Asymptotic Approximations for Radial Spheroidal Wavefunctions with Complex Size Parameter

By P. A. Martin

Radial spheroidal wavefunctions are functions of four variables, usually denoted by m, n, x, and γ, the last of which is known as the size parameter. This parameter becomes complex when the problem of scattering of a sound pulse by a spheroid is treated using a Laplace transform with respect to time together with the method of separation of variables. Several asymptotic approximations, involving modified Bessel functions, are developed and analyzed.

1. Introduction

The problem of scattering of a sound pulse by an obstacle leads to an initial boundary value problem for the three-dimensional wave equation. Application of the Laplace transform with respect to time t then gives a boundary value problem for the modified Helmholtz equation, $\nabla^2 u - (s/c)^2 u = 0$, where c is the speed of sound and s is the Laplace transform parameter. If the boundary value problem for u can be solved, the time-domain solution can then be found by inverting the Laplace transform, using a contour integral in the complex s-plane.

The method outlined above was first worked out by Jacques Brillouin in 1950 for scattering by a sphere [1]; see [2, 3] for details and references. Separation of variables in spherical polar coordinates shows that the radial

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(r) part of the solution is given in terms of modified spherical Bessel functions,

$$k_n(sr/c), \quad \text{where } k_n(z) = \sqrt{\pi/(2z)}\, K_{n+1/2}(z), \tag{1}$$

and $K_\nu(z)$ is a modified Bessel function [4, 10.47.9]. It is known that all the zeros of $k_n(z)$ lie in the left half of the z-plane, and good approximations for their locations are available. The zeros give rise to poles in the s-plane which are then exploited when the inversion integral is evaluated using the calculus of residues.

It is natural to use a similar method for scattering by a spheroid, using separation of variables in spheroidal coordinates. Let ξ denote the "radial" variable, so that the spheroid is at $\xi = \xi_0$ for some $\xi_0 > 1$. The relevant radial spheroidal wavefunctions (defined in Section 2) are

$$S_n^{m(3)}(\xi, \mathrm{i}sh/c),$$

where $2h$ is the interfocal distance of the spheroid. As before, the task is to locate the zeros of $S_n^{m(3)}(\xi_0, \mathrm{i}sh/c)$ in the complex s-plane. This is appropriate for sound-soft spheroids (Dirichlet problem). For sound-hard spheroids (Neumann problem), zeros of the ξ-derivative are needed.

For axisymmetric ($m = 0$) Neumann problems, some numerical results were given by Bollig and Langenberg [5] in 1983; we are not aware of any earlier results, which is surprising. For extensions to Dirichlet and Neumann problems (with several values for m), there are a few papers from the 1980s [6–8]; we are not aware of any later results, which is also surprising.

Spheroidal wavefunctions such as $S_n^{m(3)}(x, \gamma)$ are complicated functions of four variables implying that many different approximations covering various parameter domains are to be expected. After a brief review of basic definitions and properties in Section 2, we develop asymptotic approximations for large complex γ in Section 3. In the special case where γ is real and positive, we recover an approximation due to Miles [9].

The method used to derive our large-γ approximation is based on one found in Olver's well-known book [10]. Unfortunately, the approximation itself is not immediately useful in the context of our specific application, namely, locating zeros of $S_n^{m(3)}(\xi_0, \mathrm{i}sh/c)$ in the complex s-plane (see Section 3.6). Consequently, we develop another approximation in Section 4, one in which γ is fixed but n and x are large; the resulting approximation involves a modified spherical Bessel function. This is attractive because it permits fairly straightforward estimation of zero locations using known properties of k_n.

2. Spheroidal wavefunctions

The spheroidal wave equation can be written as [4, 30.2.1]

$$(1-x^2)\frac{\mathrm{d}^2 y}{\mathrm{d}x^2} - 2x\frac{\mathrm{d}y}{\mathrm{d}x} + \left(\lambda + \gamma^2(1-x^2) - \frac{m^2}{1-x^2}\right)y = 0, \tag{2}$$

where we assume that x is real, m is a nonnegative integer and γ is a complex parameter. The standard special cases are: associated Legendre equation, $\gamma = 0$; axisymmetric, $m = 0$; prolate, γ is real and positive; and oblate, $\gamma = \mathrm{i}u$, u is real and positive.

The first step is to determine eigenvalues $\lambda = \lambda_n^m(\gamma^2)$ so that $y(x)$ is a bounded solution of (2) for $-1 \le x \le 1$. The integer n is a counter; we take it to satisfy $n \ge m$. The eigenfunctions corresponding to the eigenvalues $\lambda_n^m(\gamma^2)$ are denoted by $\mathsf{Ps}_n^m(x, \gamma^2)$, $n = m, m+1, m+2, \ldots$, and they are called *angular spheroidal wavefunctions*.

The axisymmetric case ($m = 0$) has been studied extensively; for example, there is a book [11] dedicated to properties of $\mathsf{Ps}_n^0(x, \gamma^2)$ when γ^2 is real and positive.

In general, $\lambda_n^m(\gamma^2)$ and $\mathsf{Ps}_n^m(x, \gamma^2)$ are complex valued. Nevertheless, an argument of Sturm–Liouville type gives orthogonality,

$$\int_{-1}^{1} \mathsf{Ps}_n^m(x, \gamma^2)\, \mathsf{Ps}_{n'}^m(x, \gamma^2)\,\mathrm{d}x = 0 \quad \text{when } \lambda_n^m(\gamma^2) \ne \lambda_{n'}^m(\gamma^2).$$

Numerical methods for computing $\lambda_n^m(\gamma^2)$ are available; the paper by Barrowes et al. [12] gives a good survey. Analytically, it is known that [4, 30.3.8]

$$\lambda_n^m(\gamma^2) = n(n+1) + \sum_{k=1}^{\infty} \ell_{2k}\gamma^{2k}, \quad \left|\gamma^2\right| < r_n^m, \tag{3}$$

where the coefficients ℓ_{2k} can be computed and estimates for the radii of convergence r_n^m have been given [13, section 3.2]. It is also known that there are branch points in the complex γ-plane; these were first noted and their locations computed by Oguchi [14]. See [12, 15] for further studies and references.

Some asymptotic approximations for $\lambda_n^m(\gamma^2)$ are also available. Put $\gamma = |\gamma|\mathrm{e}^{\mathrm{i}\chi}$. For large $|\gamma|$, we have [4, 30.9.1]

$$\lambda_n^m(\gamma^2) \sim -\gamma^2 + 2\nu\gamma \quad \text{when } \chi = 0 \left(\text{prolate case; } \nu = n - m + \frac{1}{2}\right) \tag{4}$$

but [4, 30.9.4]

$$\lambda_n^m(\gamma^2) \sim 2q|\gamma| \quad \text{when } \chi = \pi/2 \text{ (oblate case);} \tag{5}$$

here, $q = n + 1$ when $n - m$ is even and $q = n$ when $n - m$ is odd. For other values of χ, it appears that one obtains either the prolate approximation or the oblate approximation, depending on the value of χ and the locations of the branch points (which depend on n and m). Quoting [12, section 3.3]: "At these branch points, two spheroidal eigenvalues merge and become analytic continuations of each other."

The complications for large γ and fixed n contrast strongly with the situation for fixed γ and large n. Then we have [4, 30.3.2]

$$\lambda_n^m(\gamma^2) = n(n+1) - \gamma^2/2 + O(n^{-2}) \quad \text{as } n \to \infty. \tag{6}$$

This simple estimate (which comes from (3)) holds for arbitrary fixed γ.

Once $\lambda_n^m(\gamma^2)$ has been determined, we can consider solving (2) for $x > 1$ so as to define so-called radial functions. We are interested in the solution that $\to 0$ as $x \to \infty$ when $\operatorname{Im}\gamma > 0$. This solution is denoted by $S_n^{m(3)}(x, \gamma)$. Specifically, we have [4, 30.11.6]

$$S_n^{m(3)}(x, \gamma) = h_n^{(1)}(\gamma x)\left(1 + O(x^{-1})\right) \quad \text{as } x \to \infty \tag{7}$$

for fixed γ, where $h_n^{(1)}$ is a spherical Hankel function. For fixed $x > 1$, $m \geq 0$, and $n \geq m$, $S_n^{m(3)}(x, \gamma)$ is an analytic function of γ. We are interested in the analytic continuation of $S_n^{m(3)}(x, \gamma)$ into the lower half of the γ-plane, because that is where we expect to find zeros.

3. Asymptotic approximations for large γ

3.1. *Prolate and oblate cases*

For the prolate case ($\chi = 0$), Miles [9, eq. (3.11)] gives the asymptotic approximation

$$S_n^{m(3)}(x, \gamma) \sim \sqrt{\frac{\pi}{2\gamma x}}\, H_m^{(1)}(\gamma X) \quad \text{as } \gamma = |\gamma| \to \infty \tag{8}$$

for $1 \leq x \leq \infty$, where

$$X = \xi - (\nu/\gamma)\arctan\xi, \qquad \xi = \sqrt{x^2 - 1}, \qquad \nu = n - m + \frac{1}{2} \tag{9}$$

(see (4)) and m and n are fixed. As a check, when x is large, $\gamma X \sim \gamma x - \nu\pi/2$. Then, using [4, 10.2.5], (8) gives

$$S_n^{m(3)}(x, \gamma) \sim \frac{\mathrm{e}^{\mathrm{i}\gamma x}}{\mathrm{i}^{n+1}\,\gamma x},$$

which agrees with (7) after use of [4, 10.52.4].

For more information and related approximations, see [16–19].

For the oblate case ($\chi = \pi/2$), some asymptotic approximations are available for large $|\gamma|$; see [20,21].

3.2. Use of Olver's method

Returning to (2), remove the first-derivative term in the usual way by writing

$$y(x) = S_n^{m(3)}(x, \gamma) = (x^2 - 1)^{-1/2} w(x). \tag{10}$$

The result is

$$\frac{\mathrm{d}^2 w}{\mathrm{d}x^2} = \left(\frac{\lambda_n^m + \gamma^2 - \gamma^2 x^2}{x^2 - 1} + \frac{m^2 - 1}{(x^2 - 1)^2} \right) w(x). \tag{11}$$

We assume that $\operatorname{Im} \gamma > 0$ (so the oblate case is included). We want to solve for $w(x)$ with $x > 1$, and we want to choose w so that $w(x) \to 0$ as $x \to \infty$. Indeed, from (7), the decay should be given by $w(x) \sim \mathrm{i}^{-n}(\mathrm{i}\gamma)^{-1}\mathrm{e}^{\mathrm{i}\gamma x}$ as $x \to \infty$; evidently, this behavior comes from the term $-\gamma^2 x^2/(x^2 - 1)$ on the right-hand side of (11).

It is convenient to put $\gamma = \mathrm{i}u$ so that $\operatorname{Re} u > 0$. In this half-plane, $w(x)$ solves

$$\frac{\mathrm{d}^2 w}{\mathrm{d}x^2} = \left(\frac{u^2 x^2 - u^2 + \lambda_n^m(-u^2)}{x^2 - 1} + \frac{m^2 - 1}{(x^2 - 1)^2} \right) w(x) \tag{12}$$

and is required to decay exponentially as $x \to \infty$.

Connecting with the notation in Olver's book [10], write (12) as

$$\frac{\mathrm{d}^2 w}{\mathrm{d}x^2} = \{u^2 f(x) + g(x)\} w(x), \quad x > 1, \tag{13}$$

where u is the large parameter,

$$f(x) = \frac{x^2 - \beta^2}{x^2 - 1}, \qquad g(x) = \frac{m^2 - 1}{(x^2 - 1)^2} \tag{14}$$

and the parameter β is defined by (cf. [19])

$$\beta^2 = 1 - u^{-2} \lambda_n^m(-u^2). \tag{15}$$

It follows from the discussion in Section 2 that the behavior of β as $\gamma \to \infty$ depends on $\arg \gamma$. In prolate-type regions of the complex γ-plane, $\beta \to 0$ as $|\gamma| \to \infty$, whereas in oblate-type regions $\beta \to 1$. These results, which follow from (4) and (5), will be used in Sections 3.4 and 3.5.

Let us apply Olver's recipe formally. Thus [10, chapter 12, section 2], introduce a new independent variable ζ and a new dependent variable W

according to

$$\frac{1}{\zeta}\left(\frac{\mathrm{d}\zeta}{\mathrm{d}x}\right)^2 = 4f(x), \qquad w = \left(\frac{\mathrm{d}\zeta}{\mathrm{d}x}\right)^{-1/2} W. \tag{16}$$

The result is

$$\frac{\mathrm{d}^2 W}{\mathrm{d}\zeta^2} = \left(\frac{u^2}{4\zeta} + \frac{m^2-1}{4\zeta^2} + \frac{\psi(\zeta)}{\zeta}\right) W, \tag{17}$$

where ψ is given in terms of f and g by [10, p. 439, eq. (2.06)]. If we neglect ψ in (17), solutions are $ZI_m(uZ)$ and $ZK_m(uZ)$, where $Z = \zeta^{1/2}$.

Integrating the first of (16),

$$Z \equiv \zeta^{1/2} = \int_1^x \{f(t)\}^{1/2}\,\mathrm{d}t = \int_1^x (t^2-\beta^2)^{1/2} \frac{\mathrm{d}t}{\sqrt{t^2-1}}. \tag{18}$$

We choose the branch so that $(t^2-\beta^2)^{1/2} \sim t$ as $t \to +\infty$, whence $Z \sim x$ as $x \to +\infty$; in detail, the substitution $y = \sqrt{t^2-1}$ gives

$$Z = \sqrt{x^2-1} + Z_0 + O(x^{-1}) \quad \text{as } x \to \infty,$$

where the constant

$$Z_0 = \int_0^\infty \left(\frac{(y^2+1-\beta^2)^{1/2}}{\sqrt{y^2+1}} - 1\right) \mathrm{d}y. \tag{19}$$

With this choice,

$$W(\zeta) \sim A_0 Z K_m(uZ) \quad \text{as } u \to \infty, \operatorname{Re} u > 0, \tag{20}$$

where A_0 is an arbitrary constant. From (16),

$$w(x) \sim A_0 \frac{(Z/2)^{1/2}(x^2-1)^{1/4}}{(x^2-\beta^2)^{1/4}} K_m(uZ) \quad \text{as } u \to \infty, \operatorname{Re} u > 0. \tag{21}$$

Hence, using (10),

$$S_n^{m(3)}(x, \mathrm{i}u) \sim A_0 (Z/2)^{1/2} \left\{(x^2-1)(x^2-\beta^2)\right\}^{-1/4} K_m(uZ) \tag{22}$$

as $u \to \infty$ with $\operatorname{Re} u > 0$. The constant A_0 can be found by letting $x \to \infty$ and then comparing with the known asymptotic behavior of $S_n^{m(3)}$. From (22) and [4, 10.25.3],

$$S_n^{m(3)}(x, \mathrm{i}u) \sim \frac{A_0\sqrt{\pi}}{2x\sqrt{u}} \mathrm{e}^{-u(x+Z_0)},$$

using $Z \sim x + Z_0$. On the other hand, it is known [4, 30.11.6 and 10.52.4] that

$$S_n^{m(3)}(x, \mathrm{i}u) \sim h_n^{(1)}(\mathrm{i}ux) \sim -\mathrm{i}^{-n} \frac{\mathrm{e}^{-ux}}{ux}, \tag{23}$$

whence $A_0 = -2\,\mathrm{i}^{-n}\mathrm{e}^{uZ_0}(\pi u)^{-1/2}$. (This calculation also provides a check on the functional form of the approximation (22).) Thus, from (22),

$$S_n^{m(3)}(x, \mathrm{i}u) \sim \frac{-(2Z)^{1/2}\,\mathrm{e}^{uZ_0}\,K_m(uZ)}{\mathrm{i}^n\,(\pi u)^{1/2}\{(x^2-1)(x^2-\beta^2)\}^{1/4}} \quad \text{as } u \to \infty, \mathrm{Re}\, u > 0. \tag{24}$$

This is our basic approximation for $S_n^{m(3)}$ for large u.

3.3. Endpoint behavior

By design, the approximation (24) behaves correctly as $x \to \infty$. It also has the correct functional form as $x \to 1+$. To see this, we note from (18) that $Z(x) \sim \{(x^2-1)(1-\beta^2)\}^{1/2}$ as $x \to 1+$. Then, using [4, 10.30.2], we find that

$$S_n^{m(3)}(x, \mathrm{i}u) \sim \frac{-2^{m/2}(m-1)!\,\mathrm{e}^{uZ_0}}{\mathrm{i}^n(2\pi u)^{1/2}\,u^m(1-\beta^2)^{m/2}}\,(x-1)^{-m/2} \quad \text{as } x \to 1+. \tag{25}$$

This can be compared with the approximation obtained by combining 16.11 (18) and 16.12 (2) in [22]; both have the same dependence on x multiplied by complicated combinations of the other variables.

3.4. Prolate case

Although (24) was derived assuming that $\mathrm{Re}\, u > 0$, let us apply it when $\mathrm{Re}\, u = 0$, which is the prolate case. From $u = -\mathrm{i}\gamma$ and [4, 10.27.8],

$$K_m(uZ) = (\pi/2)\,\mathrm{i}^{m+1}H_m^{(1)}(\gamma Z).$$

Also, from (4) and (15),

$$\beta^2 = 1 + \gamma^{-2}\lambda_n^m(\gamma^2) \sim 2\nu/\gamma \quad \text{as } \gamma \to \infty: \tag{26}$$

β^2 is small. Hence, from (18),

$$\begin{aligned} Z &= \int_0^\xi \left(1 - \frac{\beta^2}{y^2+1}\right)^{1/2} \mathrm{d}y \\ &\sim \int_0^\xi \left(1 - \frac{\beta^2}{2(y^2+1)}\right) \mathrm{d}y = \xi - \frac{\beta^2}{2}\arctan\xi, \end{aligned} \tag{27}$$

where $\xi = \sqrt{x^2-1}$. Making use of (26), we see that Z reduces to X in Miles' approximation (9). Also, $Z_0 \sim -\pi\beta^2/4 \sim -\pi\nu/(2\gamma)$. This follows from (27). Alternatively, (19) and [23, 3.169 (2)] give

$$Z_0 = (1-\beta^2)K(\beta) - E(\beta), \tag{28}$$

where K and E are complete elliptic integrals. Some further calculation then shows that we recover precisely the approximation obtained by Miles [9] (8).

3.5. *Oblate case*

In this case, u is real, positive and large. From (5) and (15), $\beta^2 \sim 1 - 2q/u$ as $u \to \infty$: β^2 is close to 1. From (28), [23, 8.113 (3)] and [23, 8.114 (3)],

$$Z_0 \sim -1 + \frac{\beta'^2}{2}\left(\frac{1}{2} + \log\frac{4}{\beta'}\right) \quad \text{with } \beta'^2 = 1 - \beta^2 \sim \frac{2q}{u}.$$

Then (24) leads to an approximation for oblate spheroidal wavefunctions. It is likely that this approximation is known although we have not found it in the literature.

3.6. *Complex u*

In the general case, we have the estimate (24) in which β, Z, and Z_0 are given by (15), (18), and (19), respectively. Also, (24) was derived assuming that $\operatorname{Re} u > 0$. The complicated branch-point structure of the eigenvalues $\lambda_n^m(-u^2)$ in the u-plane makes it difficult to use (24), unless one is interested in the behavior along a particular ray on which $\arg u$ is fixed. In the applications we have in mind, we want to continue our estimates analytically into the left half of the u-plane, $\operatorname{Re} u < 0$, where we expect to find zeros. Consequently, we proceed to look for alternative approximations.

4. Asymptotic approximations for fixed *u*

The standard methods described in Olver's book do not seem to work for large n but fixed u. To see the difficulty, write (12) as

$$\frac{\mathrm{d}^2 w}{\mathrm{d}x^2} = \left(u^2 + \frac{\lambda_n^m(-u^2)}{x^2 - 1} + \frac{m^2 - 1}{(x^2 - 1)^2}\right) w(x), \tag{29}$$

where λ_n^m is large; from (6),

$$\lambda_n^m(-u^2) = n(n+1) + u^2/2 + O(n^{-2}) \quad \text{as } n \to \infty. \tag{30}$$

When x is large, the u^2 term on the right-hand side of (29) is dominant and crucial, because it gives the required exponential decay, as e^{-ux} when $x \to \infty$. For finite x and large n, the second term on the right-hand side of (29) is dominant.

Let us follow Olver again [10, chapter 10, section 1], starting with

$$\frac{\mathrm{d}^2 w}{\mathrm{d}x^2} = \{p^2 f(x) + g(x)\} w(x), \tag{31}$$

where p is the large parameter. Comparing (29) and (31), we put

$$p^2 = \lambda_n^m(-u^2), \qquad f(x) = \frac{1}{x^2-1}, \qquad g(x) = u^2 + \frac{m^2-1}{(x^2-1)^2}. \tag{32}$$

Still following Olver, make the substitution

$$w(x) = \dot{x}^{1/2} W(\xi), \qquad \dot{x} = \mathrm{d}x/\mathrm{d}\xi \tag{33}$$

in (31). The result is [10, p. 363, eq. (1.02)]

$$\frac{\mathrm{d}^2 W}{\mathrm{d}\xi^2} = \{p^2 \dot{x}^2 f(x) + \psi(\xi)\} W, \tag{34}$$

where

$$\psi(\xi) = \dot{x}^2 g(x) + \dot{x}^{1/2}(\mathrm{d}^2/\mathrm{d}\xi^2)\dot{x}^{-1/2}. \tag{35}$$

Now, we know that one solution of

$$\frac{\mathrm{d}^2 v}{\mathrm{d}\xi^2} = \left(\mu^2 + \frac{\nu^2 - \frac{1}{4}}{\xi^2}\right) v \tag{36}$$

is $\xi^{1/2} K_\nu(\mu\xi)$; see [10, p. 374]. This solution decays exponentially with ξ, behavior that comes from the μ^2 term in (36). The analogous behavior in (34) comes from ψ, via the u^2 term in g. On the other hand, the large parameter in (34), p, is associated with f. Therefore, if we suppose that ν is large, comparing (34) with (36) suggests that we try

$$\dot{x}^2 f(x) = \xi^{-2}. \tag{37}$$

(This is not one of the three cases studied by Olver [10, p. 363].) Integrating,

$$\log \xi = \int_1^x \frac{\mathrm{d}t}{\sqrt{t^2-1}} = \operatorname{arccosh} x = \log\left(x + \sqrt{x^2-1}\right)$$

whence

$$x = \cosh(\log \xi) = \frac{\xi + \xi^{-1}}{2}, \qquad \xi = x + \sqrt{x^2-1}. \tag{38}$$

Thus

$$\begin{gathered} 2\dot{x} = 1 - \xi^{-2}, \quad 4(x^2-1) = \xi^2(1-\xi^{-2})^2 = 4\xi^2\dot{x}^2, \\ \dot{x}^{1/2}(\mathrm{d}^2/\mathrm{d}\xi^2)\dot{x}^{-1/2} = 3(\xi^2-1)^{-2}. \end{gathered} \tag{39}$$

Substituting in (35), using $(32)_3$,

$$\psi = \dot{x}^2\left(u^2 + \frac{m^2-1}{(x^2-1)^2}\right) + \dot{x}^{1/2}\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}\dot{x}^{-1/2}$$

$$= \frac{u^2}{4}\left(1-\xi^{-2}\right)^2 + \frac{m^2-1}{\xi^4\dot{x}^2} + \frac{3}{(\xi^2-1)^2}$$

$$= \frac{u^2}{4} - \frac{u^2}{2\xi^2} + \psi_4,$$

say, with

$$\psi_4(\xi) = \frac{u^2}{4\xi^4} + \frac{4m^2-1}{(\xi^2-1)^2}. \tag{40}$$

Substituting for ψ in (34), using $(32)_1$ and (37), we obtain

$$\frac{\mathrm{d}^2 W}{\mathrm{d}\xi^2} = \left\{\frac{u^2}{4} + \frac{1}{\xi^2}\left(\lambda_n^m(-u^2) - \frac{u^2}{2}\right) + \psi_4\right\} W. \tag{41}$$

This equation is exact.

We note that $\psi_4(\xi) = O(\xi^{-4})$ as $\xi \to \infty$ (thus explaining the notation "ψ_4"). If we discard ψ_4, (41) becomes (36) with

$$\mu = \frac{u}{2}, \qquad \nu^2 - \frac{1}{4} = \lambda_n^m(-u^2) - \frac{u^2}{2}, \tag{42}$$

suggesting the approximation

$$W(\xi) \simeq \xi^{1/2} K_\nu(\mu\xi) = W_0(\xi), \quad \text{say.} \tag{43}$$

By discarding ψ_4, we may expect that this approximation can be justified as $\xi \to \infty$.

For large n and fixed u, we have the estimate (30). Then (42) gives $\nu^2 - \frac{1}{4} = n(n+1) + O(n^{-2})$ as $n \to \infty$, whence

$$\nu = n + \frac{1}{2} + O(n^{-3}) \quad \text{as } n \to \infty \tag{44}$$

implying that $\nu = n + \frac{1}{2}$ to high accuracy when n is large.

4.1. Error analysis

To investigate the approximation (43), we try an analysis patterned on one given by Olver [10, chapter 6, section 2] in the context of Liouville–Green approximations.

Put $W(\xi) = W_0(\xi)\{1 + h(\xi)\}$, where h is to be estimated. We have

$$W' = W_0'(1+h) + W_0 h', \qquad W'' = W_0''(1+h) + 2W_0'h' + W_0 h''.$$

Substitute for W in (41) (with (42)). As W_0 satisfies (36), we find that $2W_0'h' + W_0 h'' = \psi_4 W_0(1+h)$, which we write as

$$\left[W_0^2 h'\right]' = \psi_4 W_0^2 (1+h).$$

Integrating once gives

$$h'(\xi) = -[W_0(\xi)]^{-2} \int_\xi^\infty \psi_4(t)[W_0(t)]^2\{1 + h(t)\}\,\mathrm{d}t.$$

Integrating again gives

$$\begin{aligned} h(\xi) &= \int_\xi^\infty [W_0(\eta)]^{-2} \int_\eta^\infty \psi_4(t)[W_0(t)]^2\{1 + h(t)\}\,\mathrm{d}t\,\mathrm{d}\eta \\ &= \int_\xi^\infty \mathcal{K}(\xi, t)\,\psi_4(t)\{1 + h(t)\}\,\mathrm{d}t, \end{aligned} \tag{45}$$

where

$$\mathcal{K}(\xi, t) = \int_\xi^t \left(\frac{W_0(t)}{W_0(\eta)}\right)^2 \mathrm{d}\eta. \tag{46}$$

Equation (45) is a Volterra integral equation of the second kind for h. Such equations can (usually) be solved by iteration.

Let us estimate $|\mathcal{K}(\xi, t)|$. From eq. (3.6) in [24] (where an extensive bibliography can be found),

$$\frac{K_\nu(x)}{K_\nu(y)} > \mathrm{e}^{y-x}\left(\frac{y}{x}\right)^{1/2}, \qquad |\nu| > \frac{1}{2}, \qquad 0 < x < y.$$

Hence,

$$\frac{W_0(t)}{W_0(\eta)} = \frac{t^{1/2}K_\nu(\mu t)}{\eta^{1/2}K_\nu(\mu\eta)} < \mathrm{e}^{\mu(\eta-t)}, \qquad 0 < \eta < t. \tag{47}$$

This holds for real μ with $\mu > 0$. We have shown elsewhere [25] that (47) can be generalized to complex μ when $\nu = n + \frac{1}{2}$ (see (44)); specifically

$$\left|\frac{W_0(t)}{W_0(\eta)}\right| = \left|\frac{t^{1/2}K_{n+1/2}(\mu t)}{\eta^{1/2}K_{n+1/2}(\mu\eta)}\right| < \mathrm{e}^{\mu_\mathrm{r}(\eta-t)}, \qquad 0 < \eta < t \tag{48}$$

for $\mu_\mathrm{r} = \mathrm{Re}\,\mu > 0$.

Using the bound (48) in (46),

$$|\mathcal{K}(\xi, t)| < \int_\xi^t \mathrm{e}^{2\mu_\mathrm{r}(\eta-t)}\,\mathrm{d}\eta = \frac{1}{u_\mathrm{r}}\left(1 - \mathrm{e}^{-u_\mathrm{r}(t-\xi)}\right) \le \frac{1}{u_\mathrm{r}}$$

as $t \ge \xi$, where $u_\mathrm{r} = \mathrm{Re}\,u$ and we have used $\mu = u/2$, (42).

Define a sequence $h_j(\xi)$, $j = 0, 1, 2, \ldots$, with $h_0 = 0$ and

$$h_j(\xi) = \int_\xi^\infty \mathcal{K}(\xi, t)\,\psi_4(t)\{1 + h_{j-1}(t)\}\,\mathrm{d}t, \quad j = 1, 2, \ldots. \tag{49}$$

In particular,

$$h_1(\xi) = \int_\xi^\infty \mathcal{K}(\xi, t)\, \psi_4(t)\, \mathrm{d}t \tag{50}$$

whence (48) gives

$$|h_1(\xi)| \le \Psi(\xi) \quad \text{with } \Psi(\xi) = \frac{1}{u_\mathrm{r}} \int_\xi^\infty |\psi_4(t)|\, \mathrm{d}t. \tag{51}$$

Next, from (49),

$$h_j(\xi) - h_{j-1}(\xi) = \int_\xi^\infty \mathcal{K}(\xi, t)\, \psi_4(t) \{h_{j-1}(t) - h_{j-2}(t)\}\, \mathrm{d}t \tag{52}$$

for $j = 2, 3, \ldots$. In particular,

$$|h_2(\xi) - h_1(\xi)| \le \frac{1}{u_\mathrm{r}} \int_\xi^\infty |\psi_4(t)|\, \Psi(t)\, \mathrm{d}t = \frac{1}{2}\, [\Psi(\xi)]^2$$

and then an inductive argument gives

$$\left| h_j(\xi) - h_{j-1}(\xi) \right| \le \frac{1}{j!}\, [\Psi(\xi)]^j, \quad j = 1, 2, 3, \ldots. \tag{53}$$

Here, we have used

$$\frac{1}{u_\mathrm{r}} \int_\xi^\infty |\psi_4(t)|\, [\Psi(t)]^j\, \mathrm{d}t = -\int_\xi^\infty \Psi'(t)\, [\Psi(t)]^j\, \mathrm{d}t = \frac{[\Psi(\xi)]^{j+1}}{j+1}.$$

Using a telescoping series and $h_0 = 0$, we have

$$h_q(\xi) = \sum_{j=1}^{q} \{h_j(\xi) - h_{j-1}(\xi)\}.$$

Letting $q \to \infty$, we put $h \equiv h_\infty$; the bound (53) gives absolute convergence for any ξ and the estimate

$$|h(\xi)| < \mathrm{e}^{\Psi(\xi)} - 1. \tag{54}$$

Olver's arguments [10, p. 195] show that the function h constructed does solve the integral equation (45) and that it is twice differentiable.

To use (54), we estimate Ψ, using (40) and (51). Thus

$$\begin{aligned} \Psi(\xi) &\le \frac{1}{u_\mathrm{r}} \int_\xi^\infty \left(\frac{|u|^2}{4t^4} + \frac{|4m^2 - 1|}{(t^2 - 1)^2} \right) \mathrm{d}t \\ &= \frac{1}{u_\mathrm{r}} \left\{ \frac{|u|^2}{12\xi^3} + \frac{|4m^2 - 1|}{4} \left(\frac{2\xi}{\xi^2 - 1} + \log \frac{\xi - 1}{\xi + 1} \right) \right\}, \end{aligned} \tag{55}$$

using [23, 2.149.2 and 2.143.3]; the bound on the right is $O(\xi^{-3})$ as $\xi \to \infty$.

4.2. *Approximations for* $S_n^{m(3)}$

Returning to (43) with $\mu = u/2$ and the large-n estimate (44), we obtain the estimate

$$W(\xi) \simeq A_1 \xi^{1/2} K_{n+1/2}(u\xi/2),$$

where A_1 is an arbitrary constant. This is justified for sufficiently large n and ξ, and it was derived for $\mathrm{Re}\, u > 0$.

From (33) and (39), $w(x) \simeq A_1(x^2-1)^{1/4} K_{n+1/2}(u\xi/2)$, and then (10) gives

$$S_n^{m(3)}(x, \mathrm{i}u) \simeq A_1(x^2-1)^{-1/4} K_{n+1/2}(u\xi/2). \tag{56}$$

The constant A_1 can be found by letting $x \to \infty$ and then comparing with (23). As $\xi \sim 2x$ (see (38)), we obtain $A_1 = -\mathrm{i}^{-n}(2/[\pi u])^{1/2}$ after using [4, 10.25.3]. Hence

$$S_n^{m(3)}(x, \mathrm{i}u) \simeq \frac{-(2\xi)^{1/2} k_n(u\xi/2)}{\mathrm{i}^n \pi (x^2-1)^{1/4}}, \tag{57}$$

where k_n is a modified spherical Bessel function (1) and $\xi = x + \sqrt{x^2-1}$.

4.3. *Discussion*

The approximation (57) is attractive because it is fairly simple, and it involves k_n; much is known about locating the zeros of $k_n(u\xi/2)$ and they are in the left half of the u-plane as expected. The functional form also gives the correct behavior as $x \to \infty$, but it is not valid as $x \to 1+$ (a limit that is not relevant in the application to scattering problems).

However, there is one surprising feature: m is absent. Looking back, we see that we lost m in two places. First, we discarded ψ_4; m occurs in the estimate (55). Second, we accepted the estimate (44) for ν. This can be improved. Thus, referring to (3) and [4, 30.3.8], we find

$$2\ell_2 = -1 - (2n)^{-2}(4m^2-1) + O(n^{-3}) \quad \text{and} \quad 2\ell_4 = (4n)^{-2} + O(n^{-3})$$

as $n \to \infty$; all higher ℓ_{2k} are smaller. Hence, (6) is refined to

$$\lambda_n^m(-u^2) = n(n+1) + u^2/2 + \Lambda n^{-2} + O(n^{-3}) \quad \text{as } n \to \infty,$$

where $\Lambda = \frac{1}{8}u^2(4m^2-1) + \frac{1}{32}u^4$. Substitution in the definition of ν, $(42)_2$, then refines (44) to

$$\nu = n + \frac{1}{2} + \frac{\Lambda}{2n^3} + O\left(n^{-4}\right) \quad \text{as } n \to \infty. \tag{58}$$

This may then be inserted in the expression for $W_0(\xi)$, (43). The resulting estimate then depends (weakly) on m (through Λ) but is no longer a modified spherical Bessel function.

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