On the Computation and Applications of Bessel Functions with Pure Imaginary Indices

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Bessel functions with pure imaginary index (order) play an important role in corpuscular optics where they govern the dynamics of charged particles in isotrjectory quadrupoles. Recently they were found to be of great importance in semiconductor material characterization as they are manifested in the strain state of crystalline material. A new algorithm which can be used for the computation of the normal and modified Bessel functions with pure imaginary index is proposed. The developed algorithm is very fast to compute and for small arguments converges after a few iterations.

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I. INTRODUCTION

Bessel functions occur in many branches of mathematical physics as solutions of differential equations when boundary conditions such as the Dirichlet or Neumann are imposed on various space domains. The Bessel functions with index (order) $\nu$ can be represented as the solutions of the following differential equation \cite{1}:

\[ x^2 y'' + xy' + \left(x^2 - v^2\right) y = 0, \]  

(1)

where $y'$ and $y''$ are the first and second derivatives (respectively) with respect to $x$ while $\nu$ is a complex constant. The solutions of eqn. (1) can be expressed as an absolute converging series that is defined in the entire complex plane:

\[ J_\nu(z) = \left(\frac{x}{2}\right)^\nu \sum_{n=0}^{\infty} (-1)^n \frac{1}{n! (\nu + n + 1)} \left(\frac{x}{2}\right)^{2n}, \]  

(2)

In order to compute the solutions of equation (1) for the case of purely imaginary indices $i\nu$, it is required to obtain the sum of a series with each coefficient being a complex number and to compute the complex value function $\Gamma(i\nu)$ which on its own is a very laborious operation. In reality, for the case of a purely imaginary index $i\nu$ and for a natural number $n$ we have:

\[ \Gamma(i\nu + n + 1) = \Gamma(i\nu) \prod_{m=0}^{n} (i\nu + m), \]  

(3)

and thereafter Bessel function \cite{2} may be re-expressed in the form:

\[ J_{i\nu}(x) = \frac{1}{\Gamma(i\nu)} \left(\frac{x}{2}\right)^{i\nu} \sum_{n=0}^{\infty} (-1)^n \frac{1}{n! \prod_{m=0}^{n} (i\nu + m)} \left(\frac{x}{2}\right)^{2n}, \]  

(4)

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where \( \nu \) and \( x \) are real and complex numbers respectively. The solution of (1) expressed in the terms of (4) represents a "difficult-to-compute" complex solution of a differential equation with the real coefficients. To the best of our knowledge there is no concrete algorithm that can enable us to compute Bessel functions with purely imaginary order as they have had no applications in areas of natural sciences till date. Only a hand full of pure mathematicians made attempts to investigate such functions.

The author of one of the most detailed treatment on Bessel functions [1] thought that these functions were of no interest though they were noticed by Lommel [4] who defined the function \( J_{\nu+i\mu}(x) \) in the form

\[
J_{\nu+i\mu}(x) = \frac{(x/2)^{\nu+i\mu}}{\Gamma(\nu+i\mu+1/2)}[K_{\nu,\mu}(x) + i S_{\nu,\mu}(x)]
\]

with \( K \) and \( S \) being real valued functions. Lommel was motivated by the following differential equation:

\[
x^2 y'' + (2\alpha - 2\beta\nu + 1)xy' + \left[ \alpha(\alpha - 2\beta\nu) + \beta^2\gamma^2x^2\beta \right] y = 0.
\]

If any real \( \beta \neq 0 \) then equation (6) has a solution

\[
y = x^{\beta\nu - \alpha} \left[ AJ_{\nu}(\gamma x^\beta) + BJ_{-\nu}(\gamma x^\beta) \right].
\]

Comparing equation (7) with the equation

\[
x^2 y'' + axy' + (b + cx^2\beta)y = 0,
\]

Lommel found a relationship between the coefficients of equation (7) and those of equation (9) and expressed them in the form:

\[
\beta\nu - \alpha = -(a - 1)/2,
\]

\[
\beta\nu = \sqrt{[(a - 1)/2]^2 - b}, \beta\gamma = \sqrt{c}.
\]

It turned out that the real valued coefficients \( (a, b, c) \) produced in a general case solution of equation (6) with a complex index \( \nu \). At the end Lommel obtained a very cumbersome solution of equation (6) as multiples of a complex valued functions. He did not propose a method for the calculation of the real valued functions \( K \) and \( S \) from (5).

Another mathematician Bocher encountered the modified Bessel function with pure imaginary index while he pondered over the solutions of Laplace’s equation using the method of variable separation in cylindrical coordinate system [5]. As opposed to Lommel [4], Bocher proposed real valued solutions with the aid of real valued series without studying the convergence of these series. Each of the term of Bocher’s series was found to be a ratio of polynomial functions in \( \nu \), with coefficients that increased in the order \( n \). This posed a major problem for the calculation and computation via his representation.

Finally the McDonald’s function \( K_{i\tau}(x) \) also having pure imaginary index was extensively used in its integral form to obtain solutions of the Laplace and wave equations for different boundary value conditions by the Soviet mathematicians M. Kantorovitch and N. Lebedev [6]. They used the integral representation

\[
K_{i\tau}(x) = \int_0^\infty \exp(-x\cosh t) \cos(\tau t) dt, x > 0.
\]

This representation are convenient only for sufficiently large values of the argument \( x \). Unfortunately, for small values of \( x \) this integral representation is not quite effective, and this is the case where Bessel functions with pure imaginary indices become applicable and useful in charge particle dynamics [2] and strain field investigations in nanostructures [3].

The above summary shows that there is no effective algorithm for the computation of Bessel functions with pure imaginary indices. In the next sections, we provide this algorithm.

II. METHOD AND CALCULATIONS

So, Bessel functions with pure imaginary indices are solutions of the equation

\[
x^2 y'' + xy' + (x^2 + \nu^2)y = 0,
\]

where \( \nu \) is a real number. The pure mathematician George Boole was not interested in Bessel functions but was the first person who, over a century and a half ago developed an operational method for solving differential equations.
Nevertheless in a small paragraph of his article [7], equation (12) was mentioned and the substitution that facilitated the solving of the problem of calculating Bessel functions with purely imaginary order was used. So expression (2) suggests the form of the solutions of equation (12):

\[ y = A(x) \cos(\nu \ln x) + B(x) \sin(\nu \ln x) \]  

(13)

where \(A(x)\) and \(B(x)\) are series with the coefficients as shown:

\[ A(x) = a_0 + a_1x + a_2x^2 + \cdots + a_nx^n + \cdots, \]

\[ B(x) = b_0 + b_1x + b_2x^2 + \cdots + b_nx^n + \cdots. \]

(14)

Substituting equation (13) into equation (12) and equating the coefficients before the linearly independent functions \(\cos(\nu \ln x)\) and \(\sin(\nu \ln x)\) to zeros, firstly we obtain the relation

\[ a_1 = b_1 = 0, \]

(15)

and secondly \(\forall n \geq 2\) the recurrent relationships

\[ a_n = -\frac{na_{n-2} - 2\nu b_{n-2}}{n(n^2 + 4\nu^2)}, \]

(16)

\[ b_n = -\frac{2\nu a_{n-2} + nb_{n-2}}{n(n^2 + 4\nu^2)}. \]

(17)

It is clearly seen from equations (16) and (17) that odd term coefficients take on zero values while those with even terms can be obtained via a recurrent relations using the values \(a_0, b_0\). The solution of the Bessel equation (12) in the form (13) was firstly introduced by Boole in [7]. However, he did not analyze the convergence of the series (14). Boole’s recurrent relationship was completely forgotten although they can be easily simplified and used to effectively calculate the functions under examination. Since only coefficients with even indices occur, we can re-define the functions \(A(x)\) and \(B(x)\) in the form:

\[ A(x) = \sum_{n=0}^{\infty} a_{2n}2^{2n} \left(\frac{x}{2}\right)^{2n} = \sum_{n=0}^{\infty} A_{2n} \left(\frac{x}{2}\right)^{2n}, \]

(18)

\[ B(x) = \sum_{n=0}^{\infty} b_{2n}2^{2n} \left(\frac{x}{2}\right)^{2n} = \sum_{n=0}^{\infty} B_{2n} \left(\frac{x}{2}\right)^{2n}. \]

(19)

Now for \(n \geq 1\) the recurrent relationship for the coefficients \(A_{2n}, B_{2n}\) can be simplified:

\[ A_{2n} = -\frac{nA_{2n-2} - \nu B_{2n-2}}{n(n^2 + \nu^2)}, \]

(20)

\[ B_{2n} = -\frac{\nu A_{2n-2} + nB_{2n-2}}{n(n^2 + \nu^2)}. \]

(21)

**III. CONSTRUCTION OF COMPUTABLE SOLUTIONS AND PROOF OF CONVERGENCE**

In order to investigate and numerically compute the strain field distribution in nanostructures, or to numerically implement these Bessel functions in other areas of physics, we need to be able to demonstrate that the solutions to this differential equation exist and above of all converges in our domain of definition and interest. We now show that the series (16), (17) converges and does so absolutely for any complex valued argument \(x\) and order \(\nu\). As a series will converge absolutely if and only if the absolute value of the \(n^{th}\) term (which we shall refer to as the majorant) converges. Let the majorant \(M_{2n}\) be defined such that

\[ M_{2n} = |A_{2n}| + |B_{2n}|. \]

(22)

It follows from (20), (21), (22) that
\[ M_{2n} \leq \left[ \frac{1}{n^2 + v^2} + \frac{|v|}{n(n^2 + v^2)} \right] M_{2n-2} \]
\[ \leq \left( \frac{1}{n^2 + \frac{|v|}{n^3}} \right) M_{2n-2}. \quad (23) \]

The last inequality provides us the possibility of studying the order of which the majorant \( M_{2n} \) decays (or grows). It can be easily shown that

\[ M_{2n} \leq C_n |\nu| (n!)^2, \quad (24) \]

where \( C \) is a positive constant dependent on the zero-th terms of the sequence. Using the d’Alembert’s test for convergence the proof of absolute convergence for all values of \( x \) and \( \nu \), is completed.

Now it is possible to form, without lost of generality, two linearly independent solutions of (12). Let us choose two pairs of the values for \( A_0, B_0 \) that generates the sequences \( A_{2n}, B_{2n} \) and its corresponding functions (18) and (19). For brevity, these two pairs provide two solutions (12) that can be easily computed numerically for a few number of iterations. In [2], it was shown that the solution spawned from the pair

\[ (A_0, B_0) = (0, 1), \quad (25) \]

represented as \( S_{\nu}(x) \) and the ones that are spawned from the pair

\[ (A_0, B_0) = (1, 0), \quad (26) \]

was also represented as \( C_{\nu}(x) \). Then an analytical expression of these functions can be easily obtained:

\[ S_{\nu}(x) = \left[ 1 - \frac{1}{1 + \nu^2} \left( \frac{x}{2} \right)^2 + \cdots \right] \sin (\nu \ln x) \]
\[ + \left[ \frac{\nu}{1 + \nu^2} \left( \frac{x}{2} \right)^2 + \cdots \right] \cos (\nu \ln x), \quad (27) \]

\[ C_{\nu}(x) = \left[ 1 - \frac{1}{1 + \nu^2} \left( \frac{x}{2} \right)^2 + \cdots \right] \cos (\nu \ln x) \]
\[ + \left[ \frac{\nu}{1 + \nu^2} \left( \frac{x}{2} \right)^2 + \cdots \right] \sin (\nu \ln x). \quad (28) \]

For \( x \to 0 \) we have two equivalent relationships

\[ S_{\nu}(x) \sim \sin (\nu \ln x), \quad (29) \]
\[ C_{\nu}(x) \sim \cos (\nu \ln x). \quad (30) \]

Now the general solution of the differential equation (12) with real coefficients may be explicitly written out via the real valued functions

\[ y = c_1 S_{\nu}(x) + c_2 C_{\nu}(x), \quad (31) \]

where \( c_1 \) and \( c_2 \) are any real constants. Provided that equation (12) has a complex valued solution in the form of the Bessel function (4). Therefore the latter must be the linear combination of the functions \( S_{\nu}(x) \) and \( C_{\nu}(x) \). It is easy to show that

\[ J_{i\nu}(x) = C_{\nu}(x) + iS_{\nu}(x). \quad (32) \]
In other words, the functions $S_{f\nu}(x)$ and $C_{f\nu}(x)$ are the real and imaginary parts of Bessel function $J_{\nu}(x)$. It follows from the following equivalent relationships:

$$J_{\nu}(x) = \frac{1}{\Gamma(i\nu + 1)} \left( \frac{x}{2} \right)^{i\nu} \left[ 1 - \frac{1}{i\nu + 1} \left( \frac{x}{2} \right)^2 + \cdots \right] \sim \frac{1}{i\nu \Gamma(i\nu)^{2\nu}} \left[ \cos(\nu \ln x) + i \sin(\nu \ln x) \right] \sim \left[ \cos(\nu \ln x) + i \sin(\nu \ln x) \right].$$

The first equivalent relationship is valid as long as $x \to 0$ and the second one is valid so long as $\nu \to 0$.

As

$$\cos (\nu \ln ix) = \cosh \left( \frac{\pi \nu}{2} \right) \cos (\nu \ln x) - \sinh \left( \frac{\pi \nu}{2} \right) \sin (\nu \ln x),$$

$$\sin (\nu \ln ix) = \cosh \left( \frac{\pi \nu}{2} \right) \sin (\nu \ln x) + \sinh \left( \frac{\pi \nu}{2} \right) \cos (\nu \ln x),$$

and as

$$C(x) = A(ix) = \sum_{n=0}^{\infty} C_{2n} \left( \frac{x}{2} \right)^{2n},$$

$$D(x) = B(ix) = \sum_{n=0}^{\infty} D_{2n} \left( \frac{x}{2} \right)^{2n},$$

it is possible to construct two linearly independent solutions for this case in the form

$$y_1 = C(x) \cos (\nu \ln x) + D(x) \sin (\nu \ln x),$$

$$y_2 = D(x) \cos (\nu \ln x) - C(x) \sin (\nu \ln x),$$

where as earlier mentioned, for $n \geq 1$ the recurrent equations for $C_{2n}, D_{2n}$ takes the expected form

$$C_{2n} = \frac{nC_{2n-2} - \nu D_{2n-2}}{n(n^2 + \nu^2)},$$

$$D_{2n} = \frac{\nu C_{2n-2} + nD_{2n-2}}{n(n^2 + \nu^2)}.$$

As the series $C(x)$ and $D(x)$ have the same majorant, these series will thus converge absolutely for any $x$ and $\nu$. One real valued solution of (12) spawns two real valued solutions for (33). Thus by choosing only one pair of values $C_0, D_0$ it is possible to obtain two real valued functions being solutions of equation (33). Let

$$(C_0, D_0) = (0, 1).$$

Substituting (36) and (37) into (38) and (39) it is possible to obtain two functions which was denoted in [2] as $S_{d\nu}(x)$ and $C_{d\nu}(x)$:

$$S_{d\nu}(x) = \left[ 1 + \frac{1}{1 + \nu^2} \left( \frac{x}{2} \right)^2 + \cdots \right] \sin (\nu \ln x)

+ \left[ -\frac{\nu}{1 + \nu^2} \left( \frac{x}{2} \right)^2 + \cdots \right] \cos (\nu \ln x),$$

(43)
\[
Cd_\nu(x) = \left[1 + \frac{1}{1 + \nu^2} \left(\frac{x}{2}\right)^2 + \cdots\right] \cos(\nu \ln x) \nonumber
\]

\[
= -\left[-\frac{\nu}{1 + \nu^2} \left(\frac{x}{2}\right)^2 + \cdots\right] \sin(\nu \ln x). \tag{44}
\]

As \(x \to 0\) we also have two equivalent relationships

\[
Cd_\nu(x) \sim \cos(\nu \ln x), \tag{45}
\]

\[
Sd_\nu(x) \sim \sin(\nu \ln x). \tag{46}
\]

It is obvious that

\[
J_\nu(ix) = Cd_\nu(x) + iSd_\nu(x), \tag{47}
\]

where \(x\) and \(\nu\) are any real numbers.

**IV. WRONSKIANS OF FUNCTIONS**

It can be easily shown that the Wronskian \(W\) of the two linearly independent solutions of the equation

\[
y'' + \frac{1}{x}y' + f(x)y = 0 \tag{48}
\]

has the form \(W = a/x\), where the constant \(a\) depends on the pair of concrete solutions. From the equivalent relationships (29), (30) and (45), (46) it follows that

\[
Cd_\nu(x)[Sf_\nu(x)]' - Sf_\nu(x)[Cd_\nu(x)]' = \frac{\nu}{x}, \tag{49}
\]

\[
Sd_\nu(x)[Cd_\nu(x)]' - Cd_\nu(x)[Sd_\nu(x)]' = \frac{\nu}{x}. \tag{50}
\]

It is clearly seen that the Wronskians (49) and (50) vanishes for \(\nu = 0\). As \(\nu \to 0\) we have

\[
Cd_\nu(x) \to J_0(x), \tag{51}
\]

\[
Sd_\nu(x) \to 0 \tag{52}
\]

and

\[
Cd_\nu(x) \to I_0(x), \tag{53}
\]

\[
Sd_\nu(x) \to 0. \tag{54}
\]

**V. ACCURACY OF PROPOSED COMPUTATIONAL ALGORITHM**

To obtain a measure of the computational error for the proposed procedure, we require a detailed study of the majorant (remainder) \(M_{2n}\). Let

\[
M_{2n} = \frac{n^{[\nu]}m_{2n}}{(n!)^2}. \tag{55}
\]

Now it is possible to obtain an estimate of remainder \(m_{2n}\) for \(n \geq 2\)

\[
\frac{m_{2n}}{m_{2n-2}} \leq \left(1 + \frac{|\nu|}{n}\right) \left(1 - \frac{1}{n}\right)^{|\nu|}. \tag{56}
\]
The Lagrange’s formula for remainder of a Taylor’s series gives for \( n \geq 2 \)

\[
\frac{m_{2n}}{m_{2n-2}} \leq 1 - \frac{\nu^2}{n^2} + \frac{\nu^2 (|\nu| - 1)}{6n^3} \left( 1 - \frac{\theta}{n} \right)^{|\nu| - 2} \times \\
\times \left[ 3 |\nu| + (|\nu| - 2) \left( 1 + \frac{|\nu|}{n} \right) \left( 1 - \frac{\theta}{n} \right)^{|\nu| - 3} \right],
\]

(57)

where \( 0 \leq \theta \leq 1 \). The last inequality may be improved by removing from the right hand side the quantity \( \theta \):

\[
\frac{m_{2n}}{m_{2n-2}} \leq 1 - \frac{\nu^2}{n^2} + \frac{F}{n^3},
\]

(58)

where

\[
F = \begin{cases} 
\frac{\nu^2 (|\nu| - 1) 2^{(1-|\nu|)}}{|\nu| (|\nu| - 1) (1 + |\nu| / 2)} & |\nu| \leq 2, \\
\frac{3 |\nu| + (|\nu| - 2)(1 + |\nu| / 2) 2^{3-|\nu|}}{6} & 2 < |\nu| \leq 3, \\
\left( |\nu| / |\nu| - 1 \right) (\nu^2/2 + 3|\nu| - 2) / 6 & |\nu| > 3.
\end{cases}
\]

(59)

As for \( \nu \neq 0 \)

\[
\frac{m_{2n}}{m_{2n-2}} \leq 1 - \frac{\nu^2}{n^2} + \frac{F}{n^3} < 1 + \frac{\nu^2}{n^2} + \frac{F}{n^3},
\]

(60)

then it is possible to obtain

\[
\ln (m_{2n}) - \ln (m_{2n-2}) < \ln(1 + \frac{\nu^2}{n^2} + \frac{F}{n^3}) < \frac{\nu^2}{n^2} + \frac{F}{n^3}.
\]

Using the well known sums

\[
\sum_{n=2}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} - 1 = 0.6449, \\
\sum_{n=2}^{\infty} \frac{1}{n^3} = \zeta(3) - 1 = 0.2021
\]

and also the values

\[
m_0 = 1, \\
m_2 = \frac{1 + |\nu|}{1 + \nu^2},
\]

it is possible finally to obtain the inequality

\[
\ln \frac{m_{2n}}{m_{2n-2}} < 0.6449\nu^2 + 0.2021F.
\]

(61)

From the last inequality it is easy to obtain a final one simplified in the form

\[
m_{2n} < \frac{1 + |\nu|}{1 + \nu^2} \exp(0.6449\nu^2 + 0.2021F) = m(\nu).
\]

(62)

Now we have
\[ M_{2n} < m(\nu) \frac{n^{2|\nu|}}{(n!)^2} \]  

and it is possible to conclude that the sum of the remaining terms for the series of functions \( A(x), B(x), C(x), D(x) \) cannot exceed the value

\[ \varepsilon = m(\nu) \sum_{n=N}^{\infty} \frac{n^{2|\nu|}}{(n!)^2} \left( \frac{x}{2} \right)^{2n} . \]  

Since the remainder \( (64) \) depends on the value of \( \nu \), let us consider for example the case \( |\nu| \leq 2 \). Then

\[ \varepsilon_N \leq m(\nu) \sum_{n=N+1}^{\infty} \frac{1}{((n-1)!)^2} \left( \frac{x}{2} \right)^{2n-2} = m(\nu) \sum_{n=N+1}^{\infty} \frac{1}{(n!)^2} \left( \frac{x}{2} \right)^{2n} . \]  

The sum at the right hand side of equation \( (65) \) is simply the remainder of the series for the modified Bessel function \( I_0(x) \). This remainder may be evaluated further as shows below:

\[ \sum_{n=N}^{\infty} \frac{1}{(n!)^2} \left( \frac{x}{2} \right)^{2n} = \sum_{n=0}^{\infty} \frac{(N!)^2}{((n+N)!)^2} \left( \frac{x}{2} \right)^{2n} = \frac{1}{(N!)^2} \left( \frac{x}{2} \right)^{2N} \left[ 1 + \frac{1}{(1+N)^2} \left( \frac{x}{2} \right)^2 + \cdots + \frac{1}{(1+N)(2+N) \cdots (n+N)^2} \left( \frac{x}{2} \right)^{2n} + \cdots \right] < \frac{1}{(N!)^2} \left( \frac{x}{2} \right)^{2N} \frac{2N}{x} I_1(x) = \frac{1}{(N!)^2} \left( \frac{x}{2} \right)^{2N-1} I_1(x) . \]  

Now for any real \( x \) and \( |\nu| < 2 \) we have

\[ \varepsilon_N \leq \frac{1+|\nu|}{1+\nu^2} \exp \left( 0.6449\nu^2 + 0.2021\nu \right) \frac{1}{(N!)^2} \left( \frac{x}{2} \right)^{2N+1} I_1(x) . \]  

Elimination of \( |\nu| \) in the last inequality gives an estimation for any \( x \) and \( |\nu| < 2 \):

\[ \varepsilon_N \leq 15 \frac{1}{(N!)^2} \left( \frac{x}{2} \right)^{2N+1} I_1(x) . \]  

For instance for \( x \leq 2 \) inequality \( (68) \) reduces to

\[ \varepsilon_N \leq \frac{24}{(N!)^2} . \]  

The last inequality shows that for the functions \( A(x), B(x), C(x), D(x) \) and for \( x \leq 2 \) and \( |\nu| \leq 2 \) a computational error less then \( \varepsilon_8 < 1.5 \times 10^{-16} \) occurs after the computation of only eight terms of the corresponding series.
VI. CONCLUSION

A new algorithm for computing the real valued solutions of some special functions namely the Gamma function with pure imaginary argument, the Bessel (and modified Bessel) function of purely imaginary orders was systematically declared. We have used these developed Bessel functions for the investigation and calculation of strain fields in semiconductor structures \[3, 8\]. In the above applied case the values of the arguments of the Bessel functions lie in the vicinity of unity. The algorithm for their computations is shown to be rapidly converging and gives a very favorable accuracy for as few as eight iterations.

The algorithm described may give an alternate approach to solving the ground state of the screened coulombs potential problem. It is also promising in solving the inverse scattering problem which is mostly approached via the inverse Green’s function. Further studies of the asymptotic behavior of these functions are still warranted as they play a great role in a wide class of boundary value problems and integral and differential problems of wave scattering.

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[9] To prove the second equivalent relationship it is necessary to use the identity

\[ \Gamma(i\nu)\Gamma(1 - i\nu) \equiv \frac{\pi}{\sin i\nu}. \]