On the $\nu$-zeros of the modified Bessel function $K_{i\nu}(x)$ of positive argument

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Abstract
The modified Bessel function of the second kind $K_{i\nu}(x)$ of imaginary order for fixed $x > 0$ possesses a countably infinite sequence of real zeros. Recently it has been shown that the $n$th zero behaves like $\nu_n \sim \pi n / \log n$ as $n \to \infty$. In this note we determine a more precise estimate for the behaviour of these zeros for large $n$ by making use of the known asymptotic expansion of $K_{i\nu}(x)$ for large $\nu$. Numerical results are presented to illustrate the accuracy of the expansion obtained.

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1. Introduction
The modified Bessel function of the second kind (the Macdonald function) $K_{i\nu}(x)$ of purely imaginary order and argument $x > 0$ is given by

$$K_{i\nu}(x) = \int_0^\infty e^{-x \cosh t} \cos \nu t \, dt = \frac{1}{2} \int_{-\infty}^{\infty} e^{-x \cosh t+i\nu t} \, dt.$$  \hspace{1cm} (1.1)

In a recent paper, Bagirova and Khanmamedov [1] have shown that $K_{i\nu}(x)$ has a countably infinite number of (simple) real zeros in $\nu$ when $x > 0$ is fixed. We label the zeros $\nu_n \equiv \nu_n(x)$ ($n = 0, 1, 2 \ldots$) and observe that it is sufficient to consider only the case $\nu > 0$ since $K_{i\nu}(x) = K_{-i\nu}(x)$. By transforming the differential equation satisfied by $K_{i\nu}(x)$ into a one-dimensional Schrödinger equation with an exponential potential, these authors employed the well-known quantisation rule to deduce the leading asymptotic behaviour of the $n$th zero given by

$$\nu_n \sim \frac{\pi n}{\log n} \quad (n \to +\infty).$$ \hspace{1cm} (1.2)

In this note, we consider the behaviour of the large-$n$ $\nu$-zeros of $K_{i\nu}(x)$ in more detail. To achieve this we make use of the known asymptotic expansion of $K_{i\nu}(x)$ for $\nu \to +\infty$ stated in Section 2. A typical plot of $e^{\pi\nu/2}K_{i\nu}(x)$ as a function of $\nu$ is shown in Fig. 1.

2. Derivation of the equation describing the large-$n$ zeros
We start with the asymptotic expansion of $K_{i\nu}(x)$ for $\nu \to +\infty$ given by [5] (see also [4] pp. 41–42)

$$e^{\pi \nu/2}K_{i\nu}(x) \sim \Re \sqrt{\frac{2\pi}{\nu \tanh \mu}} e^{\nu \phi} \sum_{k=0}^{\infty} \left(\frac{1}{2i\nu \tanh \mu}\right)^k C_k(\mu),$$ \hspace{1cm} (2.1)

1 There is a misprint in (1.4.8) of [4]: the argument of the Bessel function should be $x$.\hspace{1cm}
Figure 1: Plot of $e^{\pi \nu/2}K_{i \nu}(x)$ as a function of $\nu$ when $x = 1$.

where

$$\Phi := \nu(\mu - \tanh \mu) - \frac{\pi}{4}, \quad \cosh \mu = \frac{\nu}{x}$$

and $(a)_k = \Gamma(a + k)/\Gamma(a)$ denotes the Pochhammer symbol. The first few coefficients $C_k(\mu)$ are

$$C_0(\mu) = 1, \quad C_1(\mu) = -\frac{1}{8} + \frac{5 \coth^2 \mu}{24}, \quad C_2(\mu) = \frac{3}{128} - \frac{77 \coth^2 \mu}{576} + \frac{385 \coth^4 \mu}{3456};$$

values of $C_k(\mu)$ for $k \leq 5$ are derived in the appendix. It is important to point out that the determination of the expansion (2.1) from the integral (1.1) involves (when $\nu > x$) an infinite number of contributing saddle points. The expansion (2.1) results from the two dominant saddles, the remaining saddles yielding an exponentially small contribution of $O(e^{-\pi \nu})$. Then, from (2.1), the zeros of $K_{i \nu}(x)$ are given asymptotically by

$$\cos \Phi \left\{ 1 - \frac{3C_2(\mu)}{(\nu \tanh \mu)^2} + \frac{105C_4(\mu)}{(\nu \tanh \mu)^4} + \cdots \right\} + \sin \Phi \left\{ \frac{C_1(\mu)}{\nu \tanh \mu} - \frac{15C_3(\mu)}{(\nu \tanh \mu)^3} + \frac{945C_5(\mu)}{(\nu \tanh \mu)^5} + \cdots \right\} = 0.$$

Let

$$\Phi = (n + \frac{1}{2})\pi + \epsilon,$$

where $n$ is a large positive integer and $\epsilon$ is a small quantity. Then

$$\tan \epsilon = \frac{\frac{C_1(\mu)}{\nu \tanh \mu} - \frac{15C_3(\mu)}{(\nu \tanh \mu)^3} + \frac{945C_5(\mu)}{(\nu \tanh \mu)^5} + \cdots}{1 - \frac{3C_2(\mu)}{(\nu \tanh \mu)^2} + \frac{105C_4(\mu)}{(\nu \tanh \mu)^4} + \cdots} = \frac{1}{\nu \tanh \mu} \left\{ C_1(\mu) + \frac{3(C_1(\mu)C_2(\mu) - 5C_3(\mu))}{(\nu \tanh \mu)^2} + \frac{9C_1(\mu)C_2^2(\mu) - 45C_2(\mu)C_3(\mu) - 105C_1(\mu)C_4(\mu) + 945C_5(\mu)}{(\nu \tanh \mu)^4} + \cdots \right\},$$

so that using $\arctan z = z - z^3/3 + z^5/5 - \cdots$ ($|z| < 1$), we obtain

$$\epsilon = \frac{a_0(\mu)}{\nu} + \frac{a_1(\mu)}{\nu^3} + \frac{a_2(\mu)}{\nu^5} + \cdots,$$

where

$$a_0(\mu) = \frac{C_1(\mu)}{\tanh \mu}, \quad a_1(\mu) = \frac{3(C_1(\mu)C_2(\mu) - 5C_3(\mu)) - \frac{4C_1^2(\mu)}{\tanh^2 \mu}}{\tanh^3 \mu},$$
\[ a_2(\mu) = \frac{1}{\tanh^2 \mu} \left\{ 3(3C_1(\mu)C_2^2(\mu) - 15C_2(\mu)C_3(\mu) - 35(C_1(\mu)C_4(\mu) - 9C_5(\mu))) \\
- 3C_1^2(\mu)(C_1(\mu)C_2(\mu) - 5C_3(\mu)) + \frac{1}{5} C_1^3(\mu) \right\}. \]

Since \( \tanh \mu = \sqrt{1 - x^2/\nu^2} \), the coefficients \( a_k(\mu) \) possess expansions in inverse powers of \( \nu^2 \). Some laborious algebra shows that

\[ a_0(\mu) = \frac{1}{12} + \frac{x^2}{4\nu^2} + \frac{11x^4}{32\nu^4} + O(\nu^{-6}) \]
\[ a_1(\mu) = \frac{1}{360} - \frac{x^2}{4\nu^2} + O(\nu^{-4}) \]
\[ a_2(\mu) = \frac{1}{1260} + O(\nu^{-2}), \]

whence we obtain

\[ \epsilon = \frac{1}{12\nu} + \frac{1}{\nu^3} \left( \frac{1}{360} + \frac{x^2}{4} \right) + \frac{1}{\nu^5} \left( \frac{1}{1260} - \frac{x^2}{4} + \frac{11x^4}{32} \right) + \cdots. \]  

(2.3)

Making use of the expansion

\[ \mu - \tanh \mu = \log \lambda \nu + \frac{x^2}{4\nu^2} + \frac{x^4}{32\nu^4} + \frac{x^6}{96\nu^6} + O(\nu^{-8}), \quad \lambda := \frac{2}{ex}, \]

we then finally obtain from (2.2) and (2.3) the equation describing the large-\( n \) zeros of \( K_{\nu}(x) \) given by

\[ \nu \log \lambda \nu = m + \frac{A_0}{\nu} + \frac{A_1}{\nu^3} + \frac{A_2}{\nu^5} + \cdots, \]

(2.4)

where

\[ A_0 = \frac{1}{12} - \frac{x^2}{4}, \quad A_1 = \frac{1}{360} + \frac{x^2}{4} - \frac{x^4}{32}, \quad A_2 = \frac{1}{1260} - \frac{x^2}{4} + \frac{11x^4}{32} - \frac{x^6}{96} \]

and, for convenience, we have put \( m := (n + \frac{3}{4})\pi \).

3. Solution of the equation for the zeros

To solve (2.4) we expand \( \nu \) as

\[ \nu_n = \xi + \frac{c_0}{\xi} + \frac{c_1}{\xi^3} + \frac{c_2}{\xi^5} + \cdots, \]

where the \( c_k \) are constants to be determined and we suppose that \( \xi \) is large as \( n \to \infty \). Substitution in (2.4) then produces

\[ \xi \log \lambda \xi + \frac{c_0(1 + \log \lambda \xi)}{\xi} + \frac{c_1(1 + \log \lambda \xi)}{\xi^3} + \frac{c_2(1 + \log \lambda \xi)}{\xi^5} + \cdots = m + \frac{A_0}{\xi} + \frac{A_1 - A_0c_0}{\xi^3} + \frac{A_2 - 3A_1c_0 + A_0(c_0^2 - c_1)}{\xi^5} + \cdots. \]

Equating coefficients of like powers of \( \xi \), we obtain

\[ \xi \log \lambda \xi = m, \]

(3.1)

and

\[ c_0 = -\frac{A_0}{1 + \log \lambda \xi}, \quad c_1 = \frac{A_1 - A_0c_0 - \frac{1}{2}c_0^2}{1 + \log \lambda \xi}. \]
The solution of \((\text{3.1})\) for the lowest-order term \(\xi\) can be expressed in terms of the Lambert \(W\) function, which is the (positive) solution\(^2\) of \(W(z)e^{W(z)} = z\) for \(z > 0\). Rearrangement of \((\text{3.1})\) shows that
\[
\frac{m}{\xi} e^{m/\xi} = \lambda m,
\]
whence
\[
\xi = \frac{m}{W(\lambda m)}.
\]
(3.2)

The asymptotic expansion of \(W(z)\) for \(z \to +\infty\) is \([2, 3 \ (4.13.10)]\)
\[
W(z) \sim L_1 - L_2 + \frac{L_2 - 2 L_2}{2 L_1^2} + \frac{(6 - 9 L_2 + 2 L_2^2)L_2}{6 L_1^3} \left(\frac{-12 + 36 L_2 - 22 L_2^2 + 3 L_2^3}{12 L_1^4} + \cdots\right),
\]
where \(L_1 = \log z, L_2 = \log \log z\), from which it follows that
\[
\frac{1}{W(z)} \sim \frac{1}{L_1} \left\{ 1 + \frac{L_2}{L_1} + \frac{L_2(L_2 - 1)}{2 L_1^2} + \frac{(-6 + 21 L_2 - 26 L_2^2 + 6 L_2^3) L_2}{6 L_1^4} + \cdots \right\}.
\]

Then we have the expansion for \(\xi\) as \(\lambda m \to \infty\) given by
\[
\xi \sim \frac{m}{\log \lambda m} \left\{ 1 + \log \frac{\log \lambda m}{\log \lambda m} + \frac{\log \lambda m (\log \lambda m - 1)}{(\log \lambda m)^2} + \cdots \right\},
\]
where we recall that \(m = (n + \tfrac{3}{4})\pi\).

If we define \(\chi := \xi/m, \text{ so that by } (\text{3.1}),\)
\[1 + \log \xi \chi = (1 + \chi) / \chi\]
and introduce the coefficients
\[
B_0 = \frac{A_0}{1 + \chi}, \quad B_1 = \frac{A_1 - A_0 c_0 - \frac{1}{6} c_0^2}{\chi^2 (1 + \chi)}, \quad B_2 = \frac{A_2 - 3 A_1 c_0 + A_0 (c_0^2 - c_1) - c_0 c_1 + \frac{1}{6} c_0^3}{\chi^4 (1 + \chi)},
\]
then we finally have the result:

**Theorem 1.** The expansion for the \(n\)th \(\nu\)-zero of \(K_{\nu}(x)\) for fixed \(x > 0\) is
\[
\nu_n \sim \frac{m}{W(\lambda m)} + \frac{B_0}{m} + \frac{B_1}{m^3} + \frac{B_2}{m^5} + \cdots \quad (n \to \infty),
\]
where \(m = (n + \tfrac{3}{4})\pi, \lambda = 2/(ex)\) and the coefficients \(B_k\) are given in \((\text{3.4})\).

4. Numerical results

The leading form of \(\xi\) from \((\text{3.3})\) is, with \(\lambda = 2/(ex)\),
\[
\xi \sim \frac{(n + \tfrac{3}{4})\pi}{\log (n + \tfrac{3}{4})\pi + \log \lambda} \quad (n \to \infty),
\]
which yields the approximate estimate in \((\text{1.2})\). In numerical calculations it is found more expedient to use the expression for \(\xi\) in terms of the Lambert function in \((\text{3.2})\), rather than \((\text{3.3})\), since the asymptotic scale in this latter series is \(\log \lambda m\) and so requires an extremely large value of \(n\) to attain reasonable accuracy.

We present numerical results in Table 1 showing the zeros of \(K_{\nu}(x)\) computed using the FindRoot command in Mathematica compared with the asymptotic values determined from the expansion \((\text{3.5})\) with coefficients \(B_k, \ k \leq 2\), where \(\xi\) is evaluated from \((\text{3.2})\). The value of the zeroth-order approximation \(\xi = m/W(\lambda m)\) is shown in the final column. It is seen that there is excellent agreement with the computed zeros, even for \(n = 1\).

\(^2\)In \([3 \text{ p. 111}]\) this is denoted by \(W_p(z)\).
Table 1: Values of the zeros of $K_{i\nu}(x)$ and their asymptotic estimates when $x = 1$.

| $n$ | $\nu_n$ | Asymptotic | $\xi$ |
|-----|----------|------------|------|
| 1   | 4.5344907181 | 4.5345024086 | 4.550063 |
| 2   | 5.8798671997 | 5.8798689800 | 5.890918 |
| 4   | 8.2589364092 | 8.2589365588 | 8.265990 |
| 5   | 9.3550938258 | 9.3550938860 | 9.361083 |
| 10  | 14.3318529171 | 14.3318529198 | 14.335296 |
| 15  | 18.8230418511 | 18.8230418514 | 18.825473 |
| 20  | 23.0318794957 | 23.0318794958 | 23.033764 |
| 30  | 30.9169674670 | 30.9169674670 | 30.918273 |

Appendix: The coefficients $C_k(\mu)$ in the expansion (A.1)

The integral in (1.1) can be cast in the form

$$K_{i\nu}(x) = \frac{1}{2} \int_{-\infty}^{\infty} e^{-x \psi(t)} dt, \quad \psi(t) := \cosh t - it \cosh \mu,$$

where $\cosh \mu = \nu/x$. In the right-half plane, the dominant saddle point (where $\psi'(t) = 0$) is situated at $t_0 = \mu + \frac{1}{2} \pi i$, with a similar saddle in the left-half plane at $-\mu + \frac{1}{2} \pi i$. When $\nu > x$, there are in addition two infinite strings of subdominant saddles at $\pm \mu + (2k + \frac{1}{2})\pi i$ ($k = 1, 2, \ldots$) parallel to the positive imaginary axis over which the integration path in (A.1) is deformed; see [5], [4, pp. 41–42] for details.

We introduce the new variable $w$ by

$$w^2 = \psi(t) - \psi(t_0) = \frac{1}{2} i \sinh \mu (t - t_0)^2 + \frac{1}{6} i \cosh \mu (t - t_0)^3 + \frac{1}{24} i \sinh \mu (t - t_0)^4 + \cdots$$

to find with the help of Mathematica using the InverseSeries command (essentially Lagrange inversion)

$$t - t_0 = e^{-\pi i/4} \sqrt{\frac{2}{\sinh \mu}} w + \frac{i \coth \mu}{2 \sinh \mu} w^2 - i e^{-\pi i/4} \sqrt{\frac{2}{\sinh \mu}} \left( -\frac{3}{36 \sinh \mu} + 5 \coth^2 \mu \right) w^3 + \cdots$$

Differentiation then yields the expansion

$$\frac{dt}{dw} e^{-\pi i/4} \sqrt{\frac{2}{\sinh \mu}} \sum_{k \geq 0} \frac{C_k(\mu)}{\left( \frac{1}{2} i \sinh \mu \right)^k} w^{2k},$$

where $\equiv$ signifies the inclusion of only the even powers of $w$, since odd powers will not enter into this calculation. The first few coefficients are found to be:

$$C_0(\mu) = 1, \quad C_1(\mu) = -\frac{1}{8} + \frac{5 \coth^2 \mu}{24},$$

$$C_2(\mu) = \frac{3}{128} - \frac{77 \coth^2 \mu}{576} + \frac{385 \coth^4 \mu}{3456},$$

$$C_3(\mu) = -\frac{5}{1024} + \frac{1521 \coth^2 \mu}{25600} - \frac{17017 \coth^4 \mu}{138240} + \frac{17017 \coth^6 \mu}{248832},$$

$$C_4(\mu) = \frac{35}{32768} - \frac{96833 \coth^2 \mu}{4300800} + \frac{144001 \coth^4 \mu}{1720320} - \frac{1062347 \coth^6 \mu}{9953280} + \frac{1062347 \coth^8 \mu}{23887872},$$

$$C_5(\mu) = \frac{63}{262144} + \frac{67608983 \coth^2 \mu}{8670412800} - \frac{35840233 \coth^4 \mu}{796262400} + \frac{3094663 \coth^6 \mu}{31850496}.$$
Then the integral (A.1) resulting from the saddle \( t_0 \) can be expressed as

\[
\int_{-\infty}^{\infty} e^{-xw^2} \frac{dt}{dw} \, dw, 
\]

which, after substitution of the expansion (A.2) followed by routine integration and taking into account the contribution from the saddle at \( t = -\mu + \frac{1}{2} \pi i \), then yields the expansion for \( K_{i\nu}(x) \) stated in (2.1).

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