On the zeros of the Macdonald functions

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Abstract. We are concerned with the zeros of the Macdonald functions or the modified Bessel functions of the second kind with real index. By using the explicit expressions for the algebraic equations satisfied by the zeros, we describe the behavior of the zeros when the index moves. Results by numerical computations are also presented.

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In this article we are concerned with the zeros of the Macdonald function, or the modified Bessel function of the second kind with real index, which we denote by $K_\nu$ in the usual notation. By analytic continuation we consider $K_\nu(z)$ as a function in $z \in \mathbb{C} \setminus (-\infty, 0]$. It is well known that $K_\nu(z)$ is an entire function in $\nu$. The zeros of the Bessel functions $J_\nu, Y_\nu$ and of the other modified function $I_\nu$ are well studied and we can also carry out the numerical computations for them in several ways. However, only a few things are known about the zeros of $K_\nu$. See [2, 3, 4].

Since $K_{-\nu} = K_\nu$ and there are no zeros when $0 \leq \nu < \frac{3}{2}$ (see [3]), we throughout assume $\nu \geq \frac{3}{2}$. When $\nu = 2n + \frac{3}{2}, n = 0, 1, ..., K_{2n+\frac{3}{2}}$ is of the form $\sqrt{\pi/(2z)}z^{-(2n+1)}\varphi_n(z)$, $\varphi_n(z)$ being a polynomial of order $2n+1$ (see (2) below). $\varphi_n$ has a unique negative root and we regard it as a zero of $K_{2n+\frac{3}{2}}$. Hence $K_{2n+\frac{3}{2}}$ has $2n+1$ zeros. It is known that $K_\nu$ has $2(n+1)$ zeros when $2n+\frac{3}{2} < \nu < 2n+\frac{7}{2}$. It is also well known that the non-real zeros are complex conjugate in pairs.

Recently in [1], it has been shown that the zeros of $K_\nu$ are obtained as the roots of some algebraic equations whose coefficients are explicitly given by using $K_\nu$ and $I_\nu$. For details, see the equation (5) below. When $2n+\frac{3}{2} < \nu < 2n+\frac{7}{2}$, the equations may be taken of order $2(n+1)$. Such equations have been already shown in [1] when $\nu$ is an integer and they coincide in this special case.

Let $z_\nu$ be a non-real zero of $K_\nu$. By the formula

$$I_\nu(z)K'_\nu(z) - I'_\nu(z)K_\nu(z) = -\frac{1}{z}$$
or the uniqueness of the Bessel differential equation, we see that \( K'_\nu(z_\nu) \neq 0 \) and that \( z_\nu \) is (locally) a smooth function in \( \nu \) by the implicit function theorem.

The aim of this article is to show the continuity of the zeros from the algebraic equations, including the continuity at \( \nu = 2n + \frac{3}{2} \), and to present some numerical computations by Mathematica. The following graph shows the behavior of the zeros.

![Figure 1: Zeros of \( K_\nu(z) \)](image)

The unique zero of \( K_{\frac{3}{2}} \) is \(-1\). The two curves from \(-1\) described by the black points give the two zeros in the case of \( \frac{3}{2} < \nu < \frac{7}{2} \). The endpoints and the negative value between \(-2\) and \(-3\) found in the graph are the three zeros of \( K_{\frac{7}{2}} \). The four curves from the zeros of \( K_{\frac{7}{2}} \) described by the gray points are the zeros in the case of \( \frac{7}{2} < \nu < \frac{11}{2} \). The five zeros of \( K_{\frac{11}{2}} \) are seen in a similar manner, and so on. See also the table in the last part of this article. It should be mentioned that we find a similar graph for the zeros in [2].

In order to mention the main results, we recall some formulae obtained in [1] and prepare some further results. For \( \nu = \frac{3}{2} \), we have

\[
K_{\frac{3}{2}}(z) = \sqrt{\frac{\pi}{2z}} \frac{e^{-z}}{z} (1 + z).
\]

When \( \nu > \frac{3}{2} \), we denote the zeros of \( K_\nu \) by \( z^{(\nu)}_1, z^{(\nu)}_2, \ldots, z^{(\nu)}_{N(\nu)} \). Here the number \( N(\nu) \) of the zeros of \( K_\nu \) is equal to \( \nu - \frac{1}{2} \) if \( \nu - \frac{1}{2} \) is an integer and is the even integer closest to \( \nu - \frac{1}{2} \) otherwise as is mentioned above.

The basic formula is the following: if \( \nu - \frac{1}{2} \) is an integer,

\[
\frac{K_{\nu+1}(w)}{K_\nu(w)} = 1 + \frac{2\nu}{w} + \sum_{j=1}^{N(\nu)} \frac{1}{z^{(\nu)}_j - w}
\]
and, if \( \nu - \frac{1}{2} \) is not an integer,

\[
\frac{K_{\nu+1}(w)}{K_\nu(w)} = 1 + \frac{2\nu}{w} + \sum_{j=1}^{N(\nu)} \frac{1}{z_j^{(\nu)}} - w + \cos(\pi \nu) \int_0^\infty \frac{dx}{x(x + w)G_\nu(x)}, \tag{1}
\]

where the function \( G_\nu \) is given by

\[
G_\nu(x) = K_\nu(x)^2 + \pi^2 I_\nu(x)^2 + 2\pi \sin(\pi \nu)K_\nu(x)I_\nu(x)
\]

\[
= K_\nu(x)^2 + \pi^2 I_\nu(x)I_{-\nu}(x).
\]

These formulae have been obtained in the course of some study on the first hitting times of the Bessel diffusion processes. By considering the asymptotic expansions of the both hand sides of (1) as \( w \to \infty \), we obtain the algebraic equations (5) for the zeros \( z^{(\nu)}_j \), \( j = 1, 2, ..., N(\nu) \).

If we consider the asymptotic behavior as \( w \to 0 \), we obtain the equations for the reciprocals, which we do not mention in this paper.

We put \( \nu_n = 2n + \frac{3}{2}, \quad n = 0, 1, 2, ... \)

Then, the following is easily seen.

**Lemma 1.** When \( \nu = \nu_n \), \( G_\nu \) has a unique positive zero and it is the unique solution of

\[
K_{\nu_n}(x) = \pi I_{\nu_n}(x).
\]

When \( \nu \neq \nu_n \) for any \( n \), \( G_\nu \) does not vanish.

It should be noted that, denoting by \( x_n \) the unique solution of \( K_{\nu_n} = \pi I_{\nu_n} \), \(-x_n\) is the negative zero of \( K_{\nu_n} \), which is seen by the formula

\[
K_\nu(e^{m\pi i}z) = e^{-\nu m \pi i}K_\nu(z) - \pi i \frac{\sin \nu m \pi}{\sin(\nu \pi)} I_\nu(z) \quad (m \in \mathbb{Z}).
\]

Since \( K_{\nu_n} \) is explicitly given by

\[
K_{\nu_n}(z) = \sqrt{\frac{\pi}{2z}} e^{-z} \sum_{k=0}^{2n+1} \frac{(\nu_n, k)}{(2z)^k}, \tag{2}
\]

\(-x_n\) satisfies

\[
\sum_{k=0}^{2n+1} \frac{(\nu_n, 2n + 1 - k)}{2^{2n+1-k}} z^k = 0, \tag{3}
\]

where \( (\nu, 0) = 1 \) and

\[
(\nu, n) = \frac{(4\nu^2 - 1^2)(4\nu^2 - 3^2) \cdots (4\nu^2 - (2n - 1)^2)}{n!2^{2n}} = \frac{\Gamma(\nu + n + \frac{1}{2})}{n!\Gamma(\nu - n + \frac{1}{2})},
\]

Moreover, by the recurrence relation

\[
K_\nu(z) - K_{\nu+2}(z) = -\frac{2(\nu + 1)}{z} K_{\nu+1}(z), \quad I_\nu(z) - I_{\nu+2}(z) = \frac{2(\nu + 1)}{z} I_{\nu+1}(z),
\]

3
we can easily show that $K_{\nu_n}(x_{n+1}) - \pi I_{\nu_n}(x_{n+1}) < 0$ and that the sequence $\{x_n\}_{n=0}^\infty$ is increasing.

We set

$$\alpha_n = -K_{\nu_n}'(x_n) + \pi I_{\nu_n}'(x_n) \quad \text{and} \quad \beta_n = \left( -\frac{\partial K_{\nu_n}(x_n)}{\partial \nu} + \pi \frac{\partial I_{\nu_n}(x_n)}{\partial \nu} \right)_{\nu=\nu_n}.$$ 

Note that $\alpha_n > 0$, since $K_{\nu}$ is decreasing and $I_{\nu}$ is increasing. Then, setting $G(x, \nu) = G_{\nu}(x)$, we have

$$G(x_n, \nu_n) = 0, \quad \frac{\partial G}{\partial x}(x_n, \nu_n) = 0, \quad \frac{\partial G}{\partial \nu}(x_n, \nu_n) = 0$$

and

$$\frac{\partial^2 G}{\partial x^2}(x_n, \nu_n) = 2\alpha_n^2, \quad \frac{\partial^2 G}{\partial x \partial \nu}(x_n, \nu_n) = 2\alpha_n \beta_n, \quad \frac{\partial^2 G}{\partial \nu^2}(x_n, \nu_n) = 2\beta_n^2 + 2\pi^2 K_{\nu_n}(x_n)^2.$$ 

Moreover, we can show

$$K_{\nu_n}(x_n) = \frac{\pi}{\alpha_n x_n}.$$ 

Combining the above mentioned formulae, we obtain the following.

**Lemma 2.** For $m = 1, 2, \ldots, 2n - 1$, it holds that

$$\lim_{\nu \to \nu_n \pm 0} \cos(\pi \nu) \int_0^\infty \frac{x^{m-1}}{G(x, \nu)} dx = \pm x^n.$$

The main results are the following.

**Theorem 3.** As $\nu \downarrow \nu_n$, $n = 0, 1, 2, \ldots$, two of the zeros of $K_{\nu}$ converge to $-x_n$ and the others to the non-real zeros of $K_{\nu_n}$.

**Theorem 4.** As $\nu \uparrow \nu_n$, $n = 1, 2, \ldots$, each zero of $K_{\nu}$ converges to a non-real zero of $K_{\nu_n}$.

**Proof of Theorem 3.** At first we recall the algebraic equation for the zeros of $K_{\nu}$. For this we define $a^{(\nu)}_k$, $k = 0, 1, 2, \ldots$ inductively by

$$\frac{(\nu + 1, m)}{2^m} = \sum_{k=0}^m \frac{(\nu, m-k)}{2^{m-k}} a^{(\nu)}_k. \quad (4)$$

Moreover we define $a^{(\nu)}_m$ by $a^{(\nu)}_0 = 1$ and

$$a^{(\nu)}_m = \frac{1}{m} \sum_{k=1}^m a^{(\nu)}_{m-k} \left\{ a^{(\nu)}_{k+1} - (-1)^k \cos(\pi \nu) \int_0^\infty \frac{y^{k-1}}{G_{\nu}(y)} dy \right\}, \quad m = 1, 2, \ldots, 2n + 1.$$
Then it is shown in \[1\] that the zeros of \( K \) are the roots of

\[
\sum_{k=0}^{2n+2} a_{2n+2-k}^{(\nu)} z^k = 0
\]  

(5)

by computing the asymptotic behavior of the both hands side of \(1\) as \(w \to \infty\).

For our purpose we show that, for \(m = 0, 1, \ldots, 2n + 2\), \(\lim_{\nu \downarrow \nu_n} a_{m}^{(\nu)} \) exists and that, denoting the limit by \(c_{m}^{(n)} \),

\[
\sum_{k=0}^{2n+2} c_{2n+2-k}^{(n)} z^k = (z + x_n) \sum_{k=0}^{2n+1} \frac{(\nu_n, 2n + 1 - k)}{2^{2n+1-k}} z^k.
\]  

(6)

Then, since the roots of algebraic equations are continuous in the coefficients, we obtain the assertion of the theorem from \(3\). \(-x_n\) is the double root for the polynomial in \(4\).

For \(k = 0, 1, \ldots, 2n + 1\), \(\nu_n - k + \frac{1}{2} \geq 1\) and, hence, by \(4\), we easily see that \(a_k^{(\nu)}\) converges as \(\nu \downarrow \nu_n\) and that the limit \(a_k^{(n)}\) satisfies

\[
\frac{(\nu_n + 1, m)}{2^m} = \sum_{k=0}^{m} \frac{(\nu_n, m - k)}{2^{m-k}} a_k^{(n)}, \quad m = 0, 1, \ldots, 2n + 1.
\]

Since \((\nu_n, 2n + 2) = (\nu_n, 2n + 3) = (\nu_n + 1, 2n + 3) = 0\), we see the convergence of \(a_{2n+2}^{(\nu)}\) and \(a_{2n+3}^{(\nu)}\) again by using \(4\).

Combining the convergence of \(a_k^{(\nu)}\) with Lemma \(2\), we obtain the convergence of \(a_m^{(\nu)}\) by induction. The limit \(c_{m}^{(n)}\) satisfies

\[
c_{m}^{(n)} = \frac{1}{m} \sum_{k=1}^{m} c_{m-k}^{(n)} \{ a_{k+1}^{(n)} - (-1)^k x_n^k \}, \quad m = 1, 2, \ldots, 2n + 2.
\]

From this recurrence relation we get

\[
c_{m}^{(n)} = \frac{(\nu_n, m)}{2^m} + \frac{(\nu_n, m - 1)}{2^{m-1}} x_n.
\]  

(7)

We can check this by some lengthy computation and we omit the details.

For a proof of the second assertion, we note \(c_0^{(n)} = 1\) and \((\nu_n, 2n + 2) = 0\).

Then we get from \(7\)

\[
\sum_{k=0}^{2n+2} c_{2n+2-k}^{(n)} z^k = z^{2n+2} + \sum_{k=0}^{2n+1} \left\{ \frac{(\nu_n, 2n + 2 - k)}{2^{2n+2-k}} + \frac{(\nu_n, 2n + 1 - k)}{2^{2n+1-k}} x_n \right\} z^k
\]

\[
= z^{2n+2} + \sum_{k=0}^{2n} \frac{(\nu_n, 2n + 1 - k)}{2^{2n+1-k}} z^{k+1} + x_n \sum_{k=0}^{2n+1} \frac{(\nu_n, 2n + 1 - k)}{2^{2n+1-k}} z^k
\]

\[
= \sum_{k=0}^{2n+1} \frac{(\nu_n, 2n + 1 - k)}{2^{2n+1-k}} z^{k+1} + x_n \sum_{k=0}^{2n+1} \frac{(\nu_n, 2n + 1 - k)}{2^{2n+1-k}} z^k,
\]
which show the second assertion and Theorem 3.

**Proof of Theorem 4** We can prove in the same way as in Theorem 3 and we only give a sketch.

When \( \nu_{n-1} < \nu < \nu_n \), the zeros of \( K_{\nu} \) are the roots of

\[
\sum_{k=0}^{2n} \alpha_{2n-k}^{(\nu)} z^k = 0.
\]

We can show that each \( \alpha_{m}^{(\nu)} \), \( m = 0, 1, ..., 2n \) converges as \( \nu \uparrow \nu_n \) and that, denoting the limit by \( d_{m}^{(n)} \), \( d_0^{(n)} = 1 \) and

\[
d_m^{(n)} = \frac{1}{m} \sum_{k=0}^{m} d_{m-k}^{(n)} \{ a_{k+1}^{(n)} + (-1)^k x_n^k \}.
\]

From this recurrence relation, we obtain

\[
d_m^{(n)} = \sum_{k=0}^{m} (-1)^k \frac{(\nu_n, m-k)}{2m-k} x_n^k, \quad m = 0, 1, ..., 2n
\]

and

\[
\sum_{k=0}^{2n+1} \frac{(\nu_n, 2n-k+1)}{2^{2n-k+1}} z^k = (z + x_n) \sum_{k=0}^{2n} d_m^{(n)} z^k.
\]

The zeros of \( K_{\nu_n} \) are the roots of the polynomial on the left hand side and the limits of the zeros of \( K_{\nu} \) as \( \nu \uparrow \nu_n \) are the zeros of that on the other side. This proves Theorem 4.

**Remark 5.** It may be worthwhile noting that the algebraic equations for the zeros when \( \nu_{n-1} < \nu < \nu_n \) and when \( \nu_n < \nu < \nu_{n+1} \) are different. In fact, letting \( z_0 \) be one of the zeros of \( K_{\nu} \) when \( \nu_n < \nu < \nu_{n+1} \), we have

\[
\sum_{k=0}^{2n+2} \alpha_{2n+2-k}^{(\nu)} z_0^k = 0.
\]

If \( \sum_{k=0}^{2n} \alpha_{2n-k}^{(\nu)} z_0^k = 0 \), we have \( \sum_{k=2}^{2n+2} \alpha_{2n+2-k}^{(\nu)} z_0^k \) since \( z_0 \neq 0 \). Then, comparing this equation with the above one, we should have that \( \alpha_{2n+2}^{(\nu)} + \alpha_{2n+1}^{(\nu)} z_0 = 0 \) and that \( z_0 \) is real. This is a contradiction.

Finally we give a table of the approximate values of the zeros of \( K_{\nu} \), which are numerically computed by “Mathematica”. As is mentioned above, the algebraic equations for the reciprocals of the zeros are also given in [1]. The numerical results for the zeros of the two algebraic equations coincide and it gives a good check for our results.
| \( \nu \) | \( x^* \) | \( y^* \) |
|---|---|---|
| 1.0 | -1.06356 ± 0.0562232 | 0.05308 ± 0.0268170 |
| 1.5 | -1.22292 ± 0.1708069 | 0.05308 ± 0.0268170 |
| 1.8 | -1.1787 ± 0.2567254 | 0.05308 ± 0.0268170 |
| 2.0 | -1.21339 ± 0.3429579 | 0.05308 ± 0.0268170 |
| 2.1 | -1.28137 ± 0.4243859 | 0.05308 ± 0.0268170 |
| 2.2 | -1.32966 ± 0.5162291 | 0.05308 ± 0.0268170 |
| 2.3 | -1.37442 ± 0.6033616 | 0.05308 ± 0.0268170 |
| 2.4 | -1.41705 ± 0.6908628 | 0.05308 ± 0.0268170 |
| 2.5 | -1.5 ± 0.7860253 | 0.05308 ± 0.0268170 |
| 2.6 | -1.538 ± 0.9540271 | 0.05308 ± 0.0268170 |
| 2.7 | -1.57628 ± 1.0421238 | 0.05308 ± 0.0268170 |
| 2.8 | -1.61251 ± 1.1306434 | 0.05308 ± 0.0268170 |
| 2.9 | -1.64769 ± 1.2193241 | 0.05308 ± 0.0268170 |
| 3.0 | -1.67179 ± 1.3086101 | 0.05308 ± 0.0268170 |
| 3.1 | -1.71492 ± 1.3966996 | 0.05308 ± 0.0268170 |
| 3.2 | -1.74714 ± 1.4842976 | 0.05308 ± 0.0268170 |
| 3.3 | -1.77851 ± 1.5735636 | 0.05308 ± 0.0268170 |
| 3.4 | -1.80908 ± 1.6644884 | 0.05308 ± 0.0268170 |

Table of zeros of \( K_\nu \)

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