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# ASYMPTOTICS OF MODIFIED BESSEL FUNCTIONS OF HIGH ORDER

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**Abstract:** In this work, we present two sets of full asymptotic expansions for the modified Bessel functions $I_\nu(z)$ and $K_\nu(z)$ and a full asymptotic expansion for $I_\nu(z)K_\nu(z)$ as $\nu \to \infty$ and $z$ is fixed with $|\arg z| < \pi$. In particular, we show that

$$I_\nu(z) \sim \frac{(\frac{1}{2}z)^\nu}{\Gamma(\nu+1)} \sum_{m=0}^{\infty} \frac{b_m(z)}{\nu^m} \quad \text{as } \nu \to \infty, \quad |\arg \nu| \le \pi - \delta,$$

and

$$K_\nu(z) \sim \frac{1}{2} \frac{\Gamma(\nu)}{(\frac{1}{2}z)^\nu} \sum_{m=0}^{\infty} (-1)^m \frac{b_m(z)}{\nu^m} \quad \text{as } \nu \to \infty, \quad |\arg \nu| \le \tfrac{1}{2}\pi - \delta,$$

where, for each $m$, $b_m(z)$ is a polynomial of degree $m$ in $z^2$, whose coefficients alternate in sign. Actually,

$$b_0(z) = 1; \quad b_m(z) = \sum_{k=1}^{m} (-1)^{m-k} \frac{S(m,k)}{k!} (\tfrac{1}{4}z^2)^k, \quad m = 0, 1, \ldots,$$

where $S(m,k)$ are the Stirling numbers of the second kind. We also compare the asymptotic expansions of this work with those existing in the literature.

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## 1. Introduction

The *modified Bessel functions* $I_\nu(z)$ and $K_\nu(z)$ arise in many scientific applications. In particular, with $\nu = n + \frac{1}{2}$, $n = 0, 1, \ldots$, they arise in quantum chemistry; for such $\nu$, they are known as the *modified spherical Bessel functions.*

There is vast literature on asymptotic behavior of Bessel functions in general, and on modified Bessel functions in particular. These concern the situations in which $z \to \infty$, or $z = \nu\xi$, $\xi$ being real and $\nu \to \infty$, or $\nu = \mathrm{i}\eta$ and $\eta \to \infty$, or $\nu = \mathrm{i}\eta$ and $z = \eta\xi$, $\xi$ being real and $\eta \to \infty$, to name some. An excellent source for all these expansions is Olver [6, Chapter 10, §7], where expansions that hold uniformly in unbounded $z$ domains are given with rigorous estimates of the remainders. See also Olver et al. [7, Sections 10.25(ii), 4.2(iv)]. The purpose of this note is to contribute to the subject of their asymptotic expansions when $\nu \to \infty$ in the sectors $|\arg\nu| \leq \pi - \delta$ and $|\arg\nu| \leq \frac{1}{2}\pi - \delta$, where $\delta > 0$ is an arbitrarily small number, for finite fixed $z$, $|\arg z| \leq \pi - \delta$.

Now, it is already known that, with fixed $z$, $I_\nu(z)$ and $K_\nu(z)$ satisfy the asymptotic equalities

$$I_\nu(z) \sim \frac{(\frac{1}{2}z)^\nu}{\Gamma(\nu+1)} \quad \text{as } \nu \to \infty, \quad |\arg\nu| \leq \pi - \delta, \tag{1.1}$$

and

$$K_\nu(z) \sim \frac{1}{2}\,\frac{\Gamma(\nu)}{(\frac{1}{2}z)^\nu} \quad \text{as } \nu \to \infty, \quad |\arg\nu| \leq \tfrac{1}{2}\pi - \delta. \tag{1.2}$$

These show that, with $z$ fixed, $I_\nu(z)$ goes to zero practically as $1/\Gamma(\nu+1)$ when $\nu \to \infty$, and $K_\nu(z)$ grows to infinity practically as $\Gamma(\nu)$ when $\nu \to \infty$. The asymptotic equality in (1.1) can be found in Olver [6, p. 374], where it is obtained by analyzing the power series of $I_\nu(z)$ about $z = 0$. The asymptotic equality in (1.2) (actually, a full asymptotic expansion), with $\nu$ real positive, can also be found in Sidi [8, Example 3], where it is derived by analyzing an integral representation of $K_\nu(z)$ that involves a Mellin transform. Following the approach of Frenzen [2], it can be shown that the same asymptotic expansion is valid also in every set $S(\eta) = \{\nu : \Re\nu > 0, |\Im\nu| \leq \eta\sqrt{\Re\nu}\}$ for fixed but arbitrary $\eta > 0$. This subject is revisited in a recent paper by Sidi [9], in which a full explicit expansion for $K_\nu(z)$ for $\nu \in S(\eta)$ is also derived.

As far as we know, the full asymptotic expansions of $I_\nu(z)$ and $K_\nu(z)$ for large $\nu$, in negative powers of $\nu$, have not been presented elsewhere. Starting with suitable series and integral representations, in the next section of this work, we derive two sets of full asymptotic expansions for $I_\nu(z)$ and $K_\nu(z)$.

These are presented in Theorems 2.1 and 2.3. In Theorem 3.1 of Section 3, we derive an additional expansion for their product $I_\nu(z)K_\nu(z)$, in negative powers of $\nu$. The coefficients of all these expansions turn out to have interesting algebraic structures; for example, the coefficients in the expansions of $K_\nu(z)$ are related to the corresponding coefficients in the expansions of $I_\nu(z)$ in a simple way. We also derive asymptotic expansions for the ratios $\Gamma(\nu)/\Gamma(\nu+\frac{1}{2})$ and $\Gamma(\nu+\frac{1}{2})/\Gamma(\nu+1)$ and show that the coefficients in these expansions are also related in an interesting way.

Finally, it is important to mention that the asymptotic expansions of $I_\nu(z)$ and $K_\nu(z)$ given in Theorem 2.1 are obtained by re-expanding the power series that define these functions in negative powers of $\nu$. Actually, these power series are also generalized asymptotic expansions and provide excellent approximations for the functions involved. This point is discussed again in some detail in the proof of Theorem 2.1 of this work.

In our treatment, we make use of the *generalized Bernoulli polynomials* $B_k^{(a)}(u)$, which are defined via

$$H(t,u;a) \equiv \left(\frac{t}{e^t-1}\right)^a e^{ut} = \sum_{k=0}^{\infty} B_k^{(a)}(u)\frac{t^k}{k!}, \quad |t|<2\pi. \tag{1.3}$$

Of course, $B_k^{(a)}(u)$ is of degree $k$ in $u$, and $B_0^{(a)}(u)=1$. These polynomials satisfy

$$B_k^{(a)}(a-u) = (-1)^k B_k^{(a)}(u), \quad k=0,1,\ldots, \tag{1.4}$$

from which we also have $B_{2k+1}^{(a)}(\frac{1}{2}a)=0$, $k=0,1,\ldots$ . The constants $B_k^{(a)}(0)$ are called *generalized Bernoulli numbers* and they are denoted simply by $B_k^{(a)}$. Note that (1.3) is valid also when $a=u=0$, in which case $B_0^{(0)}(0)=1$ and $B_k^{(0)}(0)=0$, $k=1,2,\ldots$ . See [5, pp. 18–22], for example.

We also make use of the *Stirling numbers of the second kind* $S(n,k)$, which are defined via the recursion relation

$$S(n,k) = S(n-1,k-1) + kS(n-1,k), \quad n=1,2,\ldots, \quad k=0,1,\ldots, \tag{1.5}$$

with

$$\begin{aligned} &S(n,0) = \begin{cases} 1 & \text{if } n=0 \\ 0 & \text{if } n>0 \end{cases}; \quad S(n,1)=1, \quad n\geq 1; \\ &S(n,k) = 0 \quad \text{if } n<k \text{ or } n<0. \end{aligned} \tag{1.6}$$

In particular, we make use of the relation

$$\frac{1}{(\zeta+1)_k}=\sum_{n=k}^{\infty}(-1)^{n-k}S(n,k)\zeta^{-n}, \quad |\zeta|>k. \tag{1.7}$$

See, for example, Graham, Knuth, and Patashnik [4, Sections 6.1 and 7.4].

Another tool that we use is the following lemma.

**Lemma 1.1.** *Let $D_1$ and $D_2$ be two unbounded sets and let $\widehat{D}=D_1\cap D_2$ be also unbounded. Let $f(\nu)$ have the following asymptotic expansions:*

$$f(\nu)\sim\sum_{k=0}^{\infty}A_k^{(i)}\phi_k(\nu) \quad \text{as } \nu\to\infty, \quad \nu\in D_i, \quad i=1,2,$$

*where $\{\phi_k(\nu)\}_{k=0}^{\infty}$ is an asymptotic scale as $\nu\to\infty$ in both $D_1$ and $D_2$. Then*

$$A_k^{(1)}=A_k^{(2)}=A_k, \quad k=0,1,\dots,$$

*and the series $\sum_{k=0}^{\infty}A_k\phi_k(\nu)$ represents $f(\nu)$ asymptotically as $\nu\to\infty$ in $D_1\cup D_2$.*

*Proof.* Since both series $\sum_{k=0}^{\infty}A_k^{(i)}\phi_k(\nu)$, $i=1,2$, represent $f(\nu)$ asymptotically as $\nu\to\infty$ in $\widehat{D}$, they must be the same because the asymptotic expansion of a function in terms of a fixed asymptotic scale is unique (see [6, p. 17, Theorem 7.1]). □

Before going on, we would like to emphasize that the asymptotic expansions we derive are not valid uniformly in $z$; they are valid for fixed $z$ only.

## 2. Theory

We start by presenting two sets of complete asymptotic expansions for $I_\nu(z)$ and $K_\nu(z)$ as $\nu\to\infty$ in the sectors $|\arg\nu|\leq\pi-\delta$ and $|\arg\nu|\leq\frac{1}{2}\pi-\delta$, respectively, where $\delta>0$ is an arbitrarily small number, which seem to be new. In our developments, we make use of the power series representation of $I_\nu(z)$, namely,

$$I_\nu(z)=\sum_{k=0}^{\infty}\frac{(\frac{1}{2}z)^{\nu+2k}}{k!\,\Gamma(\nu+k+1)}, \tag{2.1}$$

and of the McDonald definition of $K_\nu(z)$, namely,

$$K_\nu(z)=\frac{\pi}{2}\,\frac{I_{-\nu}(z)-I_\nu(z)}{\sin\nu\pi}, \tag{2.2}$$

which is valid for noninteger $\nu$, and is defined as a limit for integer $\nu$. Since $z^\nu$ is multivalued with a branch cut along the negative real axis in the $z$-plane, we take $I_\nu(z)$ and $K_\nu(z)$ to be the principal values of the right-hand sides of (2.1) and (2.2). In addition, we recall that for each fixed $z$, both $I_\nu(z)$ and $K_\nu(z)$ are entire functions of $\nu$.

We also make use of the integral representations (see [7, Section 10.32, Eqs. 10.32.2 and 10.32.11] or Gradshteyn and Ryzhik [3, pp. 958–959])

$$I_\nu(z) = 2\,\frac{(\frac{1}{2}z)^\nu}{\sqrt{\pi}\,\Gamma(\nu+\frac{1}{2})}\int_0^1 (1-t^2)^{\nu-\frac{1}{2}}\cosh zt\,dt, \quad \Re\nu > -\frac{1}{2}, \tag{2.3}$$

that is valid for all $z \neq 0$, and

$$K_\nu(z) = \frac{\Gamma(\nu+\frac{1}{2})}{\sqrt{\pi}\,(\frac{1}{2}z)^\nu}\int_0^\infty \frac{\cos zt}{(1+t^2)^{\nu+\frac{1}{2}}}\,dt, \quad \Re\nu > -\frac{1}{2}, \quad z > 0. \tag{2.4}$$

Finally, we make use of Watson's lemma (see Olver [6], for example) as one of our analytical tools.

Our first set of asymptotic expansions provides completions of the asymptotic equalities for $I_\nu(z)$ and $K_\nu(z)$ given in (1.1) and (1.2). The resulting expansions involve the $S(m,k)$, Stirling numbers of the second kind.

**Theorem 2.1.** *Define the sets $T_\pm(\epsilon)$ via*

$$T_\pm(\epsilon) = \left\{\nu : \ |\nu \pm n| \geq \epsilon; \quad n \in \mathbb{N}, \quad \epsilon \in (0, \tfrac{1}{2})\right\}. \tag{2.5}$$

*Then, for fixed $z \neq 0$, and $|\arg z| < \pi$, the principal values of the modified Bessel functions $I_\nu(z)$ and $K_\nu(z)$ have the asymptotic expansions*

$$I_\nu(z) \sim \frac{(\frac{1}{2}z)^\nu}{\Gamma(\nu+1)}\sum_{m=0}^\infty \frac{b_m(z)}{\nu^m} \quad \text{as } \nu \to \infty, \quad \nu \in T_+(\epsilon), \tag{2.6}$$

*and*

$$K_\nu(z) \sim \frac{1}{2}\,\frac{\Gamma(\nu)}{(\frac{1}{2}z)^\nu}\sum_{m=0}^\infty (-1)^m\,\frac{b_m(z)}{\nu^m} \quad \text{as } \nu \to \infty, \quad |\arg\nu| \leq \tfrac{1}{2}\pi - \delta, \tag{2.7}$$

*where $\epsilon$ is arbitrarily small, and for each $m = 0, 1, \ldots$, $b_m(z)$ is a polynomial of degree $m$ in $z^2$, given as in*

$$b_0(z) = 1; \quad b_m(z) = \sum_{k=1}^m (-1)^{m-k}\,\frac{S(m,k)}{k!}\left(\tfrac{1}{4}z^2\right)^k, \quad m = 1, 2, \ldots\ . \tag{2.8}$$

*(Note that the $b_m(z)$ in (2.6) and (2.7) are identical. For each $m$, the coefficients of $b_m(z)$ have alternating signs.)*

*Proof.* We begin by showing that, for every fixed $z \neq 0$, the (everywhere convergent) power series of $I_\nu(z)$ in (2.1), is already an excellent asymptotic expansion as $\nu \to \infty$, in the set $T_+(\epsilon)$. For this, let us first write (2.1) in the form

$$I_\nu(z) = \frac{(\frac{1}{2}z)^\nu}{\Gamma(\nu+1)} \sum_{k=0}^{\infty} \frac{w^k}{k!\,(\nu+1)_k}; \quad w = \tfrac{1}{4}z^2, \tag{2.9}$$

and rewrite it as in

$$I_\nu(z) = \frac{(\frac{1}{2}z)^\nu}{\Gamma(\nu+1)} \left[ \sum_{k=0}^{p-1} \frac{w^k}{k!\,(\nu+1)_k} + \frac{w^p}{(\nu+1)_p} W_\nu(z;p) \right]; \quad w = \tfrac{1}{4}z^2, \tag{2.10}$$

where $p$ is a positive integer and

$$W_\nu(z;p) = \sum_{k=0}^{\infty} \frac{w^k}{(p+k)!\,(\nu+p+1)_k}.$$

We now need to show that $W_\nu(z;p)$ can be bounded independently of $\nu$. When $\Re\nu \geq 0$, we can easily show that $|W_\nu(z;p)| \leq \exp(|w|)$ independently of $\nu$, and we are done. When $\Re\nu < 0$, we proceed as follows: Let $n$ be the (unique) positive integer for which

$$-n - \tfrac{1}{2} < \Re\nu \leq -n + \tfrac{1}{2}.$$

Thus, letting also $\mu = \nu + n$, we have that $|\Re\mu| \leq \frac{1}{2}$. In addition, for any integer $m$,

$$|\nu + m| = |(m-n) + \mu| \geq \big||m-n| - |\Re\mu|\big| \geq |m-n| - \tfrac{1}{2} \geq \tfrac{1}{2}, \quad \text{if } m \neq n.$$

Therefore, taking into account also the fact that $|\nu + n| = |\mu|$,

$$|(\nu+p+1)_k| \geq \begin{cases} (\frac{1}{2})^k, & 0 \leq k \leq n-p-1, \\ |\mu|(\frac{1}{2})^{k-1}, & k \geq n-p. \end{cases}$$

Making use of these in

$$W_\nu(z;p) = \left( \sum_{k=0}^{n-p-1} + \sum_{k=n-p}^{\infty} \right) \frac{w^k}{(p+k)!\,(\nu+p+1)_k},$$

we obtain

$$|W_\nu(z;p)| \leq \sum_{k=0}^{n-p-1} \frac{|w|^k}{(p+k)!\,(\frac{1}{2})^k} + \sum_{k=n-p}^{\infty} \frac{|w|^k}{(p+k)!\,|\mu|\,(\frac{1}{2})^{k-1}}$$

$$
\begin{aligned}
&\leq \frac{1}{p!}\sum_{k=0}^{n-p-1}\frac{|2w|^k}{k!}+\frac{|2w|^{n-p}}{2|\mu|(n!)}\sum_{k=0}^{\infty}\frac{|2w|^k}{k!}\\
&\leq \left(\frac{1}{p!}+\frac{|2w|^{n-p}}{2|\mu|(n!)}\right)\exp(|2w|),\\
&\leq A(z;p)\,\exp(|2w|),\\
A(z;p) &= \frac{1}{p!}+\frac{|2w|^{-p}}{2\epsilon}\left(\sup_{m\geq 0}\frac{|2w|^m}{m!}\right)<\infty,
\end{aligned}
$$

the right-hand side of the last inequality being independent of $n$ and $\mu$, hence independent of $\nu$ as well, since $|\mu|\geq\epsilon$ when $\nu\in T_+(\epsilon)$ and $\lim_{m\to\infty}(|2w|^m/m!)=0$ for fixed $z$. We have thus shown that the right-hand side of (2.9) is an asymptotic expansion for $I_\nu(z)$ as $\nu\to\infty$, $\nu\in T_+(\epsilon)$.

Now, by (1.7), we have the expansion

$$
\frac{1}{(\nu+1)_k}=\sum_{m=k}^{\infty}(-1)^{m-k}S(m,k)\nu^{-m},\quad |\nu|>k. \tag{2.11}
$$

Note that the right-hand side of (2.11) is also an asymptotic expansion for $1/(\nu+1)_k$ as $\nu\to\infty$, $\nu\in T_+(\epsilon)$. Substituting this expansion in the series $\sum_{k=0}^{\infty}\frac{w^k}{k!\,(\nu+1)_k}$, changing the order of the summations, and invoking $S(0,0)=1$, $S(m,0)=0$ for $m\geq 1$, and (2.8), we obtain

$$
\sum_{k=0}^{\infty}\frac{w^k}{k!\,(\nu+1)_k}\sim\sum_{m=0}^{\infty}\frac{b_m(z)}{\nu^m}\quad\text{as } \nu\to\infty,\quad \nu\in T_+(\epsilon). \tag{2.12}
$$

Upon substituting this in (2.9), we obtain (2.6).

To prove (2.7), we proceed via (2.6) and (2.2). First, replacing $\nu$ in (2.6) by $-\nu$, we obtain

$$
I_{-\nu}(z)=\frac{(\frac{1}{2}z)^{-\nu}}{\Gamma(-\nu+1)}\sum_{k=0}^{\infty}\frac{w^k}{k!\,(-\nu+1)_k};\quad w=\tfrac{1}{4}z^2. \tag{2.13}
$$

It is now easy to see that, re-expanding the series $\sum_{k=0}^{\infty}\frac{w^k}{k!\,(-\nu+1)_k}$ in negative powers of $\nu$ amounts to replacing $\nu$ in (2.12) by $-\nu$. Consequently, (2.13) gives

$$
I_{-\nu}(z)\sim\frac{(\frac{1}{2}z)^{-\nu}}{\Gamma(-\nu+1)}\sum_{m=0}^{\infty}(-1)^m\frac{b_m(z)}{\nu^m}\quad\text{as } \nu\to\infty,\quad \nu\in T_-(\epsilon). \tag{2.14}
$$

Making use of the reflection formula for the Gamma function, namely,

$$\Gamma(\nu)\Gamma(1-\nu)=\frac{\pi}{\sin\nu\pi},\quad \nu\neq 0,\pm1,\pm2,\ldots,$$

(2.14) becomes

$$I_{-\nu}(z)\sim\frac{\sin\nu\pi}{\pi}\,\frac{\Gamma(\nu)}{(\frac{1}{2}z)^{\nu}}\sum_{m=0}^{\infty}(-1)^m\,\frac{b_m(z)}{\nu^m}\quad \text{as } \nu\to\infty,\quad \nu\in T_-(\epsilon). \tag{2.15}$$

From (2.6) and (2.15), it is clear that

$$\frac{I_{\nu}(z)}{I_{-\nu}(z)}\sim\frac{\pi}{\sin\nu\pi}\,\frac{(\frac{1}{2}z)^{2\nu}}{\nu[\Gamma(\nu)]^2}\quad \text{as } \nu\to\infty,\quad \nu\in T_+(\epsilon)\cap T_-(\epsilon), \tag{2.16}$$

and hence $I_{\nu}(z)/I_{-\nu}(z)$ tends to zero as $\nu\to\infty$ faster than $e^{-\lambda|\nu|}$ for all $\lambda>0$, provided $|\arg\nu|\leq\frac{1}{2}\pi-\delta$, which, by (2.2), implies that

$$\begin{aligned}&K_{\nu}(z)\sim\frac{\pi}{2\sin\nu\pi}I_{-\nu}(z)\quad \text{as } \nu\to\infty,\\ &\nu\in T_-(\epsilon),\quad |\arg\nu|\leq\tfrac{1}{2}\pi-\delta.^{1}\end{aligned} \tag{2.17}$$

Upon substituting (2.15) in (2.17), we obtain (2.7), with the restriction that $\nu\in T_-(\epsilon)$ with $\epsilon>0$ and arbitrarily small. To complete the proof of (2.7), we now have to somehow remove this restriction and show that the asymptotic expansion given in (2.7) holds for *all* $\nu$ with $|\arg\nu|\leq\frac{1}{2}\pi-\delta$. By expressing $K_{\nu}(z)$ as a Mellin transform of a suitable function with $\Re z>0$, the first author has shown in [9] that the exact same asymptotic expansion of $K_{\nu}(z)$ as $\nu\to\infty$ given in (2.7) with (2.8) is valid for $\nu$ in the set $U(\eta)=\{\nu:\ \Re\nu>0,\ |\Im\nu|\leq\eta\sqrt{\Re\nu}\}$ for fixed but arbitrary $\eta>0$.[2] Now the intersection of the sets $T_-(\epsilon)$

[1] When $|\arg\nu|=\frac{1}{2}\pi$, so that $\nu=i\eta$, $\eta$ real, we have (see [7, Section 5.4(i), equation (5.4.3)]) $|\Gamma(\nu)|^2=\dfrac{\pi}{|\eta|\sinh\pi|\eta|}$, and hence $|I_{\nu}(z)/I_{-\nu}(z)|\sim|(\frac{1}{2}z)^{2\nu}|$ as $|\eta|\to\infty$. Thus, $K_{\nu}(z)\sim\frac{\pi}{2\sin\nu\pi}I_{-\nu}(z)$ as $\nu\to\infty$, in (2.17) does not always hold in this case; in particular, it does not hold when $z$ is real and positive. See also Remark 4 following the proof of Theorem 2.1.

[2] In [8, Section 3, Example 3], the first author derived an asymptotic expansion of the form

$$K_{\nu}(z)\sim\frac{1}{2}\,\frac{\Gamma(\nu)}{(\frac{1}{2}z)^{\nu}}\sum_{k=0}^{\infty}\frac{A_k(z)}{\nu^k}\quad \text{as } \nu\to\infty,\ \ \nu \text{ real positive},$$

$A_k(z)$ being polynomials in $z$, by expressing an integral representation of $K_{\nu}(z)$ as a Mellin transform of some other function $f(t)$. Due to the complexity of the function $f(t)$, however, we were not able to give a simple explicit representation for the $A_k(z)$.

and $U(\eta)$ contains the unbounded set $\{\nu : \Re\nu \geq C,\ \epsilon \leq |\Im\nu| \leq \eta\sqrt{\Re\nu}\}$ for some sufficiently large $C > 0$. Therefore, by Lemma 1.1, (2.7) is valid as is, with the restriction $|\arg z| \leq \frac{1}{2}\pi - \delta$. [Recall that we need to show that (2.7) is valid for $|\arg z| \leq \pi - \delta$.] This last restriction on $z$ can also be removed by recalling that (see [7, Section 10.34, equation (10.34.2)])

$$K_\nu(e^{\mathrm{i}m\pi}z) = e^{-\mathrm{i}m\nu\pi}K_\nu(z) - \mathrm{i}\pi\sin(m\nu\pi)\csc(\nu\pi)I_\nu(z), \quad m \text{ integer}. \tag{2.18}$$

By (2.17) and (2.16), the asymptotic expansion of the term involving $I_\nu(z)$ in (2.18) is negligible compared to that involving $K_\nu(z)$, and hence

$$K_\nu(e^{\mathrm{i}m\pi}z) \sim e^{-\mathrm{i}m\nu\pi}K_\nu(z) \quad \text{as } \nu \to \infty.$$

Now we take $m = \pm 1$ and use the already computed asymptotic expansion of $K_\nu(z)$ to conclude that (2.7) indeed holds for $|\arg z| \leq \pi - \delta$. □

**Remarks.**

1. (2.6) applies to the sequence $\{I_{\mu-n}(z)\}_{n=0}^{\infty}$, when $\mu$ is real but not an integer. In particular, it applies to the sequence $\{I_{-n-\frac{1}{2}}(z)\}_{n=0}^{\infty}$ of modified spherical Bessel functions.

2. "$\nu \in T_+(\epsilon)$" in (2.6) can be replaced by the weaker "$|\arg\nu| \leq \pi - \delta$" since all sufficiently large $\nu$ with $|\arg\nu| \leq \pi - \delta$ are in $T_+(\epsilon)$. The opposite is not true, however.

3. (2.6) is valid also when $|\arg z| = \pi$ since $I_\nu(e^{\mathrm{i}m\pi}z) = e^{\mathrm{i}m\nu\pi}I_\nu(z)$ when $m$ is an integer. See [7, Section 10.34, equation (10.34.1)].

4. By (2.2), $K_{-\nu}(z) = K_\nu(z)$. This implies that we can restrict our attention to $K_\nu(z)$ for $\nu$ in the right half of the complex $\nu$-plane. As already mentioned, the $\Im\nu$-axis cannot be part of this half, and this is the reason for the restriction $|\arg\nu| \leq \frac{1}{2}\pi - \delta$ in (2.7).

Before we continue to the next set of asymptotic expansions for $I_\nu(z)$ and $K_\nu(z)$, we present a simple lemma concerning the asymptotic expansions of ratios of two Gamma functions. These asymptotic expansions seem to be of interest by themselves.

**Lemma 2.2.** *The ratios $\Gamma(\nu)/\Gamma(\nu+\frac{1}{2})$ and $\Gamma(\nu+\frac{1}{2})/\Gamma(\nu+1)$ satisfy*

$$\frac{\Gamma(\nu)}{\Gamma(\nu+\frac{1}{2})} \sim \sum_{k=0}^{\infty} \frac{c_k}{\nu^{k+\frac{1}{2}}} \quad \text{as } \nu \to \infty, \quad |\arg\nu| \leq \pi - \delta, \tag{2.19}$$

*and*

$$\frac{\Gamma(\nu+\frac{1}{2})}{\Gamma(\nu+1)} \sim \sum_{k=0}^{\infty}(-1)^k \frac{c_k}{\nu^{k+\frac{1}{2}}} \quad \textit{as } \nu \to \infty, \quad |\arg \nu| \le \pi - \delta, \tag{2.20}$$

*where* $\delta > 0$ *is arbitrarily small, and*

$$c_k = (-1)^k \, (\tfrac{1}{2})_k \, \frac{B_k^{(\frac{1}{2})}}{k!}, \quad k = 0, 1, \dots \, . \tag{2.21}$$

*Proof.* We start with the following result that is due to Tricomi and Erdélyi [10] (see also Luke [5, p. 33] and Andrews, Askey, and Roy [1, p. 615]):

$$\frac{\Gamma(\nu+\alpha)}{\Gamma(\nu+\beta)} \sim \sum_{k=0}^{\infty}(-1)^k \, \frac{B_k^{(\sigma)}(\alpha)}{k!} \, \frac{(\beta-\alpha)_k}{\nu^{\beta-\alpha+k}} \quad \text{as } \nu \to \infty,$$
$$|\arg \nu| \le \pi - \delta; \quad \sigma = \alpha - \beta + 1.$$

Setting first $\alpha = 0$ and $\beta = \frac{1}{2}$, and next $\alpha = \frac{1}{2}$ and $\beta = 1$, and also recalling that $B_k^{(\frac{1}{2})}(\frac{1}{2}) = (-1)^k B_k^{(\frac{1}{2})}(0) = (-1)^k B_k^{(\frac{1}{2})}$, the results follow. □

The asymptotic expansions in our second set are “symmetric” versions of those in Theorem 2.3 and involve the generalized Bernoulli numbers and polynomials.

**Theorem 2.3.** *For fixed* $z \neq 0$*, the modified Bessel functions* $I_\nu(z)$ *and* $K_\nu(z)$ *have the following asymptotic expansions:*

$$I_\nu(z) \sim \frac{(\frac{1}{2}z)^\nu}{\Gamma(\nu+\frac{1}{2})} \sum_{s=0}^{\infty} \frac{a_s(z;c)}{(\nu+c)^{s+\frac{1}{2}}} \quad \textit{as } \nu \to \infty, \quad |\arg \nu| \le \pi - \delta, \tag{2.22}$$

*and*

$$K_\nu(z) \sim \frac{1}{2} \, \frac{\Gamma(\nu+\frac{1}{2})}{(\frac{1}{2}z)^\nu} \sum_{s=0}^{\infty}(-1)^s \frac{a_s(z;c)}{(\nu-c)^{s+\frac{1}{2}}} \quad \textit{as } \nu \to \infty,$$
$$|\arg \nu| \le \tfrac{1}{2}\pi - \delta, \tag{2.23}$$

*where* $\delta > 0$ *is arbitrarily small,* $c$ *is an arbitrary constant and, for each* $s = 0, 1, \dots,$ $a_s(z;c)$ *is a polynomial of degree* $s$ *in* $z^2$*, given by*

$$a_s(z;c) = (\tfrac{1}{2})_s \sum_{k=0}^{s}(-1)^{s-k} \frac{B_{s-k}^{(-k+\frac{1}{2})}(\frac{1}{2}-c)}{(s-k)!} \, \frac{z^{2k}}{(2k)!}. \tag{2.24}$$

*Clearly,* $a_0(z;c) = 1$*. [Note that the* $a_s(z;c)$ *in* (2.22) *and* (2.23) *are identical.]*

*Proof.* That there exist asymptotic expansions of the forms given in (2.22) and (2.23) can be shown as follows: Let us rewrite (2.6) and (2.7) as in

$$I_\nu(z) \sim \frac{(\frac{1}{2}z)^\nu}{\Gamma(\nu+\frac{1}{2})}\left[\frac{\Gamma(\nu+\frac{1}{2})}{\Gamma(\nu+1)}\sum_{m=0}^{\infty}\frac{b_m(z)}{\nu^m}\right] \quad \text{as } \nu \to \infty, \tag{2.25}$$

and

$$K_\nu(z) \sim \frac{1}{2}\frac{\Gamma(\nu+\frac{1}{2})}{(\frac{1}{2}z)^\nu}\left[\frac{\Gamma(\nu)}{\Gamma(\nu+\frac{1}{2})}\sum_{m=0}^{\infty}(-1)^m\frac{b_m(z)}{\nu^m}\right] \quad \text{as } \nu \to \infty. \tag{2.26}$$

Now invoke Lemma 2.2, and re-expand the terms inside the square brackets in negative powers of $\nu \pm c$; this produces the required asymptotic expansions. As for the conditions on $\arg\nu$, it is easy to see that these must be the same as those in (2.6) and (2.7) since the corresponding conditions in Lemma 2.2 contain $|\arg\nu| \le \pi - \delta$ both in (2.19) and in (2.20).

We now want to obtain the explicit expressions given in (2.24) for the coefficients $a_s(z;c)$. Because these are polynomials in $z$, and because asymptotic expansions are unique, it suffices to obtain these by working with real $\nu$ and $z$.

*1. Proof of* (2.22). Making the substitution $1-t^2 = e^{-\tau}$ in the integral of (2.3), we obtain

$$D_\nu(z) = 2\int_0^1 (1-t^2)^{\nu-\frac{1}{2}}\cosh zt\,dt = \int_0^\infty e^{-\nu\tau}\Phi(\tau;z)\,d\tau, \tag{2.27}$$

where

$$\Phi(\tau;z) = \frac{e^{-\tau/2}\cosh\left(z\sqrt{1-e^{-\tau}}\right)}{\sqrt{1-e^{-\tau}}}. \tag{2.28}$$

Now, $\Phi(\tau;z)$ can be expanded in an infinite series as in

$$\Phi(\tau;z) = \frac{e^{-\tau/2}}{\sqrt{1-e^{-\tau}}}\sum_{k=0}^{\infty}\frac{z^{2k}(1-e^{-\tau})^k}{(2k)!}, \tag{2.29}$$

which, for arbitrary constant $c$, can be rewritten as

$$\Phi(\tau;z) = \sum_{k=0}^{\infty}\frac{z^{2k}}{(2k)!}\,\tau^{k-\frac{1}{2}}H(\tau,-k+c;-k+\tfrac{1}{2})e^{-c\tau}, \tag{2.30}$$

with $H(t,u;a)$ as in (1.3). Hence, by (1.3), $\Phi(\tau;z)$ has the convergent Maclaurin series

$$\Phi(\tau;z)=\sum_{k=0}^{\infty}\sum_{i=0}^{\infty}\frac{z^{2k}}{(2k)!}\,\frac{B_i^{(-k+\frac{1}{2})}(-k+c)}{i!}\,\tau^{i+k-\frac{1}{2}}e^{-c\tau}.$$

Rearranging this series, and invoking (1.4), we have

$$\Phi(\tau;z)=\sum_{s=0}^{\infty}\left[\sum_{k=0}^{s}(-1)^{s-k}\frac{z^{2k}}{(2k)!}\,\frac{B_{s-k}^{(-k+\frac{1}{2})}(\frac{1}{2}-c)}{(s-k)!}\right]\tau^{s-\frac{1}{2}}e^{-c\tau}.$$

On account of this series, we can now apply Watson's lemma to the integral representation of $D_\nu(z)$ given in (2.27), and obtain the asymptotic expansion

$$D_\nu(z)\sim\sum_{s=0}^{\infty}\left[\sum_{k=0}^{s}(-1)^{s-k}\frac{z^{2k}}{(2k)!}\,\frac{B_{s-k}^{(-k+\frac{1}{2})}(\frac{1}{2}-c)}{(s-k)!}\right]\frac{\Gamma(s+\frac{1}{2})}{(\nu+c)^{s+\frac{1}{2}}},\qquad\text{as }\nu\to\infty,$$

that is valid for $|\arg\nu|\leq\frac{1}{2}\pi-\delta$. Substituting this expansion in (2.3), and recalling that

$$\Gamma(\tfrac{1}{2})=\sqrt{\pi}\quad\text{and}\quad\Gamma(\zeta+n)/\Gamma(\zeta)=(\zeta)_n,$$

the result in (2.22) and (2.24) follows.

*2. Proof of* (2.23). Making the substitution $1+t^2=e^\tau$ in the integral of (2.4), we obtain

$$E_\nu(z)=2\int_0^\infty\frac{\cos zt}{(1+t^2)^{\nu+\frac{1}{2}}}\,dt=\int_0^\infty e^{-\nu\tau}\Psi(\tau;z)\,d\tau,\tag{2.31}$$

where

$$\Psi(\tau;z)=\frac{e^{\tau/2}\cos\left(z\sqrt{e^\tau-1}\right)}{\sqrt{e^\tau-1}}.\tag{2.32}$$

Now, $\Psi(\tau;z)$ can be expanded in an infinite series as in

$$\Psi(\tau;z)=\frac{e^{\tau/2}}{\sqrt{e^\tau-1}}\sum_{k=0}^{\infty}(-1)^k\frac{z^{2k}(e^\tau-1)^k}{(2k)!},\tag{2.33}$$

which can be rewritten as

$$\Psi(\tau;z)=\sum_{k=0}^{\infty}(-1)^k\frac{z^{2k}}{(2k)!}\,\tau^{k-\frac{1}{2}}\,H(\tau,\tfrac{1}{2}-c;-k+\tfrac{1}{2})e^{c\tau}.$$

Hence, by (1.3), $\Psi(\tau;z)$ has the convergent Maclaurin series

$$\Psi(\tau;z)=\sum_{k=0}^{\infty}\sum_{i=0}^{\infty}(-1)^k\frac{z^{2k}}{(2k)!}\frac{B_i^{(-k+\frac{1}{2})}(\frac{1}{2}-c)}{i!}\tau^{i+k-\frac{1}{2}}e^{c\tau}.$$

Rearranging this series, and invoking (1.4), we have

$$\Psi(\tau;z)=\sum_{s=0}^{\infty}\left[\sum_{k=0}^{s}(-1)^k\frac{z^{2k}}{(2k)!}\frac{B_{s-k}^{(-k+\frac{1}{2})}(\frac{1}{2}-c)}{(s-k)!}\right]\tau^{s-\frac{1}{2}}e^{c\tau}.$$

The proof of (2.23) and (2.24) can now be achieved exactly as that of (2.22) and (2.24). □

**Remarks.**

1. The cases $c=0$ and $c=\frac{1}{2}$ seem to be interesting. Letting $c=0$, we have the asymptotic expansions

$$I_\nu(z)\sim\frac{(\frac{1}{2}z)^\nu}{\Gamma(\nu+\frac{1}{2})}\sum_{s=0}^{\infty}\frac{\hat{a}_s(z)}{\nu^{s+\frac{1}{2}}}\quad\text{as }\nu\to\infty,\quad|\arg\nu|\le\pi-\delta,\tag{2.34}$$

and

$$K_\nu(z)\sim\frac{1}{2}\frac{\Gamma(\nu+\frac{1}{2})}{(\frac{1}{2}z)^\nu}\sum_{s=0}^{\infty}(-1)^s\frac{\hat{a}_s(z)}{\nu^{s+\frac{1}{2}}}\quad\text{as }\nu\to\infty,$$
$$|\arg\nu|\le\tfrac{1}{2}\pi-\delta,\tag{2.35}$$

where

$$\hat{a}_s(z)=(\tfrac{1}{2})_s\sum_{k=0}^{s}(-1)^{s-k}\frac{B_{s-k}^{(-k+\frac{1}{2})}(\frac{1}{2})}{(s-k)!}\frac{z^{2k}}{(2k)!}.\tag{2.36}$$

With $c=\frac{1}{2}$ in (2.22) and (2.23), we have $B_{s-k}^{(-k+\frac{1}{2})}(\frac{1}{2}-c)=B_{s-k}^{(-k+\frac{1}{2})}$ in (2.24).

2. In addition, the $\hat{a}_s(z)=a_s(z;0)$ and the $b_m(z)$ of Theorem 2.1 are related through

$$\hat{a}_s(z)=\sum_{m=0}^{s}(-1)^{s-m}c_{s-m}b_m(z),\quad s=0,1,\dots,\tag{2.37}$$

and

$$b_m(z) = \sum_{s=0}^{m} c_{m-s}\,\hat{a}_s(z), \quad m = 0, 1, \dots\ . \tag{2.38}$$

Here, the $c_k$ are those introduced in Lemma 2.2.

To prove (2.37), we substitute (2.20) in (2.25), expand in negative powers of $\nu$ via the Cauchy product, and equate with (2.34). To prove (2.38), we proceed analogously. We leave the details to the reader.

3. Interestingly, from Theorems 2.1 and 2.3, we can also derive a relation between Stirling numbers of the second kind and generalized Bernoulli polynomials and numbers. Substituting (2.24) and (2.21) in (2.38), and rearranging and then invoking (2.8), we obtain

$$S(m,k) = \sum_{s=k}^{m} \frac{(\frac{1}{2})_{m-s}(\frac{1}{2})_s}{(\frac{1}{2})_k} \frac{B_{m-s}^{(\frac{1}{2})}}{(m-s)!} \frac{B_{s-k}^{(-k+\frac{1}{2})}(\frac{1}{2})}{(s-k)!}. \tag{2.39}$$

This identity seems to be new.

## 3. Asymptotic expansion of $I_\nu(z)K_\nu(z)$

Finally, we give a *full* asymptotic expansion for the product of the functions $I_\nu(z)$ and $K_\nu(z)$ as $\nu \to \infty$.

**Theorem 3.1.** *For fixed $z \neq 0$, the product $I_\nu(z)K_\nu(z)$ has the asymptotic expansion*

$$I_\nu(z)K_\nu(z) \sim \frac{1}{2\nu} \sum_{s=0}^{\infty} \frac{p_s(z)}{\nu^{2s}} \quad \text{as } \nu \to \infty, \quad |\arg \nu| \leq \tfrac{1}{2}\pi - \delta, \tag{3.1}$$

*where $p_s(z)$ is a polynomial of degree $s$ in $z^2$, given by*

$$p_0(z) = 1; \quad p_s(z) = \sum_{k=1}^{s} \gamma_{s,k}\, w^k, \quad s = 1, 2, \dots,; \quad w = \tfrac{1}{4}z^2, \tag{3.2}$$

*where*

$$\gamma_{s,k} = (-1)^k \binom{2s}{2k} \binom{2k}{k} B_{2s-2k}^{(-2k)}(-k), \quad k = 1, \dots, s. \tag{3.3}$$

*Moreover, $(-1)^k \gamma_{s,k} > 0$, $k = 1, \dots, s$.*

**Remark.** Note that, multiplying the two asymptotic expansions given in Theorem 2.1, we obtain

$$I_\nu(z)K_\nu(z) \sim \frac{1}{2\nu}\left[\sum_{m=0}^{\infty}\frac{b_m(z)}{\nu^m}\right]\left[\sum_{m=0}^{\infty}(-1)^m\frac{b_m(z)}{\nu^m}\right] \quad \text{as } \nu \to \infty,$$
$$|\arg\nu| \le \tfrac{1}{2}\pi - \delta. \tag{3.4}$$

The result in (3.1) can be obtained by realizing that the Cauchy product of the two summations in (3.4) contains only even powers of $\nu^{-1}$. Clearly, the polynomials $p_s(z)$ in (3.1) are given as in

$$p_s(z) = \sum_{m=0}^{2s}(-1)^m b_{2s-m}(z)b_m(z). \tag{3.5}$$

¿From this discussion, it is also clear that (3.1) is valid for all $\nu$ such that $|\arg\nu| \le \frac{1}{2}\pi - \delta$ and for $z \ne 0$ since the asymptotic expansions of Theorem 2.1 are. Now, all we can say about $p_s(z)$ in (3.5) is that it is a polynomial in $z^2$ of degree at most $2s$. Thus, our result that the degree of $p_s(z)$, as a polynomial in $z^2$, is exactly $s$ comes as a surprise.

*Proof.* We start with the integral representation (see [7, Section 10.32(iii), equation (10.32.16)])

$$I_\nu(z)K_\nu(z) = \int_0^\infty J_{\mu\pm\nu}(2z\sinh t)e^{(-\mu\pm\nu)t}\,dt;$$
$$\Re(\mu\mp\nu) > \tfrac{1}{2}, \quad \Re(\mu\pm\nu) > -1, \quad z > 0,$$

which, upon letting $\mu = \nu$ and choosing the lower sign in $\pm$ and $\mp$, becomes

$$I_\nu(z)K_\nu(z) = \int_0^\infty J_0(2z\sinh t)e^{-2\nu t}\,dt; \quad \Re\nu > \tfrac{1}{4}, \quad z > 0. \tag{3.6}$$

Here, $J_0(\xi)$ is the Bessel function of the first kind of order zero. Letting $\tau = 2t$ in (3.6), we obtain

$$I_\nu(z)K_\nu(z) = \frac{1}{2}\int_0^\infty J_0\left(2z\sinh\frac{\tau}{2}\right)e^{-\nu\tau}\,d\tau; \quad \Re\nu > \tfrac{1}{4}, \quad z > 0. \tag{3.7}$$

We can apply Watson's lemma to this integral and obtain the asymptotic expansion of $I_\nu(z)K_\nu(z)$ as $\nu \to \infty$, $|\arg\nu| \le \frac{1}{2}\pi - \delta$. For this, we need the asymptotic expansion of $J_0(2z\sinh\frac{\tau}{2})$ as $\tau \to 0$. By the fact that

$$J_0(\xi) = \sum_{k=0}^{\infty}(-1)^k\frac{(\frac{1}{2}\xi)^{2k}}{(k!)^2},$$

which is also an asymptotic expansion for $J_0(\xi)$ as $\xi \to 0$, we first have

$$J_0\left(2z\sinh\frac{\tau}{2}\right) = \sum_{k=0}^{\infty}(-1)^k\frac{z^{2k}}{(k!)^2}\left(\sinh\frac{\tau}{2}\right)^{2k}. \tag{3.8}$$

Next, using the fact that $\sinh t = \frac{1}{2}(e^t - e^{-t})$, after some simple algebra, we obtain

$$\left(\sinh\frac{\tau}{2}\right)^{2k} = \left(\frac{\tau}{2}\right)^{2k}\left(\frac{\tau}{e^\tau - 1}\right)^{-2k} e^{-k\tau},$$

which, by invoking (1.3) and (1.4), can be expressed in the form

$$\left(\sinh\frac{\tau}{2}\right)^{2k} = \sum_{j=0}^{\infty}\frac{B_{2j}^{(-2k)}(-k)}{4^k\,(2j)!}\tau^{2(j+k)}. \tag{3.9}$$

Note that, $B_{2j}^{(-2k)}(-k) > 0$ for all $j \geq 0$ and $k \geq 1$, since $2k$ is a positive integer and since the Maclaurin expansion of $\sinh\frac{\tau}{2}$ contains only odd powers of $\tau$ with positive coefficents. Substituting (3.9) in (3.8), and re-expanding , we finally obtain the (convergent) asymptotic expansion (as $\tau \to 0$)

$$J_0\left(2z\sinh\frac{\tau}{2}\right) = \sum_{s=0}^{\infty}\left[\sum_{k=0}^{s}(-1)^k\frac{w^k}{(k!)^2}\frac{B_{2s-2k}^{(-2k)}(-k)}{(2s-2k)!}\right]\tau^{2s}. \tag{3.10}$$

Applying now Watson's lemma to the integral in (3.7), and observing from (1.3) that $B_k^{(0)}(u) = u^k$, so that $B_0^{(0)}(0) = 1$ and $B_k^{(0)}(0) = 0$ for $k = 1, 2, \ldots,$ we obtain the result in (3.1)–(3.3).

Even though we have obtained the result in (3.1) under the restriction that $z$ is real and positive, this result is nevertheless true for all $z \neq 0$, as concluded in the remark preceding this proof. $\square$

## 4. Concluding Remarks

As already mentioned in the proof of Theorem 2.1, the infinite series representation of $I_\nu(z)$ in (2.1) is already an excellent generalized asymptotic expansion as $\nu \to \infty$ in the sense described in (2.10). This series can be used to compute $I_\nu(z)$ for finite $z$ and large $\nu$, within the limitations of finite-precision arithmetic on a computer.

A similar argument applies to $K_\nu(z)$. For example, when $\nu = n$ is a nonnegative integer, the convergent series (see [7, Section 10.31, equation (10.31.1)])

$$K_n(z) = \frac{1}{2}\,(\tfrac{1}{2}z)^{-n}\sum_{k=0}^{n-1}\frac{(n-k-1)!}{k!}(-\tfrac{1}{4}z^2)^k + (-1)^{n+1}\log(\tfrac{1}{2}z)\,I_n(z)$$
$$+ (-1)^n\frac{1}{2}(\tfrac{1}{2}z)^n\sum_{k=0}^{\infty}[\psi(k+1)+\psi(n+k+1)]\frac{(\tfrac{1}{2}z)^{2k}}{k!(n+k)!}. \quad (4.1)$$

serves as a good (generalized) asymptotic expansion for $K_n(z)$ as $n \to \infty$. It can be used to compute $K_n(z)$ for finite $z$ and large $n$, again within the limitations of finite-precision arithmetic on a computer.

In contrast, the expansions given in this work are asymptotic but divergent, and they are not meant to be used for computational purposes. They are useful in theoretical work, however. For example, all three expansions given in Theorems 2.3 and 3.1, in addition to being new and of interest by themselves, enable us to provide a precise and refined asymptotic analysis of certain important functions, called Barnett–Coulson–Löwdin functions, that arise in quantum chemistry and that are expressed in terms of the modified spherical Bessel functions $I_{n+\frac{1}{2}}(z)$ and $K_{n+\frac{1}{2}}(z)$, $n = 0, 1, \ldots$ . It is precisely this topic that has motivated the study we present in this note.

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