Therefore, here we may replace $\sum_{k=0}^{\ell}$ by $\sum_{k=0}^{\ell-1}$. Re-indexing $q = k + 1$, yields

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

Main Result: careful proof continued...(5)

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

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

Main Result: careful proof continued...(6)

Through re-indexing of sums we get to

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

which is the desired form. Recalling that we have set $r = r_B$,

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

and we may express that last equation as

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

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

- Numerical check using **Mathematica**
- Watson's argument showing poles are simple and in left-half plane.

real and imaginary parts of roots for $\ell = 20$

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-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
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