Solutions to a generalized spheroidal wave equation: Teukolsky's equations in general relativity, and the two-center problem in molecular quantum mechanics

Edward W. Leaver
Department of Physics and the College of Science Computer, University of Utah, Salt Lake City, Utah 84112
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The differential equation

$$x(x-x_0)\frac{d^2y}{dx^2}+(B_1+B_2x)\frac{dy}{dx}+\left[\omega^2x(x-x_0)-2\eta\omega(x-x_0)+B_3\right]y=0$$

arises both in the quantum scattering theory of non-relativistic electrons from polar molecules and ions, and, in the guise of Teukolsky's equations, in the theory of radiation processes involving black holes. This article discusses analytic representations of solutions to this equation. Previous results of Hylleraas [E. Hylleraas, Z. Phys. **71**, 739 (1931)], Jaffé [G. Jaffé, Z. Phys **87**, 535 (1934)], Baber and Hassé [W.G. Baber and H.R. Hassé, Proc. Cambridge Philos. Soc. **25**, 564 (1935)], and Chu and Stratton [L.J. Chu and J.A. Stratton, Journal of Mathematics and Physics, **20**, 259, (1941)] are reviewed, and a rigorous proof is given for the convergence of Stratton's spherical Bessel function expansion for the ordinary spheroidal wavefunctions. An integral is derived that relates the eigensolutions of Hylleraas to those of Jaffé. The integral relation is shown to give an integral equation for the scalar field quasi-normal modes of black holes, and to lead to irregular second solutions to the equation. New representations of the general solutions are presented as series of Coulomb wavefunctions and confluent hypergeometric functions. The Coulomb wavefunction expansion may be regarded as a generalization of Stratton's representation for ordinary spheroidal wave functions, and has been fully implemented and tested on a digital computer. Both solutions given by the new algorithms are analytic in the variable x and the parameters B_1, B_2, B_3, ω, x_0, and η, and are uniformly convergent on any interval bounded away from x_0. They are the first representations for generalized spheroidal wave functions which allow the direct evaluation of asymptotic magnitude and phase.

I. INTRODUCTION

Generalized Spheroidal Wave Equations have been the topic of much applied mathematical research. They are usually characterized as being second order linear differential equations having two regular singular points and one confluently irregular singular point. In this article the problem of generating general solutions to the specific equation

$$x(x-x_0)\frac{d^2y}{dx^2}+(B_1+B_2x)\frac{dy}{dx}+\left[\omega^2x(x-x_0)-2\eta\omega(x-x_0)+B_3\right]y=0 \tag{1}$$

(where B_1, B_2, B_3, ω, η, and x_0 are constants) is approached from the point of view of the computational physicist. Equation (1) will hereafter be refered to as "the generalized spheroidal wave equation." The intervals of physical interest are both $[0 \leq x \leq x_0]$ and $[x_0 \leq x < \infty)$. Representations for solutions on the bounded interval $[0 \leq x \leq x_0]$ are well understood, and are reviewed here only to illustrate properties of three-term recurrence relations. The purpose of this paper is to present new representations for solutions on the semi-infinite interval $[x_0 \leq x < \infty)$.

The differential equation (1) arises in two specific physical contexts: the separation of the one particle Schrödinger equation in prolate spheroidal coordinates, and the separation of linearized perturbation equations on the backgrounds of Schwarzschild and Kerr black holes. (Teukolsky's equations governing perturbations of the Kerr metric are generalized spheroidal wave equations.) This paper is an exposition on neither quantum mechanics nor general relativity, and the physics underlying these equations will be mentioned only in the context of boundary conditions relevant to the solutions.

Researchers in both astrophysics and molecular physics have long recognized the frequent inadequacy of numerical integration techniques in supplying satisfactory solutions to generalized spheroidal wave equations.[1,2,3] The original goal of this study was the development of analytic representations for solutions to equation (1) on the interval $[x_0 \leq x < \infty)$ that would be useful in the investigation of resonance phenomena in low energy molecular scattering processes. For that end I sought a representation that was both analytic in the independent variable x and the parameters B_1, B_2, B_3, ω, x_0, and η, and from which the analytic behavior of the solutions as $x \to \infty$ could readily be inferred. The power of the resulting Coulomb wavefunction expansion is demonstrated in an article on the spectral decomposition of the perturbation response of Schwarzschild black holes.[4] The present paper presents the new algorithm, and how I arrived at it.

In the process it reviews earlier work of Hylleraas, Jaffé, Baber and Hassé, Chu and Stratton, and Morse. These authors' results form a natural starting point for this study, which may be considered to be a continuation of their previous efforts, and are a seemingly forgotten topic in themselves. Review of their work is particularly worthwhile in view of enduring misconceptions concerning the convergence properties of some of their representations.

Lastly, I have included discussion of two representations that I have not yet used in computational problems, nor verified numerically. They are the second solutions of Jaffé's type presented in Sec. IV C, and the confluent hypergeometric function expansions of Sec. VII. The first of these (if it is correct) may eventually be of considerable computational utility. The second is more difficult to evaluate. The representations of which I have made extensive computational use are the regular Jaffé series discussed in Sec. IV A, and the Coulomb wave function expansion presented in Sec. VI. The present (July, 1985) computer implementation of these algorithms is discussed briefly in the Summary. The paper is outlined as follows:

Section II shows the equivalence of the separated parts of the one-particle Schrödinger equation in prolate spheroidal coordinates to the Teukolsky equations that describe the perturbations of the Weyl tensor for Kerr black holes. The angular and radial parts of both sets of equations are cast in the common form of equation (1), and solutions at the singular points $x = 0$, $x = x_0$, and $x = \infty$ are discussed.

Section III briefly reviews the theory of three-term recurrence relations and illustrates the usefulness thereof in generating spheroidal harmonics and in obtaining the eigenvalues of the angular differential equation on the interval $[0 \leq x \leq x_0]$. The origins of the method are lost in antiquity, and most of the material in this section is stolen from more recent articles by W.G. Baber and H.R. Hassé,[5] and W. Gautschi.[6]

Section IV turns to the study of solutions on the interval $[x_0 \leq x < \infty)$, and starts with a review of the eigensolutions of Egil Hylleraas[7] and George Jaffé.[8] Convergence properties of both representations are discussed in detail, and an integral relating the two is derived. Jaffé's solution is of critical importance since it can be generalized to all values of the frequency ω, and provides solutions that are regular and analytic as $x \to x_0$. Section IV C contains a rather lengthly digression on the possibility of generating second solutions to the differential equation by means of a confluent hypergeometric function expansion related to the Laguerre polynomial expansion of Hylleraas. The resulting expressions have yet to be verified numerically.

Section V reviews Stratton's classic solution to the ordinary spheroidal wave equation, and generalizes Stratton's solution to the case of the Schrödinger's equation for an electron in the field of a finite dipole. Rigorous proofs of the convergence of the resulting spherical Bessel function expansions are discussed in detail, and form the basis for the full generalization in terms of Coulomb wave functions presented in Sec. VI. The discussion in Sec. V is important because it shows for the first time how analytic solutions may be constructed for a spheroidal wave equation in a space with a nonzero potential.

Section VI presents the ultimate result of this study: the expansion of solutions to the fully generalized spheroidal wave equation (1) in convergent series of Coulomb wavefunctions. The solutions provided by this representation are both irregular as $x \to x_0$, but are analytic in the operational sense that they allow the asymptotic (large x) behavior of any solution to the generalized spheroidal wave equation to be computed directly from the value of the solution and its derivative at any finite x greater than x_0. The algorithm has seen full computational implementation, and has been used to characterize the nature of the perturbation response of the Schwarzschild black hole to an appreciably greater extent than has previously been possible.[4] Sections V and VI may be read independently from section IV.

Section VII presents another expansion for the generalized spheroidal wavefunctions as series of confluent hypergeometric functions.

Section VIII looks at what happens to the generalized spheroidal wave equation and its Coulomb wavefunction solutions (Sec. VI) in the confluence as $x_0 \to 0$. This happens at the extreme Kerr limit of black hole rotation, and concludes the present analysis of generalized spheroidal wave functions.

Section IX is a Summary and contains a brief description of the computer programs that generate the Jaffè solutions and the Coulomb wave-function expansions.

Lastly, it has not been possible for the present paper to reference all the literature pertaining to spheroidal wave functions, much of which is due to the efforts of Josef Miexner, Friedrich Schäfke, and Gerhard Wolf. The interested reader will find a comprehensive bibliography in their recent monograph.[9]

II. ORIGINS OF THE EQUATION AND ASYMPTOTIC SOLUTIONS

Generalized Spheroidal Wave Equations are ordinary differential equations with two regular singular points and one confluently irregular singular point. Although the Helmholtz equation separates in spheroidal coordinates into particular, and special, examples of such equations (ordinary spheroidal wave equations),[10] the earliest physical context of a *generalized* spheroidal wave equation arose in the consideration of the quantum mechanics of hydrogen molecule-like ions. Early investigations into this subject are reviewed by Baber and Hassé,[5] and much of the discussion in this and the following two sections is excerpted from their article. Generalized spheroidal wave equations also result from the separation of linearized covariant wave equations on black hole background metrics, and the quasi-normal modes of the perturbations of these geometries may be found by the same techniques used to determine the bound-state eigenfunctions of the hydrogen molecule ion.[11] This section explores the similarity of the differential equations in the astrophysical problem to corresponding differential equations in the molecular ion problem, and reduces them both to the form of equation (1).

A. Schrödinger's Equation for Hydrogen Molecule-like Ions

If N_1 and N_2 are the charges on two fixed nuclei A and B, $2a$ is the distance AB between them, and r_1 and r_2 are the distances of an electron from A and B respectively, then the prolate spheroidal coordinates λ and μ are defined by $\lambda = (r_1 + r_2)/2a$ and $\mu = (r_1 - r_2)/2a$. At large values of r_1 and r_2, λ becomes a simple measure of the distance from the molecule or ion, and is referred to as the "radial coordinate." Under the same conditions μ reduces to the cosine of the usual polar angle θ, and μ is termed the "angular coordinate." The time-independent Schrödinger equation $\bigtriangledown^2\psi + (E - V)\psi = 0$ separates if $\psi = \Psi(\lambda)\Phi(\mu)\exp(im\phi)$, where ϕ is the azimuthal angle about the axis AB. A description of this separation is given in Eyring, Walter, and Kimball.[12] The resulting ordinary differential equations for Ψ and Φ are

$$\frac{d}{d\lambda}\left[(\lambda^2 - 1)\frac{d\Psi}{d\lambda}\right] + \left[\omega^2\lambda^2 + 2a(N_1 + N_2)\lambda - A_{lm} - \frac{m^2}{\lambda^2 - 1}\right]\Psi = 0 \tag{2}$$

and

$$\frac{d}{d\mu}\left[(1 - \mu^2)\frac{d\Phi}{d\mu}\right] + \left[-\omega^2\mu^2 - 2a(N_1 - N_2)\mu + A_{lm} - \frac{m^2}{1 - \mu^2}\right]\Phi = 0 \tag{3}$$

where $\omega^2 = 2a^2E$ in atomic units.

Equations (2) and (3) are generalized spheroidal wave equations. If we write $\Psi = (\lambda^2 - 1)^{m/2}f(\lambda)$ and $\Phi = (1 - \mu^2)^{m/2}g(\mu)$, the differential equations for f and g are

$$(\lambda^2 - 1)f_{,\lambda\lambda} + 2(m + 1)\lambda f_{,\lambda} + \left[\omega^2\lambda^2 + 2a(N_1 + N_2)\lambda + m(m + 1) - A_{lm}\right]f = 0 \tag{4}$$

and

$$(1 - \mu^2)g_{,\mu\mu} - 2(m + 1)\mu g_{,\mu} - \left[\omega^2\mu^2 + 2a(N_1 - N_2)\mu + m(m + 1) - A_{lm}\right]g = 0 \quad . \tag{5}$$

The form (1) is obtained if we let $x = \lambda + 1$ in equation (4), and $x = \mu + 1$ in equation (5) :

$$\begin{aligned} &x(x - 2)f_{,xx} + 2(m + 1)(x - 1)f_{,x} \ + \\ &\quad \left[\omega^2x(x - 2) + 2a(N_1 + N_2)(x - 2) + \omega^2 + 2a(N_1 + N_2) + m(m + 1) - A_{lm}\right]f = 0 \end{aligned} \tag{6}$$

$$\begin{aligned} &x(x - 2)g_{,xx} + 2(m + 1)(x - 1)g_{,x} \ + \\ &\quad \left[\omega^2x(x - 2) + 2a(N_1 - N_2)(x - 2) + \omega^2 + 2a(N_1 - N_2) + m(m + 1) - A_{lm}\right]g = 0 \quad . \end{aligned} \tag{7}$$

Generalized spheroidal wave equations are characterized by two regular and one confluently irregular singular points. These occur at $x = 0$, $x = x_0$, and at $x = \infty$, respectively. For equations (6) and (7) the regular singularities correspond to the physical locations of the two nuclei, which are at the foci of the coordinate system, $\lambda = 1$ and $\mu = \pm 1$. If

$$\lim_{x\to 0} y \sim x^{k_1} \ , \ \text{ and } \ \lim_{x\to x_0} y \sim (x-x_0)^{k_2} \ ,$$

then the indices k_1 and k_2 take the values

$$k_1 = 0,\ 1 + B_1/x_0 \ , \qquad \text{and} \qquad k_2 = 0,\ 1 - B_2 - B_1/x_0 \ \ .$$

For equations (6) and (7) these values are $0, -m$ both for k_1 and for k_2.

B. Covariant Wave Equation on Schwarzschild and Kerr Backgrounds

A separable linearized partial differential wave equation obeyed by components of weak electromagnetic and gravitational fields on the background geometry of the Schwarzschild black hole was derived through the efforts of Wheeler,[13] Regge and Wheeler,[14] Zerilli,[15] Chandrasekhar,[16] and Chandrasekhar and Detweiler.[17] Analysis of wave equations on the Kerr geometry of rotating black holes was provided by Teukolsky.[18] Generalized Spheroidal Wave Equations result in each case.

Schwarzschild Geometry

The Schwarzschild Geometry is spherically symmetric, and the partial differential equation for the field components separates in polar spatial coordinates r, θ, and ϕ, and Schwarzschild's time coordinate t. These are the Schwarzschild coordinates.

Denote either a massless scalar field or a component of the electromagnetic or gravitational fields by a generic field function $\Phi(t, r, \theta, \phi)$. Fourier analyze and expand Φ in spherical harmonics as

$$\Phi(t, r, \theta, \phi) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} \left(\sum_l \frac{1}{r} \psi_l(r, \omega) Y_{l0}(\theta, \phi) \right) d\omega \ . \tag{8}$$

The homogeneous differential equation obeyed by the fourier component $\psi_l(r)$ is

$$r(r-1)\psi_{l,rr} + \psi_{l,r} + \left[\frac{\omega^2 r^3}{r-1} - l(l+1) + \frac{s^2-1}{r} \right] \psi_l = 0 \ , \tag{9}$$

where the coordinates t and r have been scaled so that the horizon, which usually appears at $r = 2M$, is now at $r = 1$. The parameter s is the spin of the field, and takes the values 0, 1, or 2 depending on whether Φ is respectively a component of the massless scalar, electromagnetic, or gravitational field.

The history of the derivation of these perturbation equations is long and rich. The derivation of the radial component of the scalar wave equation [$s = 0$ in Eq. (9)] on the Schwarzschild background is a straightforward exercise in perturbation theory.[19,20] The $s = 1$ equation for electromagnetic perturbations was derived by Wheeler in 1955,[13] and the $s = 2$ equation for odd parity gravitational perturbations by Regge and Wheeler a few years later.[14] A very similar equation obeyed by even parity gravitational perturbations was obtained by Zerilli in 1970,[15] and the equivalence of Zerilli's even parity equation to Regge and Wheeler's odd parity equation (Eq. (9) with $s = 2$) was demonstrated by Chandrasekhar[16] and Chandrasekhar and Detweiler in 1975.[17] This twenty years of effort has been summarized by Professor Chandrasekhar in chapter 4 of his recent book.[21]

Equation (9) may be put in the form of equation (1) by means of the substitution

$$\psi_l(r, \omega) = r^{1+s}(r-1)^{-i\omega} y(r, \omega) \quad . \tag{10}$$

The differential equation for y is

$$r(r-1)y_{,rr} + [2(s+1-i\omega)r - (2s+1)]y_{,r} + \\ [\omega^2 r(r-1) + 2\omega^2(r-1) + 2\omega^2 - l(l+1) + s(s+1) - (2s+1)i\omega]y = 0 \tag{11}$$

and the indicial structure at the regular singular points $r = 0$ and $r = 1$ is given by

$$y \overset{r\to 0}{\longrightarrow} r^{k_1} \ , \qquad y \overset{r\to 1}{\longrightarrow} (r-1)^{k_2} \ ,$$

where $k_1 = 0, -2s$ and $k_2 = 0,\ 2i\omega$. With the signs for ω chosen in equations (8) and (10), the exterior (i.e., $1 \le r < \infty$) solution y that is regular at $r = 1$ corresponds, for $Re(\omega) > 0$, to a field function that radiates into the horizon. This is the physically meaningful case, but a second exterior solution may be found simply by replacing ω by $-\omega$ in equations (10) and (11).

Kerr Geometry

The geometry of the rotating black hole has oblate spheroidal nature, and the wave equation for the components of the massless fields can be separated in the oblate spheroidal spatial coordinates λ, μ, and ϕ, and a time-like coordinate t. The coordinates λ and μ may be defined as in Sec. II A for prolate spheroids, but the axis of oblate rotation is the semi-minor axis of the family of ellipses parameterized by constant values of λ. The oblate spheroidal coordinate ϕ measures the azimuthal angle about the semi-minor axis. The singularities of the coordinate system, which are the fixed locations of the two foci for prolate spheroids, become a singular ring of radius a when the foci rotate about the semi-minor axis.

Kerr's spatial coordinates r and θ are simply related to the oblate spheroidal coordinates λ and μ by[22]

$$r = a(\lambda^2 - 1)^{1/2} \ \text{ and } \ \theta = \sin^{-1}\mu \quad .$$

Simplification of the Kerr metric is obtained by the introduction of the Boyer-Lindquist azimuthal coordinate $\bar{\phi}$, which is related to the azimuthal angle ϕ and the "radial" coordinate r by

$$d\bar{\phi} = d\phi + a(r^2 - 2Mr + a^2)^{-1} dr \ .$$

I will follow the usual convention of dropping the "$^-$" from $\bar{\phi}$ and denote the Boyer-Lindquist coordinates simply by t, r, θ, and ϕ. These coordinates reduce to Schwarzschild's coordinates as $a \to 0$. The Kerr metric in Boyer-Lindquist coordinates is

$$ds^2 = \begin{array}{l} (1 - 2Mr/\Sigma)dt^2 + (4Mar\sin^2(\theta)/\Sigma)dtd\phi - (\Sigma/\Delta)dr^2 - \Sigma d\theta^2 \\ \qquad - \sin^2(\theta)(r^2 + a^2 - 2Ma^2 r\sin^2(\theta)/\Sigma)d\phi^2 \end{array} \tag{12}$$

where

$$\Sigma = r^2 + a^2\cos^2\theta \ ,$$

and

$$\Delta = r^2 - 2Mr + a^2 \ .$$

It is convenient to define one last angular coordinate $u = \cos(\theta) = \pm(1-\mu^2)^{\frac{1}{2}}$. The field function $\Phi(t, r, u, \phi)$ can then be expanded as

$$\Phi(t, r, u, \phi) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\omega t} \sum_{l=|s|}^{\infty} \sum_{m=-l}^{l} e^{im\phi} S_{lm}(u) R_{lm}(r) d\omega \tag{13}$$

and, after a rescaling of t and r so that $2M = 1$, the following differential equations obtained[18,1] for the angular function $S(u)$ and the radial function $R(r)$:

$$\left[(1-u^2)S_{lm,u}\right]_{,u} + \left[a^2\omega^2u^2 - 2a\omega su + s + A_{lm} - \frac{(m+su)^2}{1-u^2}\right] S_{lm} = 0 \tag{14}$$

and

$$\Delta R_{lm,rr} + (s+1)(2r-1)R_{lm,r} + V(r)R_{lm} = 0 \tag{15}$$

where

$$V(r) = \left\{ \begin{array}{c} \left[(r^2+a^2)^2\omega^2 - 2am\omega r + a^2m^2 + is\left(am(2r-1) - \omega(r^2-a^2)\right)\right]\Delta^{-1} \\ + \left[2is\omega r - a^2\omega^2 - A_{lm}\right] \end{array} \right\}$$

Equations (14) and (15) are the Kerr geometry linearized wave equation analogs to the Schrödinger prolate spheroidal equations (2) and (3) . The functions R_{lm} and and S_{lm} are referred to as "Teukolsky's functions",[21] and I will now show that they are, in fact, generalized spheroidal wave functions.

Define an auxiliary rotation parameter b by $b = (1-4a^2)^{1/2}$, and define r_+ and r_- to be the zeros of Δ, so that $\Delta = (r-r_-)(r-r_+)$. Then $r_\pm = (1 \pm b)/2$, and $r = r_+$ corresponds to the event horizon. The solutions of equations (15) and (14) at the regular singularities $u = \pm 1$ and $r = r_\pm$ can be found in the usual way: if

$$\lim_{u\to -1} S_{lm} \sim (1+u)^{k_1}, \text{ and } \lim_{u\to +1} S_{lm} \sim (1-u)^{k_2}, \tag{16}$$

then

$$k_1 = \pm\frac{1}{2}(m-s) \; , \text{ and } k_2 = \pm\frac{1}{2}(m+s) \; .$$

Similarly if

$$\lim_{r\to r_-} R_{lm} \sim (r-r_-)^{k_-}, \text{ and } \lim_{r\to r_+} R_{lm} \sim (r-r_+)^{k_+},$$

then

$$k_- = -\frac{i}{b}(\omega r_- - am) \; , \quad -s + \frac{i}{b}(\omega r_- - am) \; ,$$

and

$$k_+ = \frac{i}{b}(\omega r_+ - am) \; , \quad -s - \frac{i}{b}(\omega r_+ - am) \; .$$

The physically meaningful solutions to the angular equation (14) are regular at the axis ($u = \pm 1$), so the usual choices for k_1 and k_2 are $k_1 = |m-s|/2$ and $k_2 = |m+s|/2$. Similarly, the usual exterior solutions to the radial equation are those which correspond to fields radiating into the event horizon at $r = r_+$. This corresponds to $k_+ = -s - i(\omega r_+ - am)/b$. Boyer-Lindquist coordinates are not well suited to analysis of the physics of the interior problem, but the choice $k_- = -s + i(\omega r_- - am)/b$ turns out to be convenient for the present study restricted to just the differential equation. Letting

$$R_{lm} = (r-r_-)^{-s+\frac{i}{b}(\omega r_- - am)}(r-r_+)^{-s-\frac{i}{b}(\omega r_+ - am)}y(r-r_-) \tag{17}$$

and

$$S_{lm} = (1+u)^{\frac{1}{2}|m-s|}(1-u)^{\frac{1}{2}|m+s|}g(u) \tag{18}$$

then the differential equations for y and g are

$$\begin{aligned} &x(x-b)y_{,xx} + [2(1-s-i\omega)x + (s-1+2i\omega)b - 2i(\omega r_+ - am)]y_{,x} + \\ &\quad [\omega^2 x(x-b) + 2(\omega+is)\omega(x-b) + (1+b-a^2)\omega^2 + (2s-1)i\omega + is\omega b - 2s - A_{lm}]y = 0 \; , \end{aligned} \tag{19}$$

where $x = r - r_-$, and

$$\begin{aligned} &z(z-2)g_{,zz} + [2(k_1+k_2+1)z - 2(2k_1+1)]g_{,z} + [-a^2\omega^2 z(z-2) + \\ &\quad 2a\omega sz - s - A_{lm} - (s+a\omega)^2 + (k_1+k_2)(k_1+k_2+1)]g = 0 \; , \end{aligned} \tag{20}$$

where $z = u + 1$. These are generalized spheroidal wave equations of form (1).

C. Exponents of the Solutions Near the Regular Singular Points $x = 0$ and $x = x_0$, and Asymptotic Solutions

We may now take equation (1) to be our standard form for the generalized spheroidal wave equation:

$$x(x - x_0)\frac{d^2y}{dx^2} + (B_1 + B_2 x)\frac{dy}{dx} + \left[\omega^2 x(x - x_0) - 2\eta\omega(x - x_0) + B_3\right] y = 0 \ .$$

I recapitulate the solution forms at the regular singular points. If

$$\lim_{x\to 0} y \sim x^{k_1}, \ \text{ and } \ \lim_{x\to x_0} y \sim (x - x_0)^{k_2}, \tag{21}$$

then

$$k_1 = 0, 1 + B_1/x_0 \ \text{ and } \ k_2 = 0, 1 - B_2 - B_1/x_0 \ .$$

Asymptotic solutions are found through the substitution

$$y(x) = x^{B_1/2x_0}(x - x_0)^{-\frac{1}{2}(B_2 + B_1/x_0)} v(x).$$

The differential equation for $v(x)$ as $x \to \infty$ is approximately

$$\frac{d^2v}{dx^2} + \left[\omega^2 - \frac{2\eta\omega}{x} - \frac{\frac{1}{2}B_2(\frac{1}{2}B_2 - 1) - B_3}{x^2} + \mathcal{O}(x^{-3})\right] v = 0$$

so that two independent asymptotic solutions for equation (1) are

$$\lim_{x\to\infty} y_+(x) = x^{B_1/2x_0}(x - x_0)^{-\frac{1}{2}(B_2 + B_1/x_0)} \left[G_{\nu_a}(\eta, \omega x) + iF_{\nu_a}(\eta, \omega x)\right] \left[1 + \mathcal{O}(x^{-3})\right] \tag{22}$$

and

$$\lim_{x\to\infty} y_-(x) = x^{B_1/2x_0}(x - x_0)^{-\frac{1}{2}(B_2 + B_1/x_0)} \left[G_{\nu_a}(\eta, \omega x) - iF_{\nu_a}(\eta, \omega x)\right] \left[1 + \mathcal{O}(x^{-3})\right] \tag{23}$$

where $F_{\nu_a}(\eta, \omega x)$ and $G_{\nu_a}(\eta, \omega x)$ are the Coulomb wave functions of (usually complex) order $\nu_a = \frac{1}{2}[-1 \pm (1 + B_2(B_2 - 2) - 4B_3)^{1/2}]$. To lower order the asymptotic approximations simplify to

$$\lim_{x\to\infty} y_\pm(x) \sim x^{-(\frac{1}{2}B_2 \pm i\eta)} e^{\pm i\omega x} \left[1 + \mathcal{O}(1/x)\right] \ . \tag{24}$$

Coulomb wave functions will be discussed further in Sec. VI.

III. THREE-TERM RECURRENCE RELATIONS AND THE ANGULAR EIGENVALUE PROBLEM

Every representation of generalized spheroidal wavefunctions discussed in this paper will involve either a power series expansion, or an expansion in a series of special functions. Since the expansion coefficients in each case will be defined by a three-term recurrence relation, a review of some properties of such relations is in order. The discussion here will be quite brief, and is excerpted primarily from the first few sections of the excellent article on three-term recurrence relations by Walter Gautschi.[6] I illustrate the theory by a simple and relevant example of a sequence determined by a three-term recurrence relation: the coefficients for a power series solution to equation (1) about the regular singular point $x = 0$.

A. Power Series Solutions on $[0 \leq x \leq x_0]$

Equation (1) was

$$x(x-x_0)\frac{d^2y}{dx^2} + (B_1 + B_2 x)\frac{dy}{dx} + \left[\omega^2 x(x-x_0) - 2\eta\omega(x-x_0) + B_3\right] y = 0 \quad .$$

Following Baber and Hassé,[5] a power series solution about $x = 0$ may be obtained by letting

$$y(x) = e^{i\omega x}\sum_{n=0}^{\infty} a_n^\theta x^n \tag{25}$$

I use the superscript θ in this solution to denote its usual association with the angular equations (3) and (14). The sequence of expansion coefficients $\{a_n^\theta : n = 1, 2, \ldots\}$ is defined by the three-term recurrence relation

$$\begin{array}{rcl} \alpha_0^\theta a_1^\theta \;\; + \beta_0^\theta a_0^\theta & = & 0 \\ \alpha_n^\theta a_{n+1}^\theta + \beta_n^\theta a_n^\theta + \gamma_n^\theta a_{n-1}^\theta & = & 0 \quad n = 1, 2 \ldots \end{array} \tag{26}$$

where

$$\begin{array}{rcrcrcl} \alpha_n^\theta & = & -x_0 n^2 & + & (B_1 - x_0)n & + & B_1 \\ \beta_n^\theta & = & n^2 & + & (B_2 - 2i\omega x_0 - 1)n & + & 2\eta\omega x_0 + i\omega B_1 + B_3 \\ \gamma_n^\theta & = & & & 2i\omega n & + & i\omega(B_2 - 2) - 2\eta\omega \quad . \end{array} \tag{27}$$

Equations (26) and (27) are equivalent to Baber and Hassé's equation 10. I will take equation (26) to be my standard form for a three-term recurrence relation. In Sec. 5 and Sec. 6 I will also discuss double-ended sequences in which the index n runs from $-\infty$ to $+\infty$, as opposed to the single-ended variety considered here.

Three-term recurrence relations, like second-order differential equations, possess two independent solution sequences $\{A_n : n = 1, 2 \ldots\}$ and $\{B_n : n = 1, 2 \ldots\}$. The two sequences frequently have the property that $\lim_{n\to\infty} A_n/B_n = 0$. The sequence $\{A_n : n = 1, 2 \ldots\}$ is then referred to as the "solution sequence minimal as $n \to \infty$", or briefly, as *minimal*. Any nonminimal solution sequence $\{B_n : n = 1, 2 \ldots\}$ is referred to as *dominant* (Gautschi, page 25). Dominant sequences are not unique, as any multiple of the minimal solution may be added to them without destroying their dominant property. I typically denote either type of sequence by the general sequence $\{a_n : n = 1, 2 \ldots\}$. Whether the a_n are minimal or dominant will be seen to depend on the ratio a_1/a_0.

The large n behavior of the expansion coefficients $\{a_n^\theta : n = 1, 2 \ldots\}$ may be analyzed by writing equation (26) as

$$\alpha_n^\theta \frac{a_{n+1}^\theta}{a_n^\theta} + \beta_n^\theta + \gamma_n^\theta \frac{a_{n-1}^\theta}{a_n^\theta} = 0 \ , \tag{28}$$

dividing by n^2, and keeping only the leading order terms in the result:

$$-x_0 \frac{a_{n+1}^\theta}{a_n^\theta} + 1 + \frac{2i\omega}{n}\frac{a_{n-1}^\theta}{a_n^\theta} \approx 0 \ . \tag{29}$$

We then see that the a_n^θ are elements of the minimal solution sequence if

$$\lim_{n\to\infty} \frac{a_n^\theta}{a_{n-1}^\theta} \sim -\frac{2i\omega}{n} \tag{30}$$

and the a_n^θ are dominant if

$$\lim_{n\to\infty} \frac{a_n^\theta}{a_{n-1}^\theta} = \frac{1}{x_0} \; . \tag{31}$$

The ratio of successive elements of the minimal solution sequence to the recurrence relation (26) is given by the continued fraction[6]

$$\frac{a_{n+1}^\theta}{a_n^\theta} = \frac{-\gamma_{n+1}^\theta}{\beta_{n+1}^\theta -}\,\frac{\alpha_{n+1}^\theta\gamma_{n+2}^\theta}{\beta_{n+2}^\theta -}\,\frac{\alpha_{n+2}^\theta\gamma_{n+3}^\theta}{\beta_{n+3}^\theta -}\,\ldots \tag{32}$$

which for $n = 0$ gives

$$\frac{a_1^\theta}{a_0^\theta} = \frac{-\gamma_1^\theta}{\beta_1^\theta -}\,\frac{\alpha_1^\theta\gamma_2^\theta}{\beta_2^\theta -}\,\frac{\alpha_2^\theta\gamma_3^\theta}{\beta_3^\theta - \ldots} \; . \tag{33}$$

However, for single-ended sequences such as arise out of power series expansions, the first of equations (26) requires that

$$\frac{a_1^\theta}{a_0^\theta} = -\frac{\beta_0^\theta}{\alpha_0^\theta} \; . \tag{34}$$

Equations (33) and (34) cannot both be satisfied for arbitrary values of the recurrence coefficients α_n^θ, β_n^θ, and γ_n^θ, so that the general solution sequence to equation (26) is a dominant one and can usually be generated by simple forward recursion from a chosen value of a_0^θ. The resulting power series (25) will converge for all x of magnitude less than the magnitude of x_0, but will diverge when $|x| \geq |x_0|$.

A power series solution for equation (1) about the singular point $x = x_0$ may be obtained simply by letting $z = x - x_0$. Then equation (1) in this new variable becomes

$$z(z + x_0)y_{,zz} + (B_1 + B_2x_0 + B_2z)y_{,z} + [\omega^2 z(z + x_0) - 2\eta\omega z + B_3]y = 0 \tag{35}$$

which is of the same form as equation (1), and a power series solution about $z = 0$ can be generated in the same manner as before. Such a solution could be useful in obtaining the behavior near $x = x_0$ of solutions on the exterior interval $[x_0 \leq x < \infty)$. However, the radius of convergence of this series expansion is just $|x_0|$. It is no more useful in obtaining eigensolutions on $[0 \leq x \leq x_0]$ as the series (25), and is vastly inferior to Jaffé's solution on $[x_0 \leq x < \infty)$. Second power-series solutions, in the cases when $1 + B_1/x_0$ or $1 - B_2 - B_1/x_0$ are integers, may be found by the method of Frobenius.

B. The Angular Eigenvalue Problem

The prolate angular coordinate $\mu = (r_1 - r_2)/2a$ of equation (3) and the oblate angular coordinate $u = \pm(1 - \mu^2)^{1/2}$ of equation (14) play the same role in their respective wavefunctions, and the physically meaningful solutions to either of equations (7) or (20) are those that are finite both at $x = 0$ and at $x = x_0$ (*i.e.*, μ or u equal ± 1). These solutions are simple Sturmian eigensolutions, and are obtained for a given value of ω if the angular separation constant A_{lm}, which appears as part of the equation parameter B_3 in the β_n^θ, can be adjusted so that equations (33) and (34) are both satisfied. If so, the resulting solution sequence $\{a_n^\theta : n = 1, 2\ldots\}$ will be purely minimal, and the power series (25) will converge at $x = x_0$. Equating the right-hand sides of equations (33) and (34) yields an implicit continued fraction equation for the angular separation constant A_{lm} :

$$0 = \beta_0^\theta - \frac{\alpha_0^\theta\gamma_1^\theta}{\beta_1^\theta -}\,\frac{\alpha_1^\theta\gamma_2^\theta}{\beta_2^\theta -}\,\frac{\alpha_2^\theta\gamma_3^\theta}{\beta_3^\theta - \ldots} \tag{36}$$

The α, β, and γ are defined as explicit functions of B_3 and the other parameters of the differential equation in equations (27), and equation (36) may be solved for A_{lm} (that is, B_3) by standard nonlinear root-search techniques. The expansion coefficients a_n^θ are then generated by downward recursion on (26), starting from ratios given by (32) at a suitably large value of n.

Fackerell and Crossman[23] have obtained a continued fraction equation for the eigenvalues of the spin-weighted angular spheroidal equation (14) by expanding $S_{lm}(u)$ in a series of Jacobi polynomials, and discuss the normalization properties of these functions (see also Breuer, Ryan, and Waller[24]). There is probably an integral relating Fackerell and Crossman's Jacobi polynomial solution with the power series solution reviewed here. Hunter and Guerrieri[25] have done a detailed Wentzel-Kramer-Brillouin-Jeffreys (WKBJ) analysis of the angular equation for large values of A_{lm}, which has provided analytic insight into branch points associated with these eigenvalues. Their work might complement Ferrari and Mashoon's[26] WKBJ analysis of the Schwarzschild quasi-normal frequencies to provide useful insight into the large l behavior of the Kerr quasi-normal frequencies. It is interesting that none of these recent studies of the angular equation reference the early results of Wilson,[27] or of Baber and Hassé.[5] Fackerell and Crossman's expansions (19) and (20), for instance, apparently are independently derived generalizations of Baber and Hassé's expansions (30) and (33). The power series expansion I have given here (cf. equation (25)) is equivalent to Baber and Hassé's equation (34).

IV. THE SOLUTIONS OF HYLLERAAS AND JAFFÉ, INTEGRAL RELATIONS, AND SECOND SOLUTIONS

Although Egil Hylleraas is generally given credit for the first solution to the bound state problem of the hydrogen molecule ion in 1931,[7] the solution to equation (2) derived by George Jaffé in 1934[8] was the first to contain a proof of convergence. Such proof did not exist for Hylleraas' representation until W.G. Baber and H.R. Hassé provided one in 1935.[5] (Baber and Hassé apparently also made independent discovery of Jaffé's solution.) This section will discuss the eigensolutions of Hylleraas and Jaffé, and their convergence properties. In particular, Jaffé's representation will be shown to be simply convergent for noneigenfunction solutions to equation (1), in addition to being uniformly convergent for eigenfunctions. An integral equation for Sturmian eigenfunctions is derived and used to illuminate the relationship between the representations of Hylleraas and Jaffé, and to express the solution to equation (1) that is regular as $x \to \infty$ in terms of the solution that is regular at $x = x_0$.

A. The Solutions of Hylleraas and Jaffé on $[x_0 \le x < \infty)$

Equation (1) was

$$x(x - x_0)\frac{d^2y}{dx^2} + (B_1 + B_2 x)\frac{dy}{dx} + \left[\omega^2 x(x - x_0) - 2\eta\omega(x - x_0) + B_3\right] y = 0 \ \ .$$

Hylleraas, using hydrogen atom eigenfunctions as *Ansätze*, expanded the solution $y(x)$ that is regular at $x = x_0$ in a series of Laguerre polynomials:

$$y = e^{i\omega x} \sum_{n=0}^{\infty} \frac{n! a_n^r}{\Gamma(\frac{1}{2}B_2 + i\eta + B_1/x_0 + 1 + n)} L_n^{B_2 + B_1/x_0 - 1}(-2i\omega(x - x_0)) \ \ . \quad (37)$$

(The superscript (r) on the expansion coefficients a_n^r denotes they are related to solutions of "radial" equations, such as (2), (9), and (15).)

Jaffé took a more rigorous approach and reasoned that since a power series expansion of solutions to a differential equation about one regular singular point generally has a radius of convergence equal to the distance from the point of expansion to the next nearest singular point, and that since the singular point at $x = 0$ obstructs the convergence of a power series between x_0 and ∞, the obvious solution to the power series convergence problem was to rearrange the singular points so that the point $x = x_0$ was moved to 0, the point at ∞ was moved to 1, and the bothersome singular point at 0 was shuffled off to oblivion. Jaffé effected this rearrangement with the variable change $u = (x - x_0)/x$ and then let

$$y(x) = e^{i\omega x} x^{-\frac{1}{2}B_2 - i\eta} f(u) \ \ .$$

The differential equation for f in terms of the variable u is

$$u(1 - u)^2 f_{,uu} + (c_1 + c_2 u + c_3 u^2) f_{,u} + (c_4 + c_5 u) f = 0 \ , \quad (38)$$

where

$$\begin{aligned}
c_1 &= B_2 + B_1/x_0 \\
c_2 &= -2[c_1 + 1 + i(\eta - \omega x_0)] \\
c_3 &= c_1 + 2(1 + i\eta) \\
c_5 &= (\tfrac{1}{2}B_2 + i\eta)(\tfrac{1}{2}B_2 + i\eta + 1 + B_1/x_0) \\
c_4 &= -c_5 - \tfrac{1}{2}B_2(\tfrac{1}{2}B_2 - 1) + \eta(i - \eta) + i\omega x_0 c_1 + B_3 \ \ .
\end{aligned}$$

The function $f(u)$ can then be expanded in a power series in u, $f(u) = \sum_{n=0}^{\infty} a_n u^n$, and Jaffé's solution to the generalized spheroidal wave equation is

$$y_1(x) = e^{+i\omega x} x^{-\frac{1}{2}B_2 - i\eta} \sum_{n=0}^{\infty} a_n^r \left(\frac{x - x_0}{x} \right)^n \quad . \tag{39}$$

With the Laguerre polynomials defined in Appendix A the coefficients a_n^r in the Hylleraas expansion (37) and the coefficients a_n^r in the Jaffé expansion (39) have the amusing property of being identical. They obey the same three-term recurrence relation

$$\begin{array}{rcl} \alpha_0^r a_1^r \quad + \beta_0^r a_0^r & = & 0 \\ \alpha_n^r a_{n+1}^r + \beta_n^r a_n^r + \gamma_n^r a_{n-1}^r & = & 0 \quad n = 1, 2 \ldots \end{array} \tag{40}$$

where

$$\begin{array}{rcl} \alpha_n^r & = & (n+1)(n + B_2 + B_1/x_0) \\ \beta_n^r & = & \left\{ \begin{array}{l} -2n^2 - 2[B_2 + i(\eta - \omega x_0) + B_1/x_0]n \\ -(\frac{1}{2}B_2 + i\eta)(B_2 + B_1/x_0) + i\omega(B_1 + B_2 x_0) + B_3 \end{array} \right\} \\ \gamma_n^r & = & (n - 1 + \frac{1}{2}B_2 + i\eta)(n + \frac{1}{2}B_2 + i\eta + B_1/x_0) \quad . \end{array} \tag{41}$$

The normalization of the Laguerre polynomials is important. The convention here is that used by Slater,[28] and by Gradshteyn and Ryzhik.[29] Relevant recurrence and differential properties, as well alternate normalizations, will be found in Appendix A.

Convergence of the Hylleraas and Jaffé expansions may be analyzed by determining the behavior of the expansion coefficients at large n and applying the ratio test to successive terms in the series. To this end divide recurrence relation (40) by $n^2 a_n^r$, retain terms to $\mathcal{O}(1/n)$, and expand

$$\lim_{n \to \infty} \frac{a_{n+1}^r}{a_n^r} = 1 + \frac{a}{\sqrt{n}} + \frac{b}{n} + \ldots \tag{42}$$

The resulting approximate recurrence relation can be written

$$\left(1 + \frac{u}{n}\right)\left(1 + \frac{a}{\sqrt{n}} + \frac{b}{n}\right) - \left(2 + \frac{v}{n}\right) + \left(1 + \frac{w}{n}\right)\left(1 - \frac{a}{\sqrt{n}} + \frac{a^2 - b}{n} + \frac{2ab - a/2 - a^3}{n^{3/2}}\right) \approx 0 \tag{43}$$

where u, v, and w are constants given by $u = B_2 + B_1/x_0 + 1$, $v = 2[B_2 + B_1/x_0 + i(\eta - \omega x_0)]$, and $w = B_2 + B_1/x_0 + 2i\eta - 1$. Retaining terms to $\mathcal{O}(n^{-3/2})$ and solving for a and b we find $a^2 = v - u - w$ and $b = \frac{1}{4} + v/2 - u$, or

$$a^2 = -2i\omega x_0 \quad , \quad b = i(\eta - \omega x_0) - 3/4 \quad . \tag{44}$$

The large n behavior of the a_n^r may then be deduced by writing (42) as

$$\lim_{n \to \infty} \frac{a_{n+1}^r - a_n^r}{a_n^r} = \frac{a}{\sqrt{n}} + \frac{b}{n} \quad , \tag{45}$$

and integrating with respect to n. The result[5] is

$$\lim_{n \to \infty} a_n^r \approx n^b e^{2a\sqrt{n}} = n^{i(\eta - \omega x_0) - 3/4} e^{\pm 2\sqrt{-2i\omega x_0 n}} \quad . \tag{46}$$

The two signs ($\pm$) in the exponent indicate the asymptotic behavior of the two independent solution sequences to the recurrence relation. It is apparent that one solution sequence will be dominant and the other minimal for all ωx_0 that are not pure negative imaginary.

The Laguerre polynomials $L_n(z)$ are a dominant solution to the recurrence relation

$$(n+1)L^{\alpha}_{n+1}(z) - (2n+\alpha+1-z)L^{\alpha}_{n}(z) + (n+\alpha)L^{\alpha}_{n-1}(z) = 0 \quad . \tag{47}$$

Repeating the procedure that found $\lim a^r_{n+1}/a^r_n$, we find

$$\lim_{n\to\infty} \frac{L^{\alpha}_{n+1}(z)}{L^{\alpha}_{n}(z)} = 1 + \sqrt{-\frac{z}{n}} + \frac{z+1-\alpha}{2n}$$

where $z = -2i\omega(x - x_0)$. The limiting form of the ratio of successive terms of the series (37) is

$$\begin{aligned}\lim_{n\to\infty} \frac{\Gamma(\frac{1}{2}B_2 + B_1/x_0 + i\eta + n + 1)}{\Gamma(\frac{1}{2}B_2 + B_1/x_0 + i\eta + n + 2)} \frac{(n+1)!a^r_{n+1}L^{\alpha}_{n+1}(z)}{n!a^r_n L^{\alpha}_n(z)} &= \\ 1 + \frac{\sqrt{2i\omega(x-x_0)} \pm \sqrt{-2i\omega x_0}}{\sqrt{n}} &+ \mathcal{O}(1/n) \quad .\end{aligned} \tag{48}$$

The $(\pm)$ arises from the ratio a^r_{n+1}/a^r_n, and is $(-)$ only for sequences a^r_n that are minimal. Hence the only condition under which Hylleraas' expansion (37) can converge is if *both* (i) $2i\omega(x - x_0)$ is purely negative real, *and* (ii) the sequence $\{a^r_n : n = 0, 1, 2\ldots\}$ is minimal. (We will not consider cases in which $2i\omega(x - x_0)$ and $-2i\omega x_0$ are both purely negative real. Analysis of that condition hinges on the $\mathcal{O}(1/n)$ terms, and in light of the much stronger convergence properties of Jaffé's expansion, is not terribly relevant.) In the context of the quantum mechanics of hydrogen molecule ion condition (i) is automatically satisfied for any negative real energy $E = -\rho^2/2a$ (where $\rho = -i\omega$ in the usual notation), and the fulfillment of condition (ii) becomes the quantization condition on ω. (The continued fraction equation (53) must be satisfied for the recurrence coefficients given in (41)). Hence the Hylleraas expansion successfully represents the eigenfunctions of the bound states of hydrogen molecule-like ions, but very little else.

Jaffé's expansion, on the other hand, is absolutely convergent on $[x_0 \le x < \infty)$, and is uniformly convergent there if $\sum a^r_n$ is finite (usually only if the a^r_n are minimal). Proof of absolute convergence is trivial: choose an x from the half-plane in which $|(x - x_0)/x| < 1$. Then

$$\lim_{n\to\infty} \left| \frac{a^r_{n+1}[(x-x_0)/x]^{n+1}}{a^r_n[(x-x_0)/x]^n} \right| = \left| \frac{x-x_0}{x} \right| < 1 \quad ,$$

and convergence at any finite x is assured.

The condition for uniform convergence is similarly demonstrated:

$$\lim_{n\to\infty} \left[\lim_{x\to\infty} \left| \frac{a^r_{n+1}[(x-x_0)/x]^{n+1}}{a^r_n[(x-x_0)/x]^n} \right| \right] = \lim_{n\to\infty} \frac{a^r_{n+1}}{a^r_n} = 1 \pm \frac{\sqrt{-2i\omega x_0}}{\sqrt{n}} - \frac{1 - i(\eta - \omega x_0)}{n} \quad .$$

Convergence is guaranteed if (i) the $(-)$ sign is obtained, which is the case if the sequence $\{a^r_n : n = 1, 2\ldots\}$ is minimal, or (ii) if $Re(\sqrt{2i\omega x_0}) = 0$ and $Im(\eta - \omega x_0) > 0$. The first case again defines the quantization condition for the hydrogen molecule-like ions, and has also been used to characterize the quasi-normal modes of black holes — a problem for which $2i\omega x$ is complex and the Hylleraas expansion is useless. The second case can arise in the consideration of hydrogen molecule-like ion wavefunctions for negative noneigenenergies if one defines ρ by $E = -\rho^2/2a$ (i.e., $\rho = -i\omega$) as before, and expands the solution $y(x)$ as

$$y_2(x) = e^{-i\omega x} x^{-\frac{1}{2}B_2 + i\eta} \sum_{n=0}^{\infty} b^r_n \left(\frac{x - x_0}{x} \right)^n \quad . \tag{49}$$

The expansion coefficients b^r_n are generated by a three-term recurrence relation

$$\begin{aligned} \tilde{\alpha}_0 b^r_1 \quad + \tilde{\beta}_0 b^r_0 \qquad\qquad &= \;\; 0 \\ \tilde{\alpha}_n b^r_{n+1} + \tilde{\beta}_n b^r_n + \tilde{\gamma}_n b^r_{n-1} &= \;\; 0 \quad n = 1, 2 \ldots \end{aligned} \tag{50}$$

where now the recurrence coefficients $\tilde{\alpha}_n$, $\tilde{\beta}_n$, and $\tilde{\gamma}_n$ are given by

$$\begin{aligned}
\tilde{\alpha}_n &= (n+1)(n+B_2+B_1/x_0) \\
\tilde{\beta}_n &= \left\{ \begin{array}{l} -2n^2 - 2[B_2 - i(\eta - \omega x_0) + B_1/x_0]n \\ -(\frac{1}{2}B_2 - i\eta)(B_2 + B_1/x_0) - i\omega(B_1 + B_2 x_0) + B_3 \end{array} \right\} \\
\tilde{\gamma}_n &= (n - 1 + \tfrac{1}{2}B_2 - i\eta)(n + \tfrac{1}{2}B_2 - i\eta + B_1/x_0) \quad .
\end{aligned} \tag{51}$$

The $\tilde{\alpha}_n$, $\tilde{\beta}_n$, and $\tilde{\gamma}_n$ of equation (51) are the complex conjugates of the α_n, β_n, and γ_n of equation (41) only if the parameters B_1, B_2, B_3, ω, x_0, and η are purely real. When $\omega = i\rho$ lies on the positive imaginary axis the independent solutions sequences to recurrence relation (50) are neither minimal nor dominant, so this expression is not well-suited to determine the exact hydrogen molecule-like ion eigenfunctions – but it does generate the general negative energy solutions in a stable manner, and was useful in the numerical verification of the integral relationships to be discussed forthwith (Sec. 4c).

B. The Radial Eigenvalue Problem

The eigensolutions of the generalized spheroidal wave equation (1) on the interval $[0 \leq x < \infty)$ are those functions $y_1(x)$ or $y_2(x)$ of equations (39) and (49) for which $\sum a_n^r$ or $\sum b_n^r$ converge. The function $y_1(x)$ then describes an eigenfunction that is regular at $x = x_0$ and has purely $e^{+i(\omega x - \eta \ln x)}$ behavior as $x \to \infty$, and $y_2(x)$ describes an eigenfunction that is regular at $x = x_0$ and has purely $e^{-i(\omega x - \eta \ln x)}$ behavior as $x \to \infty$. The sums over a_n^r or b_n^r will usually converge iff the a_n^r or b_n^r are minimal solutions to their respective recurrence relations (40) and (50), and this will happen only for certain characteristic values of the frequency ω. (The values of ω for which the a_n^r are minimal will not be the same as the values of ω for which the b_n^r are minimal.) As in our previous discussion of the angular eigenvalue problem, the coefficients a_n^r will be minimal iff they satisfy the continued fraction equation

$$\frac{a_{n+1}^r}{a_n^r} = \frac{-\gamma_{n+1}^r}{\beta_{n+1}^r -}\,\frac{\alpha_{n+1}^r\gamma_{n+2}^r}{\beta_{n+2}^r -}\,\frac{\alpha_{n+2}^r\gamma_{n+3}^r}{\beta_{n+3}^r -}\,\ldots \tag{52}$$

which in turn will require that ω be a root of

$$0 = \beta_0^r - \frac{\alpha_0^r\gamma_1^r}{\beta_1^r -}\,\frac{\alpha_1^r\gamma_2^r}{\beta_2^r -}\,\frac{\alpha_2^r\gamma_3^r}{\beta_3^r -}\,\ldots \tag{53}$$

Here the α_n^r, β_n^r, and γ_n^r are defined as functions of ω in equations (41). Analogous equations can be written concerning the b_n^r and the $\tilde{\alpha}_n$, $\tilde{\beta}_n$, and $\tilde{\gamma}_n$ in the instances when eigensolutions of the type y_2 are desired.

In most physical situations both the α_n^θ, β_n^θ, and γ_n^θ for the angular eigenvalue equation (36) and the α_n^r, β_n^r, and γ_n^r for the radial eigenvalue equation (53) are functions of both the angular separation constant A_{lm} and of the frequency ω. This will then require the simultaneous solution of equations (36) and (53), which usually is not difficult numerically. Such solutions were demonstrated for the electronic spectra of the hydrogen molecule-ion by Hylleraas,[7] Jaffé,[8] and Baber and Hassé.[5] Analogous solutions for the quasi-normal modes of black holes are given by Leaver.[11] With use of eigensolutions of type y_2 a similar approach can be taken to the "algebraically special" black hole perturbations discussed by Chandrasekhar.[30]

C. Second Solutions by way of an Integral Transform

If we express the solutions to equation (1) near the singular point $x = x_0$ as

$$\lim_{x \to x_0} y(x) = (x - x_0)^{k_2} \tag{54}$$

then the exponent k_2 takes the values 0 and $1 - B_2 - B_1/x_0$. If $B_2 + B_1/x_0$ is not an integer, a second solution to equation (1) may be found through the substitution $y(x) = (x - x_0)^{1-B_2-B_1/x_0} g(x)$. The differential equation for g will be

$$\begin{aligned} x(x-x_0)g_{,xx} + [B_1 + (2 - B_2 - 2B_1/x_0)x]g_{,x} \ + \\ \{\omega^2 x(x-x_0) - [2\eta\omega + (1 - B_2 - B_1/x_0)B_1/x_0](x - x_0) + B_3\}g = 0 \end{aligned} \tag{55}$$

which is of the same form as equation (1), and a regular solution for f may be found by the method of Jaffé. If $B_2 + B_1/x_0$ is an integer, then a second solution to equation (38) may be found by the method of Frobenius. The expansion coefficients for the resulting second solution will obey an inhomogeneous three-term recurrence relation, and contain a free parameter that may be empirically adjusted to vary the amount of the first solution that appears in the second. This property is interesting, but the procedure is tedious and will not be dealt with here (see Rabenstein[31] for a discussion of Frobenius' method).

A more entertaining approach to the second solutions is open to those who remain curious about the equality of the Hylleraas and Jaffé expansion coefficients. Wilson[27] speculated that "the solution of (a generalized spheroidal wave equation) is probably expressible as a homogeneous integral equation." One such integral had already been given by Ince[32] for the particular parameters choice $\eta = \pm i(B_1+B_2)/2$, and although the contour used by Ince was $[-1, 1]$, his expressions can be made valid on $[1, \infty)$. Another integral relation for a different, though still specific, choice $\eta = \pm i(B_2/2 - 1)$ is arrived at through consideration of the equality of the Hylleraas and Jaffé expansion coefficients, and leads directly to a representation for a second solution to the differential equation as a series of irregular confluent hypergeometric functions. The new representation is valid for arbitrary η. The argument goes as follows:

Start with equation (1)

$$x(x-x_0)\frac{d^2y}{dx^2} + (B_1 + B_2 x)\frac{dy}{dx} + \left[\omega^2 x(x-x_0) - 2\eta\omega(x-x_0) + B_3\right] y = 0$$

and make the substitution $y = e^{i\omega x} f(x)$. The differential equation for $f(x)$ is

$$x(x-x_0)f_{,xx} + [B_1 + B_2 x + 2i\omega x(x-x_0)]f_{,x} + [(B_2 + 2i\eta)i\omega x + 2\eta\omega x_0 + i\omega B_1 + B_3]f = 0 \tag{56}$$

and f admits to the expansions

$$f(x) = \sum_{n=0}^{\infty} \frac{n! a_n^r}{\Gamma(\frac{1}{2}B_2 + i\eta + B_1/x_0 + 1 + n)} L_n^{B_2+B_1/x_0-1}(-2i\omega(x - x_0)) \tag{57}$$

(Hylleraas) and

$$\bar{f}(x) = x^{-\frac{1}{2}B_2 - i\eta} \sum_{n=0}^{\infty} a_n^r \left(\frac{x - x_0}{x}\right)^n \tag{58}$$

(Jaffé). The coefficients a_n^r are the same for each expansion and $\bar{f}(x)$ is proportional to $f(x)$ when both are eigenfunctions such that $\sum a_n^r$ converges. Specializing to the case $i\eta = B_2/2 - 1$, these expressions respectively become

$$f(x) = \sum_{n=0}^{\infty} \frac{n! a_n^r}{\Gamma(B_2 + B_1/x_0 + n)} L_n^{B_2+B_1/x_0-1}(-2i\omega(x - x_0)) \tag{59}$$

and

$$\bar{f}(x) = x^{1-B_2} \sum_{n=0}^{\infty} a_n^r \left(\frac{x - x_0}{x}\right)^n \quad . \tag{60}$$

Perusal of standard integral tables[33] reveals

$$\int_0^\infty e^{-st} t^\alpha \mathbf{L}_n^\alpha(t) dt = \frac{\Gamma(\alpha+n+1)}{n!}\, s^{-\alpha-1} \left(\frac{s-1}{s}\right)^n \quad , \tag{61}$$

so that with the associations $\alpha = B_2 + B_1/x_0 - 1,\ t = -2i\omega(x - x_0)$, and $s = x/x_0$, we conclude

$$\bar{f}(x) = x^{1+B_1/x_0} \int_c e^{2i\omega x(t-x_0)/x_0} (t - x_0)^{B_2+B_1/x_0-1} f(t) dt \tag{62}$$

for some contour c that includes x_0 and ∞. Multiplicative constants have been omitted from the integration. This result is verified *via* the theory of integral transforms in Appendix B. The important result of that derivation is the procurement of the bilinear concomitant

$$P(x,t) = \left\{ \begin{array}{c} t(t-x_0)[f(t)\frac{d}{dt}K(x,t) - K(x,t)\frac{d}{dt}f(t)] \quad + \\ \qquad (2i\omega t^2 + (B_2 + 2B_1/x_0 - 2i\omega x_0)t - B_1 - x_0)K(x,t)f(t) \end{array} \right\} \tag{63}$$

where the kernel $K(x,t)$ is given by

$$K(x,t) = e^{2i\omega x(t-x_0)/x_0} (t - x_0)^{-s_2}$$

and

$$s_2 = 1 - B_2 - B_1/x_0 \quad .$$

The exponent s_2 takes the second of the allowed values of k_2 of equation (54). The bilinear concomitant must vanish at each end of the integration contour.

On such an integration contour equation (62) is an integral relation among solutions $f(x)$ and $\bar{f}(x)$ to equation (56). This does not necessarily mean that f and $\bar{f}$ are the same solution to the differential equation, however. Equation (62) is an integral equation only for functions $f(x)$ that have the decreasing exponential behavior at $x = \infty$. If such an $f(x)$ should also happen to be regular at $x = x_0$, then $f(x)$ is an eigenfunction of equation (56) and one endpoint of the contour c can be taken directly to $t = x_0$. In this case $f(x)$ and $\bar{f}(x)$ are proportional and equation (62) becomes an integral equation for eigenfunctions. It may be noted that the quasi-normal modes of black holes can be described by this kind of eigenfunction, although the requirement $i\eta = B_2/2 - 1$ restricts the applicability of (62) to consideration only of scalar fields ($s = 0$ in equations (11) and (19)).

The integration contour c is determined by the requirement that the bilinear concomitant $P(x,t)$ vanish at its endpoints. If $f(x) \to (x - x_0)^{s_i}$ as $x \to x_0$, then the allowed values for the exponent s_i are $s_1 = 0$ and $s_2 = 1 - B_2 - B_1/x_0$. We consider two general cases:

i. $f(x) \stackrel{x \to x_0}{\longrightarrow}$ (constant) and either $Re(s_2) < 0$ or $s_2 = 0$. In this case $P(x,t)$ vanishes at $t = x_0$ and the contour c may be taken to be that shown in Figure 1a. The approach angle θ is chosen such that $Re(2i\omega xt/x_0) < 0$. The kernel $K(x,t)$ is then an exponentially decreasing function of x and equation (62) expresses the solution $\bar{f}(x)$ regular as $x \to \infty$ in terms of the solution $f(t)$ that is regular as $t \to x_0$. If $f(t)$ is also regular as $t \to \infty$, then ω is an eigenfrequency, $\bar{f}$ is proportional to f, and equation (62) becomes an integral equation for the eigenfunctions. We can see how this works by substituting the Jaffé expansion for $f(t)$ into equation (62):

$$\bar{f}(x) = x^{1+B_1/x_0} \int_{x_0}^\infty e^{2i\omega x(t-x_0)/x_0} (t - x_0)^{-s_2} t^{1-B_2} \left[\sum_{n=0}^\infty a_n^r \left(\frac{t - x_0}{t}\right)^n \right] dt \tag{64}$$

The behavior of $\bar{f}(x)$ near $x = x_0$ is determined by the large t behavior of the integrand. If ω is an eigenfrequency the series $\sum a_n^r[(t - x_0)/t]^n$ is uniformly convergent as $t \to \infty$ and the integral for large t, $x \to x_0$, looks like

$$\bar{f}(x) \stackrel{x \to x_0}{\longrightarrow} x^{1+B_1/x_0} \int^\infty e^{2i\omega x(t-x_0)/x_0} t^{B_1/x_0} dt$$

(since $s_2 = 1 - B_2 - B_1/x_0$) and is always finite with the aforementioned choice of approach angle θ. Hence $\bar{f}(x)$ is finite as $x \to x_0$. If ω is not an eigenfrequency then $\sum a_n^r (t-x_0)/t)^n \stackrel{t\to\infty}{\longrightarrow} t^{B_2-2} e^{-2i\omega t}$, the integral looks like

$$\bar{f}(x) \stackrel{x\to x_0}{\longrightarrow} x^{1+B_1/x_0} \int^{\infty} e^{2i\omega(x-x_0)t/x_0} t^{-s_2-1} dt$$

and

$$\lim_{x\to x_0} \bar{f}(x) \sim (x-x_0)^{s_2}$$

as required for the independent second solution. Note that while in physical contexts the variable x is a spatial coordinate and is positive and real, the flexibility afforded in the choice of the approach angle allows equation (62) to describe functions f for which $Im(\omega) \leq 0$.

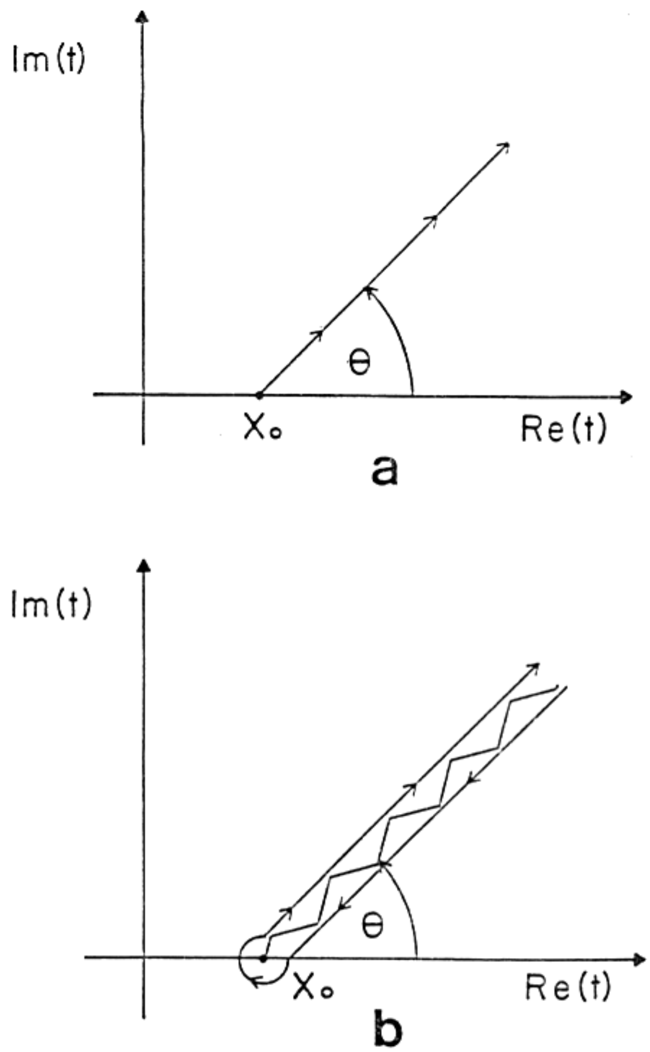

Figure 1: Contours for use with integral relation (62).

ii. $f(x) \stackrel{x \to x_0}{\longrightarrow} (x - x_0)^{s_2}$ or $Re(s_2) > 0$. Note that the restriction $Re(s_2) > 0$ is artificial, since one can always obtain $Re(s_2) < 0$ for a function $g(x)$ by substituting $f(x) = (x - x_0)^{s_2} g(x)$ in equation (56). Either way $P(x,t)$ is not zero at $t = x_0$ and the contour c is chosen to be that illustrated in Figure 1b. This contour has the appearance of being all-purpose and do-everything, but we shall see that if one actually had the information necessary to use it, one would also have the information to convert the problem to that considered in case(1) above, and would end up using the contour of Figure 1a.

The branch cut arises from the factor $(t - x_0)^{-s_2}$ in $K(x,t)$ if s_2 is not an integer, and from the logrithmic term inherent in f if s_2 is an integer. The function $\bar{f}(x)$ is regular as $x \to \infty$ regardless of the behavior of $f(t)$, so that given any solution $f(x)$ to equation (56), equation (62) will always give the solution $\bar{f}(x)$ that is regular as $x \to \infty$ for the chosen contour c. On this contour equation (62) is an integral equation for all functions f that are regular at $t = \infty$, but is of limited computational utility as an integral equation for non-eigenfunctions because a solution that is irregular at $x = x_0$ and regular at $x = \infty$ must be a weighted sum of two component functions, one regular and the other irregular at $x = x_0$, and both irregular at $x = \infty$. Detailed knowledge of the weighting factors in the sum is necessary, since the product of only one of the component functions and the kernel $K(x,t)$ will contribute to the integral. The product of the other component function and the kernel will have the same value on each side of the branch cut, and will give no contribution.

To see how this works, first consider s_2 not an integer. Then $f(t)$ can be written

$$f(t) = t^{1-B_2} \left[\sum_{n=0}^{\infty} a_n^r \left(\frac{t - x_0}{t} \right)^n + (t - x_0)^{s_2} \sum_{n=0}^{\infty} b_n^r \left(\frac{t - x_0}{t} \right)^n \right] \tag{65}$$

which is just the sum of two independent Jaffé solutions. Only the product of $K(x,t)$ and the function corresponding to the first sum will contribute to the integral, and if that function were known (i.e., if we knew the value of a_0^r), we could use case (1) above. Similarly, if s_2 is an integer, then any solution irregular at x_0 is expressible as

$$f(t) = t^{1-B_2} \left[\log \left(\frac{t - x_0}{t} \right) \sum_{n=0}^{\infty} a_n^r \left(\frac{t - x_0}{t} \right)^n + (t - x_0)^{s_2} \sum_{n=0}^{\infty} b_n^r \left(\frac{t - x_0}{t} \right)^n \right] \tag{66}$$

which is the form of the second Jaffé solution as obtained by the method of Frobenius. Here again only the product of $K(x,t)$ and the term containing the first sum will contribute to the integral. If the product of the logarithm and the first solution were known we again would revert to case (1) since the difference of the logarithm across the branch cut is just the constant $2\pi i$, and the integrand becomes effectively integrable at x_0. Either way we are required to know the function that is regular at $x = x_0$ in order to evaluate the difference across the branch cut, and if that solution is known (such as by Jaffé's method), then the problem reduces to the one considered in case (1).

As noted previously, Hylleraas' expansion converges only when ω is a purely imaginary eigenfrequency. We have shown how in that case the relation of the Hylleraas expansion coefficients to the Jaffé coefficients leads to an integral equation for eigenfunctions (at least when $i\eta = B_2/2 - 1$) and how, when ω is not an eigenfrequency, the same integral will transform the first solution that is regular at $x = x_0$ into a second independent solution that is regular at $x = \infty$. Jaffé's method always gives a convergent expansion for the regular first solution, and it is interesting to examine the result of transforming Jaffé's expansion term by term.

We interchange the summation and the integration to explicitly evaluate the the right hand side of equation (64):

$$
\begin{aligned}
\bar{f}(x) &= x^{1+B_1/x_0}\sum_{n=0}^{\infty} a_n^r \left\{\int_{x_0}^{\infty} e^{2i\omega x(t-x_0)/x_0} t^{1-B_2-n}(t-x_0)^{B_2+B_1/x_0+n-1}dt\right\} \\
&= x^{1+B_1/x_0}\sum_{n=0}^{\infty} a_n^r \Gamma(B_2+B_1/x_0+n)U(B_2+B_1/x_0+n, 2+B_1/x_0, -2i\omega x) \qquad (67) \\
&= \sum_{n=0}^{\infty} a_n^r \Gamma(B_2+B_1/x_0+n)U(B_2-1+n, -B_1/x_0, -2i\omega x) \quad .
\end{aligned}
$$

Here $U(a,b,z)$ is the irregular confluent hypergeometric function defined by the integral representation

$$\Gamma(a)U(a,b,z) = \int_0^{\infty} e^{-zt}t^{a-1}(t+1)^{b-a-1}dt \qquad (68)$$

and obeys the Kummer relation[28]

$$U(a,b,z) = z^{1-b}U(1+a-b, 2-b, z) \quad . \qquad (69)$$

The normalization in $\bar{f}(x)$ is not important here, and the constant multiplying factors were dropped during the integration.

The last of equations (67) may also be arrived at by the usual eigenfunction expansion method of solving ordinary differential equations (see Appendix C), which produces a result that holds for arbitrary η:

$$\bar{f}(x) = \sum_{n=0}^{\infty} a_n^r \Gamma(B_2+B_1/x_0+n)U(B_2/2+i\eta+n, -B_1/x_0, -2i\omega x) \quad . \qquad (70)$$

The expansion coefficients a_n^r are the same as Jaffé's (equation (41)), and since $y(x) = e^{i\omega x}\bar{f}(x)$, we now have a second independent solution to the generalized spheroidal wave equation (1). Expansion (70) is absolutely convergent on any interval bounded away from x_0, is uniformly convergent as $x \to \infty$, diverges at $x = x_0$ when ω is not an eigenfrequency, and is uniformly convergent as $x \to x_0$ when ω is an eigenfrequency.

The derivations for the second solutions may again be repeated with the substitutions $y(x) = e^{-i\omega x}f(x)$. We then have our first four convergent representations for solutions to the generalized spheroidal wave equation:

$$y_1(x) = e^{+i\omega x}x^{-B_2/2-i\eta}\sum_{n=0}^{\infty} a_n^r \left(\frac{x-x_0}{x}\right)^n \qquad (71)$$

$$y_2(x) = e^{-i\omega x}x^{-B_2/2+i\eta}\sum_{n=0}^{\infty} b_n^r \left(\frac{x-x_0}{x}\right)^n \qquad (72)$$

$$y_3(x) = e^{+i\omega x}\sum_{n=0}^{\infty} a_n^r (B_2+B_1/x_0)_n U(\tfrac{1}{2}B_2+i\eta+n, -B_1/x_0, -2i\omega x) \qquad (73)$$

$$y_4(x) = e^{-i\omega x}\sum_{n=0}^{\infty} b_n^r (B_2+B_1/x_0)_n U(\tfrac{1}{2}B_2-i\eta+n, -B_1/x_0, +2i\omega x) \quad . \qquad (74)$$

Here y_3 and y_4 have been normalized by a factor $1/\Gamma(B_2+B_1/x_0)$ and $(z)_n \equiv \Gamma(z+n)/\Gamma(z)$ is Pochhammer's symbol. The a_n^r are defined by equations (40) and (41), and the b_n^r by equations (50) and (51). The solutions $y_1(x)$ and $y_2(x)$ are both regular as $x \to x_0$, and are proportional by the factor $e^{2i\omega x_0}a_0^r/b_0^r$.

However, convergence properties and growth behavior of individual terms in the series will differ markedly if $Im(\omega)$ is not zero. Solutions $y_3(x)$ and $y_4(x)$ are independent and are both irregular as $x \to x_0$ when ω is not an eigenfrequency. When ω is an eigenfrequency then one or the other of $y_3(x)$ and $y_4(x)$ will be regular at $x = x_0$ (see Appendix C). Solutions $y_3(x)$ and $y_4(x)$ should have the limiting forms

$$\lim_{|x|\to\infty} y_3(x) = a_0^r x^{-\frac{1}{2}B_2} e^{+i(\omega x - \eta \ln x)} \tag{75}$$

and

$$\lim_{|x|\to\infty} y_4(x) = b_0^r x^{-\frac{1}{2}B_2} e^{-i(\omega x - \eta \ln x)} \tag{76}$$

(see Slater,[28] equation 13.5.2). Although I have made extensive computational use of equations (71) and (72) — they are the basis of my standard algorithm for generating regular solutions to the generalized spheroidal wave equation near $x = x_0$ — I have not yet (as of July, 1985) been able to verify expansions (73) and (74) and their asymptotic forms (75) and (76) with a computer. But they do look as if they might be useful.

D. Computational Limitations of the Jaffé Solutions

As might be expected, the absolute convergence property of Jaffé's expansion makes (39) an extremely useful expression for the numerical evaluation of the generalized spheroidal wavefunction that is regular at $x = x_0$, and for those eigenfunctions for which convergence is uniform it provides the algorithm of choice. However, for arbitrary ω the a_n^r are dominant, and it behooves one to graph the behavior of the sequence $\{a_n^r[(x-x_0)/x]^n : n = 0, 1, 2\ldots\}$ as a function of n before concluding one really can sum its terms. Assume that the a_n are dominant. If the sequence is normalized such that $a_0^r = 1$, the sum

$$\sum_{n=0}^{\infty} a_n^r \left(\frac{x - x_0}{x}\right)^n$$

will typically have magnitude of $\mathcal{O}(1 + |\omega^{-1}|)$. For a rough estimate ignore the n^b term in equation (46). Then for large x

$$\lim_{n\to\infty} \left| a_n^r \left(\frac{x - x_0}{x}\right)^n \right| \approx \left|\frac{x - x_0}{x}\right|^n \left| e^{2\rho\sqrt{n}} \right| \quad , \tag{77}$$

(where $\rho = \sqrt{-2i\omega x_0}$), and $|a_n^r[(x-x_0)/x]^n|$ has a maximum at $n_{max} \approx (\rho x/x_0)^2$. To give an idea of the numerical problems lurking in wait of the unwary, consider the not unreasonable case of $\rho = 1$, $x/x_0 = 5$. Then $n_{max} \approx 25$ and

$$a_{n_{max}}^r \left(\frac{x - x_0}{x}\right)^{n_{max}} \approx 80$$

which is only two orders of magnitude greater than the sum of all the terms. But if $x/x_0 = 20$

$$a_{n_{max}}^r \left(\frac{x - x_0}{x}\right)^{n_{max}} \approx 3 \times 10^8$$

and rounding considerations dictate the use of extended precision if the series (39) is to be summed with any accuracy.

V. THE STRATTON SOLUTIONS TO THE ORDINARY SPHEROIDAL WAVE EQUATION, AND A PRELIMINARY GENERALIZATION

The separated parts of the one-particle Schrödinger equation simplify in free space where there is no potential and $N_1 = N_2 = 0$. Equations (2) and (3) are then the same as those resulting from the separation of the Helmholtz equation in spheroidal coordinates, and Stratton's[34] representations of the ordinary spheroidal wave functions are a natural starting point for investigation of solutions to more general forms of the equation. I was originally attracted to Morse's spherical Bessel function expansion for two reasons. First, the asymptotic magnitude and phase of any convergent series of spherical Hankel functions $\sum a_n h_n^{(1)}(z)$ or $\sum a_n h_n^{(2)}(z)$ can readily be calculated. Second, numerical algorithms to generate Bessel functions for a variety of orders and a wide range of magnitudes of the argument are reasonably well understood. The first property will be dealt with in full generality in Sec. VI. The second will be touched upon in the Summary. The present section reviews the Stratton representation for ordinary spheroidal wavefunctions, and generalizes it to the case of the equations that arise for an electron in the field of a finite dipole: $N_1 = -N_2 \neq 0$. A detailed discussion of convergence properties is given which will serve as a model for the convergence proofs of the general Coulomb wavefunction expansions presented in section VI, and which (I hope) will dispel misconceptions concerning the convergence of Stratton's solutions to the ordinary spheroidal wave equation.

A. The Ordinary Spheroidal Wave Equation

The ordinary spheroidal wave equation results from the separation of the Helmholtz and free-particle Schrödinger equations in spheroidal coordinates. It is a special case of equations (2) and (3) for which N_1 and N_2 are both zero, and for which equations (2) and (3) become the same. The angular equation (3) simplifies to

$$\frac{d}{d\mu}\left[(1-\mu^2)\frac{d\Phi}{d\mu}\right] + \left[-\omega^2\mu^2 + A_{lm} - \frac{m^2}{1-\mu^2}\right]\Phi = 0 \quad , \tag{78}$$

and the solution function $\Phi(\mu)$ can be expanded in a series of Gegenbauer polynomials[35]:

$$\Phi(\mu) = (1-\mu^2)^{m/2} \sum_{n=0,1}^{\infty}{}' d_n T_n^m(\mu) \quad . \tag{79}$$

The " $'$ " indicates the sum is to be taken over even values of n if l is even and over odd values of n if l is odd. The Gegenbaur polynomials are generated[36] by

$$\sum_{n=0}^{\infty} h^n T_n^m(z) = \frac{2^m \Gamma(m+\frac{1}{2})}{\sqrt{\pi}(1+h^2-2hz)^{m+\frac{1}{2}}} \qquad (|h|<1) \quad ,$$

and are related to the regular Gauss hypergeometric series ${}_2F_1$ by

$$T_n^m(z) = \frac{(n+2m)!}{2^m n! m!}\, {}_2F_1\left(n+2m+1, -n; m+1; \frac{1-z}{2}\right) \quad .$$

The expansion coefficients $\{d_n : n = 0, 2, 4\ldots \text{ or } n = 1, 3, 5\ldots\}$ obey the recurrence relation[37]

$$\begin{aligned} \alpha_0 d_2 \quad + \beta_0 d_0 &= 0 \\ \alpha_1 d_3 \quad + \beta_1 d_1 &= 0 \\ \alpha_n d_{n+2} + \beta_n d_n + \gamma_n d_{n-2} &= 0 \quad n = 2, 3, 4\ldots \end{aligned}$$

where

$$\begin{aligned}\alpha_n &= \omega^2\frac{(n+2m+1)(n+2m+2)}{(2n+2m+3)(2n+2m+5)}\\ \beta_n &= \omega^2\frac{2[(n+m)(n+m+1)-m^2]-1}{(2n+2m+3)(2n+2m-1)}+(n+m)(n+m+1)-A_{lm} \\ \gamma_n &= \omega^2\frac{n(n-1)}{(2n+2m-1)(2n+2m-3)}\end{aligned} \tag{80}$$

In order for the series to converge at $\mu = \pm 1$, the separation constant A_{lm} must be chosen such that the d_n are minimal and the continued fraction equation

$$\beta_0 = \frac{\alpha_0\gamma_2}{\beta_2 -}\,\frac{\alpha_2\gamma_4}{\beta_4 -}\,\frac{\alpha_4\gamma_6}{\beta_6 -}\ldots \tag{81}$$

is satisfied.

The simplified spheroidal radial equation (2) becomes

$$\frac{d}{d\lambda}\left[(\lambda^2-1)\frac{d\Psi}{d\lambda}\right]+\left[\omega^2\lambda^2 - A_{lm} - \frac{m^2}{\lambda^2-1}\right]\Psi = 0 \tag{82}$$

which is the same as (78) but in the coordinate λ instead of μ. Next, if $\Phi(\mu)$ is a solution to (78), then

$$\Psi(\lambda) = (\lambda^2-1)^{m/2}\int_{-1}^{+1} e^{i\omega\lambda\mu}(1-\mu^2)^{m/2}\Phi(\mu)d\mu \tag{83}$$

is a solution also, but in the variable λ (Ince, page 201). Integrating the series (79) for Φ term by term and using the relation

$$\int_{-1}^{+1} e^{i\omega zt}(1-t^2)^m T_n^m(t)dt = i^n\frac{2(n+2m)!}{n!(\omega z)^m}j_{n+m}(\omega z)$$

(Morse and Feshbach, page 643 — the j_{n+m} are spherical Bessel functions), we obtain the final result

$$\Psi(\lambda) = \left(\frac{\lambda^2-1}{\lambda^2}\right)^{\frac{m}{2}}\sum_{n=0,1}^{\infty}{}' i^n d_n\frac{(n+2m)!}{n!}j_{n+m}(\omega\lambda) \tag{84}$$

(see Morse and Feshbach, Eq. 11.3.91. We have left off the normalization factors). The d_n are the same as in the expansion (79) for Φ and satisfy recurrence relation (80). A second solution to equation (82) is obtained by substituting the irregular spherical Bessel functions $y_n(\omega\lambda)$ in place of the $j_n(\omega\lambda)$ in expression (84).

The convergence properties of both solutions will be discussed in Sec. Vc. The important point for now is that the series (84) converges only if the d_n form a minimal solution to the recurrence relation (80), which can happen only for specific values of the parameter A_{lm}.

B. Preliminary Generalization: Schrodinger's Equation for an Electron in the Field of a Finite Dipole

The simplest generalization of the ordinary spheroidal wave equation is the removal of the freedom to choose A_{lm}. The physical context wherein this complexity arises is the separation of the Schrödinger equation for an electron in the dipole field of two fixed but oppositely charged nuclei. In this consideration $N_2 = -N_1$ in equations (2) and(3), so that equation (2) still simplifies to equation (82). However, equation (3) becomes more complicated, and while it is still readily solvable by the power series method described in Sec. III, the resulting separation constant A_{lm} is now dependent on the dipole moment $2aN_1$ in addition to ω. If we again try to expand the solution to equation (82) as

$$\Psi(\lambda) = \left(\frac{\lambda^2-1}{\lambda^2}\right)^{\frac{m}{2}}\sum_{n=0,1}^{\infty}{}' i^n d_n\frac{(n+2m)!}{n!}j_{n+m}(\omega\lambda) \tag{85}$$

we find that although the d_n still satisfy the recurrence relation (80), they will in general form a dominant solution sequence since A_{lm} can no longer have a value that will force them to be minimal. The series (85) will then diverge.

The convergence problem can be solved if we can find some other parameter in the recurrence relation that may be adjusted so that the expansion coefficients d_n form a minimal solution sequence. There are no free parameters left in the differential equation (82) itself, so a new parameter must be introduced in the representation of the solution. Consideration of the physical problem of the electron in the dipole field leads to the suspicion that the natural choice for such a parameter will have something to do with the asymptotic phase of the solution function $\Psi(\lambda)$, since the asymptotic phase of the Schrödinger wave function will be shifted as the dipole moment $2aN_1$ of the source potential increases away from zero. Specifically, a solution to equation (82) for arbitrary values of A_{lm} and ω may be expressed as a generalized Neumann expansion[38]:

$$\Psi_1(\lambda) = \left(\frac{\lambda^2 - 1}{\lambda^2}\right)^{\frac{m}{2}} \sum_{L=-\infty}^{\infty}{}' a_L j_{L+\nu}(\omega\lambda) \quad . \tag{86}$$

The $j_{L+\nu}$ are again spherical Bessel functions. A second solution may be obtained by substituting the irregular spherical Bessel functions $y_{L+\nu}$ for the $j_{L+\nu}$:

$$\Psi_2(\lambda) = \left(\frac{\lambda^2 - 1}{\lambda^2}\right)^{\frac{m}{2}} \sum_{L=-\infty}^{\infty}{}' a_L y_{L+\nu}(\omega\lambda) \quad . \tag{87}$$

The phase (or order) parameter ν in expansions (86) and (87) is free to be adjusted to make the a_L minimal, and thus to obtain convergence of the series. The recurrence relation obeyed by the a_L is

$$\alpha_L a_{L+2} + \beta_L a_L + \gamma_L a_{L-2} = 0 \quad , \tag{88}$$

where

$$\begin{aligned}
\alpha_L &= -\omega^2 \frac{(L+\nu-m+1)(L+\nu-m+2)}{(2L+2\nu+3)(2L+2\nu+5)} \\
\beta_L &= +\omega^2 \left[\frac{2[(L+\nu)(L+\nu+1)-m^2]-1}{(2L+2\nu-1)(2L+2\nu+3)}\right] + (L+\nu)(L+\nu+1) - A_{lm} \\
\gamma_L &= -\omega^2 \frac{(L+\nu+m)(L+\nu+m-1)}{(2L+2\nu-1)(2L+2\nu-3)} \quad .
\end{aligned}$$

If ν should equal m, then this recurrence relation is exactly the same as the recurrence relation (80) obeyed by the d_n if we make the substitution $a_L = i^L[(L+2m)!/L!]d_L$. In this case the series (86) must be started at $L = 0$ or $L = 1$ instead of $L = -\infty$, and the solution representation (86) reduces to the representation (84) for the ordinary spheroidal wave functions. Convergence properties of the two representations are therefore the same.

In the more general case when $N_1 = -N_2 \neq 0$, the values of the parameter ν for which the series (86) and (87) converge will not be integers, and the sequence $\{a_L : L = \ldots -2, -1, 0, +1, +2 \ldots\}$ must be made minimal both as $L \to \infty$ and as $L \to -\infty$. The ratios of successive a_L must then satisfy both

$$\frac{a_L}{a_{L-2}} = \frac{-\gamma_L}{\beta_L -}\ \frac{\alpha_L \gamma_{L+2}}{\beta_{L+2} -}\ \frac{\alpha_{L+2}\gamma_{L+4}}{\beta_{L+4} -}\ \ldots \tag{89}$$

for $L = +2, +4, +6 \ldots$ and

$$\frac{a_L}{a_{L+2}} = \frac{-\alpha_L}{\beta_L -}\ \frac{\alpha_{L-2} \gamma_L}{\beta_{L-2} -}\ \frac{\alpha_{L-4}\gamma_{L-2}}{\beta_{L-4} -}\ \ldots \tag{90}$$

for $L = -2, -4, -6\ldots$ The recursion equation at $L = 0$ requires

$$\beta_0 = -\alpha_0 \frac{a_2}{a_0} - \gamma_0 \frac{a_{-2}}{a_0} \quad . \tag{91}$$

Substituting the right hand sides of equations (89) and (90) into (91), we obtain an implicit characteristic equation for ν that must be satisfied if the series (86) is to converge[38]:

$$\beta_0 = \left\{ \begin{array}{c} \dfrac{\alpha_{-2}\gamma_0}{\beta_{-2}-} \, \dfrac{\alpha_{-4}\gamma_{-2}}{\beta_{-4}-} \, \dfrac{\alpha_{-6}\gamma_{-4}}{\beta_{-6}-} \ldots \\ + \\ \dfrac{\alpha_0\gamma_2}{\beta_2-} \, \dfrac{\alpha_2\gamma_4}{\beta_4-} \, \dfrac{\alpha_4\gamma_6}{\beta_6-} \ldots \end{array} \right\} \tag{92}$$

The α_L, β_L, and γ_L are given by equations (88).

Existence and Uniqueness: I do not have a formal proof that equation (92) actually has solutions in the parameter ν. However, solutions can be found numerically, so they must exist. Expansions (86) and (87) must reduce to the solutions (84) in the limit as the dipole moment $2aN_1$ goes to zero, so $\nu = m$ must be a solution to (92) at that limit. Knowing the approximate location of a root to a nonlinear equation is the first step towards finding it, and it is not difficult to start at a given ω with $\nu = m$, $N_1 = -N_2 = 0$, A_{lm} an eigenvalue of the ordinary prolate spheroidal wave equation, and then track the values of ν that solve equation (92) as the dipole moment is gradually increased.

The solutions ν are not unique, but rather are periodic with period 1: if ν is a solution to equation (92), then so is $\nu \pm n$, where n is any integer. The correct choice of ν depends on how the coefficients a_L are generated. The a_L are to be minimal as $L \to \pm\infty$, and if the a_L are generated by forward recursion from $L = -\infty$ upward to $L = 0$ and by backward recursion from $L = +\infty$ downward to $L = 0$, then the largest a_L will be $a_{\max} = a_0$. As $\omega \to 0$ this $a_{\max} = a_0$ becomes the only coefficient that contributes to the series, and *with this choice* of $a_{\max} = a_0$ the correct limiting value of ν as the dipole moment $2aN_1$ reduces to zero is $\nu = l + m$. Solutions ν that do not reduce to $l + m$ as $2aN_1 \to 0$ are spurious: they will enable expansions (86) and (87) to converge, but the resulting expressions will not solve the differential equation. That $\nu = l+m$ is the correct limit as $\omega \to 0$ or as $2aN_1 \to 0$ will be demonstrated at the end of the section. This value may appear inconsistent with expansion (84), but it is not. For $|\omega| \ll 1$ the d_n of (84) will have a maximum at $d_{\max} = d_l$ or d_{l-1}, and for $2aN_1 = 0$ and $\omega \neq 0$ the a_L of (86) will become zero only for $L < -l$ or $-l+1$. The two expansions are the same: it is only the indexing that is different.

C. Convergence Properties

To establish the convergence of the series (86) and (87) it is necessary to examine the ratios

$$\lim_{L \to \pm\infty} \frac{a_L f_{L+\nu}(\omega\lambda)}{a_{L-2} f_{L+\nu-2}(\omega\lambda)}$$

where $f_{L+\nu}$ is either $j_{L+\nu}$ or $y_{L+\nu}$. We assume that ν has been chosen to satisfy equation (92), so that the a_L are minimal as $L \to \pm\infty$ and have the limiting behavior

$$\lim_{L \to +\infty} \frac{a_L}{a_{L-2}} = \frac{\omega^2}{4L^2} \left[1 - \frac{2\nu+1}{L} + \mathcal{O}(1/L^2) \right]$$

and

$$\lim_{L \to -\infty} \frac{a_L}{a_{L+2}} = \frac{\omega^2}{4L^2} \left[1 - \frac{2\nu+1}{L} + \mathcal{O}(1/L^2) \right] \quad . \tag{93}$$

The $j_{L+\nu}$ and the $y_{L+\nu}$ are both solutions to the recurrence relation

$$\begin{aligned} &\frac{1}{2L+2\nu+3} f_{L+\nu+2} \\ &\quad + \frac{1}{2L+2\nu-1} f_{L+\nu-2} \\ &\qquad + \left[\frac{4L+4\nu+2}{(2L+2\nu+3)(2L+2\nu-1)} - \frac{2L+2\nu+1}{\omega^2\lambda^2} \right] f_{L+\nu} = 0 \quad , \end{aligned} \tag{94}$$

the $j_{L+\nu}$ being the particular solution sequence that is minimal as $L \to +\infty$. In general the $j_{L+\nu}$ and the $y_{L+\nu}$ will both be dominant as $L \to -\infty$ (the exception being the inconsequential case when ν is an odd multiple of $1/2$), and we consider the following three cases:

1. $f_{L+\nu}(\omega\lambda) = j_{L+\nu}(\omega\lambda)$ and $L \to +\infty$. From equation (94) the ratio $j_{L+\nu}/j_{L+\nu-2}$ has the limiting forms:

$$\lim_{L\to\infty} \frac{j_{L+\nu}(\omega\lambda)}{j_{L+\nu-2}(\omega\lambda)} = \begin{cases} \dfrac{\omega^2\lambda^2}{4L^2}\left[1 - \dfrac{2\nu}{L} + \mathcal{O}(1/L^2)\right] & (L \gg |\omega\lambda|) \\ -1 & (L \ll |\omega\lambda|) \end{cases}$$

In either case

$$\lim_{L\to\infty} \left| \frac{a_L j_{L+\nu}(\omega\lambda)}{a_{L-2} j_{L+\nu-2}(\omega\lambda)} \right| < \left| \frac{\omega^2}{4L^2} \right| \quad , \tag{95}$$

and this part of the series is absolutely convergent for all λ. If ν is an integer the negative L part of the series (86) truncates, and (95) describes the convergence of the regular solution (84) to the ordinary spheroidal wave equation.

2. $f_{L+\nu}(\omega\lambda) = y_{L+\nu}(\omega\lambda)$ and $L \to +\infty$. Again from equation (94) we find

$$\lim_{L\to\infty} \frac{y_{L+\nu}(\omega\lambda)}{y_{L+\nu-2}(\omega\lambda)} = \begin{cases} \dfrac{4L^2}{\omega^2\lambda^2}\left[1 + \dfrac{2\nu}{L} + \mathcal{O}(1/L^2)\right] & (L \gg |\omega\lambda|) \\ -1 & (L \ll |\omega\lambda|) \end{cases}$$

Hence

$$\lim_{L\to\infty} \frac{a_L y_{L+\nu}(\omega\lambda)}{a_{L-2} y_{L+\nu-2}(\omega\lambda)} = \begin{cases} \dfrac{1}{\lambda^2}\left[1 - \dfrac{1}{L} + \mathcal{O}(1/L^2)\right] & (L \gg |\omega\lambda|) \\ -\dfrac{\omega^2}{4L^2} & (L \ll |\omega\lambda|) \end{cases}$$

and the series (87) converges rapidly for large λ and mediocre ω, but diverges when $|\lambda| = 1$. Explicitly:

For every λ such that $|\lambda| > 1$ and for every $\epsilon > 0$ there exits an $N(\omega, \lambda, \epsilon)$ such that

$$\sum_{L=N}^{\infty}{}' a_L y_{L+\nu}(\omega\lambda) < \epsilon \; .$$

For each $\epsilon > 0$, N will increase without bound as $\lambda \to 1$.

Contrary assertions[39] notwithstanding, $\sum' a_L y_{L+\lambda}(\omega\lambda)$ is absolutely convergent for all $|\lambda| > 1$, and is in no sense asymptotic: N does not go to zero as $\lambda \to \infty$. This convergence was demonstrated numerically by Sinha and MacPhie,[40] but to my knowledge the present analysis constitutes the first rigorous proof. Jen and Hu[41] have recently derived accurate approximations for the ordinary spheroidal wave functions (both regular and irregular) that are rapidly convergent for large values of ω, where the convergence of Stratton's expansion is rather slow.

3. $f_{L+\nu}(\omega\lambda) = j_{L+\nu}(\omega\lambda)$ or $f_{L+\nu}(\omega\lambda) = y_{L+\nu}(\omega\lambda)$ and $L \to -\infty$. This case is similar to the one just discussed. Equation (94) once more yields

$$\lim_{L\to-\infty} \frac{f_{L+\nu}(\omega\lambda)}{f_{L+\nu+2}(\omega\lambda)} = \begin{cases} \dfrac{4L^2}{\omega^2\lambda^2}\left[1 + \dfrac{2\nu+4}{L} + \mathcal{O}(1/L^2)\right] & (|L| \gg |\omega\lambda|) \\ -1 & (|L| \ll |\omega\lambda|) \end{cases}$$

which together with equation (93) gives

$$\lim_{L\to-\infty} \frac{a_L f_{L+\nu}(\omega\lambda)}{a_{L+2} f_{L+\nu+2}(\omega\lambda)} = \begin{cases} \dfrac{1}{\lambda^2}\left[1 + \dfrac{3}{L} + \mathcal{O}(1/L^2)\right] & (|L| \gg |\omega\lambda|) \\ -\dfrac{\omega^2}{4L^2} & (|L| \ll |\omega\lambda|) \end{cases} .$$

Therefore the negative L part of either series (86) or (87) behaves like the positive L part of the series (87) discussed previously, and series (86) and (87) are two independent and convergent irregular solutions to our preliminary generalization of the ordinary spheroidal wave equation.

D. Solutions as $\omega \to 0$

1. $N_1 = -N_2 = 0$. When $N_1 = -N_2 = 0$ and ω is very small, equation (78) reduces to

$$\frac{d}{d\mu}\left[(1-\mu^2)\frac{d\Phi}{d\mu}\right] + \left[A_{lm} - \frac{m^2}{1-\mu^2}\right]\Phi = 0 \tag{96}$$

and with the substitution $\Phi(\mu) = (1-\mu^2)^{m/2} g(\mu)$ the differential equation for g becomes

$$(1-\mu^2) g_{,\mu\mu} - 2(m+1)\mu g_{,\mu} - [m(m+1) - A_{lm}]\, g = 0 \ . \tag{97}$$

Hence

$$\lim_{\omega\to 0} \Phi(\mu) = (1-\mu^2)^{m/2} T_l^m(\mu) \ .$$

and

$$\lim_{\omega\to 0} A_{lm} = (l+m)(l+m+1) \ .$$

This limiting value for A_{lm} may also be obtained by setting $\omega = 0$ and $B_2 = 2m+2$ in equation (27), then finding the B_3 that truncates the series (25) by making $\beta_l^\theta = 0$. Equation (83) then gives

$$\lim_{\omega\to 0} \Psi(\lambda) = \left(\frac{\lambda^2 - 1}{\lambda^2}\right)^{\frac{m}{2}} j_{l+m}(\omega\lambda)$$

and we must have $\nu \to l + m$ as $\omega \to 0$ when N_1 and N_2 are zero if we are to keep a_0 the maximum term in series (86).

2. $N_1 = -N_2 \neq 0$. By equations (89) and (90) we see that if we fix the largest expansion coefficient to be $a_{\max} = a_0 = 1$ in (86), then all the other a_L must become zero as $\omega \to 0$ and the series will reduce to the single term

$$\lim_{\omega\to 0} \Psi_1(\lambda) = \left(\frac{\lambda^2 - 1}{\lambda^2}\right)^{\frac{m}{2}} a_0 j_{\nu_0}(\omega\lambda) \ . \tag{98}$$

This single term must also suffice as $\omega\lambda \to \infty$ ($|\omega|$ still $\ll 1$), and ν_0 may be determined by looking at this limit. Asymptotic solutions to equation (82) are

$$\lim_{\lambda\to\infty} \Psi_1(\lambda) = \left(\frac{\lambda+1}{\lambda-1}\right)^{\frac{1}{2}} j_{\nu_a}(\omega(\lambda+1)) \quad [1 + \mathcal{O}(\lambda^{-3})] \tag{99}$$

and

$$\lim_{\lambda\to\infty} \Psi_2(\lambda) = \left(\frac{\lambda+1}{\lambda-1}\right)^{\frac{1}{2}} y_{\nu_a}(\omega(\lambda+1)) \quad [1+\mathcal{O}(\lambda^{-3})] \tag{100}$$

where ν_a is a function of ω and takes the value $(-1+\sqrt{1+4A_{lm}})/2$ when $\omega = 0$ (see equations (6) and (22) with $zj_\nu(z) = F_\nu(0,z)$). The $\omega \to 0$ limit ν_0 must equal this ν_a, which is consistent with our previous determination that ν_0 should equal $l+m$ in the special case when $N_1 = -N_2 = 0$ and $A_{lm} = (l+m)(l+m+1)$. That ν_0 must equal ν_a may be recognized by considering λ large enough that $[(\lambda+1)/(\lambda-1)]^{1/2} \approx [1-\lambda^{-2}]$, and ω small enough that $\omega\lambda \ll 1$. The asymptotic solutions (99) and (100) are valid in this region, but can represent the regular solution (98) only if the orders ν_a and ν_0 are the same. This is because $j_\nu(x) \propto x^\nu$ for small x. We should not be surprised to find that ν_0 will become complex when the dipole moment $2aN_1$ is greater than the critical value that makes $A_{lm} < -1/4$. Only those values of ν that are solutions to equation (92) and are contiguous with ν_a as $\omega \to 0$ can be used to generate a sequence a_L that allow expansions (86) and (87) to give true solutions to the differential equation (82). In other words, if one wants to find a ν with which to generate solutions to the differential equation (82) *via* expansions (86) and (87) for some nonzero (and perhaps even complex) ω, one should first solve equation (91) for an ω very near zero using the ν_a given at equation (23) as a starting point, then move ω toward the desired value in small increments, re-solving (91) at each step to make certain the final value of ν obtained is on the correct branch.

VI. SOLUTIONS BY EXPANSION IN SERIES OF COULOMB WAVEFUNCTIONS

Heartened by success with the preliminary generalization discussed in the previous section, one is immediately tempted to try an expansion of the same sort as (86) and (87) for the general case of equation (2) when $2a(N_1 + N_2) \neq 0$. In terms of the problem of the two-center Schrödinger equation, this full generalization implies a net Coulomb charge on the nuclei, hence the expansion must be in terms of Coulomb wavefunctions rather than spherical Bessel functions. This is not a great conceptual complication, since the Coulomb wavefunction $F_L(\eta, \rho)$ and the spherical Bessel function $j_L(\rho)$ are related when $\eta = 0$ by $F_L(0, \rho) = \rho j_L(\rho)$. Unfortunately, if the expansion

$$\Psi(\lambda) = \frac{1}{\lambda}\left(\frac{\lambda^2 - 1}{\lambda^2}\right)^{\frac{m}{2}} \sum_{L=-\infty}^{\infty} a_L F_{L+\nu}(\eta, \omega\lambda)$$

(with $\eta = -a(N_1 + N_2)/\omega$) is substituted into the differential equation (2), the resulting recurrence relation amongst the a_L will have five terms instead of three, being of the form

$$-\frac{\omega^2}{4}\alpha_L a_{L+2} - \frac{\omega^2}{L^2}\eta m \alpha'_L a_{L+1} + L^2 \beta_L a_L + \frac{\omega^2}{L^2}\eta m \gamma'_L a_{L-1} - \frac{\omega^2}{4}\gamma_L a_{L-2} = 0$$

where the α_L, α'_L, β_L, γ'_L, and γ_L are functions of L, ν, and the parameters of the differential equation and are normalized such that they each approach 1 as $L \to \infty$. Exact expressions for these recurrence coefficients are nearly as ghastly to derive as they are to contemplate once written down, and as I know of no reasonable computational method for dealing with five-term recurrence relations, I will spare the reader the agony of their further consideration and turn instead to the presentation of a more elegant representation for the generalized spheroidal wavefunctions.

A. The Coulomb Wavefunction Expansion

Equation (1) was

$$x(x - x_0)\frac{d^2y}{dx^2} + (B_1 + B_2 x)\frac{dy}{dx} + \left[\omega^2 x(x - x_0) - 2\eta\omega(x - x_0) + B_3\right] y = 0 \quad .$$

With the substitutions $y(x) = x^{-B_2/2}h(x)$ and $z = \omega x$ the differential equation becomes

$$z(z - \omega x_0)[h_{,zz} + (1 - 2\eta/z)h] + C_1\omega h_{,z} + (C_2 + C_3\omega/z)h = 0 \tag{101}$$

where

$$\begin{aligned} C_1 &= B_1 + B_2 x_0 \\ C_2 &= B_3 - \tfrac{1}{2}B_2\left(\tfrac{1}{2}B_2 - 1\right) \\ C_3 &= -\tfrac{1}{2}B_2\left[x_0\left(\tfrac{1}{2}B_2 + 1\right) + B_1\right] \quad . \end{aligned} \tag{102}$$

The function $h(z)$ can then be expanded in a series of Coulomb wavefunctions:

$$h(z) = \sum_{L=-\infty}^{\infty} a_L \boldsymbol{u}_{L+\nu}(z) \tag{103}$$

where $\boldsymbol{u}_{L+\nu}(z)$ is any combination of the Coulomb wavefunctions $F_{L+\nu}(\eta, z)$ and $G_{L+\nu}(\eta, z)$. The $\eta = 0$, $\nu = l + m$ ordinary spheroidal wavefunction limit of this expansion can no doubt be obtained by an integral transformation of Baber and Hassé's equation 30 or 33, but there is little to be gained by further consideration of such special cases. The Coulomb wavefunctions satisfy the recurrence relation

$$\frac{1}{2L + 2\nu + 1}R_{L+1}\boldsymbol{u}_{L+\nu+1} - (1/z + Q_L)\,\boldsymbol{u}_{L+\nu} + \frac{1}{2L + 2\nu + 1}R_L \boldsymbol{u}_{L+\nu-1} = 0 \tag{104}$$

and the differential relation

$$\frac{d}{dz}\boldsymbol{u}_{L+\nu} = -\frac{L+\nu}{2L+2\nu+1}R_{L+1}\boldsymbol{u}_{L+\nu+1} - Q_L\boldsymbol{u}_{L+\nu} + \frac{L+\nu+1}{2L+2\nu+1}R_L\boldsymbol{u}_{L+\nu-1} \tag{105}$$

where

$$Q_L = \frac{\eta}{(L+\nu)(L+\nu+1)} \qquad \text{and} \qquad R_L = \frac{\left[(L+\nu)^2+\eta^2\right]^{1/2}}{L+\nu} \quad , \tag{106}$$

and are solutions of the differential equation

$$\frac{d^2}{dz^2}\boldsymbol{u}_{L+\nu} + \left[1 - \frac{2\eta}{z} - \frac{(L+\nu)(L+\nu+1)}{z^2}\right]\boldsymbol{u}_{L+\nu} = 0 \quad . \tag{107}$$

The $F_{L+\nu}(z)$ form a solution sequence to recurrence relation (104) that is minimal as $L \to +\infty$, and are the solution to the Coulomb wave equation (107) that is proportional to $z^{L+\nu+1}$ as $z \to 0$. The $G_{L+\nu}(z)$ are irregular solutions to the Coulomb wave equation, are proportional to $z^{-L-\nu}$ as $z \to 0$, and form a dominant solution sequence to recurrence relation (104). $F_{L+\nu}(z)$ and $G_{L+\nu}(z)$ are normalized such that the Wronskian

$$F_{L+\nu,z}G_{L+\nu} - G_{L+\nu,z}F_{L+\nu} = 1 \tag{108}$$

and have the asymptotic form

$$G_{L+\nu}(\eta,z) \pm iF_{L+\nu}(\eta,z) \overset{z\to\infty}{\longrightarrow} \exp\left[\pm i(z - \eta\ln 2z - (L+\nu)\tfrac{\pi}{2} + \sigma_L)\right] \tag{109}$$

where

$$\sigma_L = -\frac{i}{2}\ln\left[\frac{\Gamma(L+\nu+1+i\eta)}{\Gamma(L+\nu+1-i\eta)}\right] \quad . \tag{110}$$

Coulomb wavefunctions are defined by the integral representations

$$G_{L+\nu} \pm iF_{L+\nu} = \frac{e^{\pi\eta/2}e^{\pm iz}(2z)^{-L-\nu}}{\left[\Gamma(L+\nu+1+i\eta)\Gamma(L+\nu+1-i\eta)\right]^{\frac{1}{2}}}\int_0^\infty e^{-t}t^{L+\nu\pm i\eta}(t\mp 2iz)^{L+\nu\mp i\eta}dt \quad , \tag{111}$$

and afford an alternate way of expressing the confluent hypergeometric functions. (The Coulomb wavefunctions have usually been defined only for non-negative integer orders and real charge parameter η. Equations (110) and (111) were obtained from the discussion of Coulomb wavefunctions and confluent hypergeometric functions given by Morse and Feshbach, who define Coulomb wavefunctions in a completely analytic manner.)

The expansion coefficients a_L in series (103) are defined by the recurrence relation

$$\alpha_L a_{L+1} + \beta_L a_L + \gamma_L a_{L-1} = 0 \quad , \tag{112}$$

where

$$\begin{aligned}
\alpha_L &= -\frac{\omega R_{L+1}}{2L+2\nu+3}\left[(L+\nu+1)(L+\nu+2)x_0 - (L+\nu+2)C_1 - C_3\right] \\
\beta_L &= (L+\nu)(L+\nu+1) + C_2 + \omega Q_L\left[(L+\nu)(L+\nu+1)x_0 - C_1 - C_3\right] \\
\gamma_L &= -\frac{\omega R_L}{2L+2\nu-1}\left[(L+\nu)(L+\nu-1)x_0 + (L+\nu-1)C_1 - C_3\right] \quad .
\end{aligned}$$

The C_1, C_2, and C_3 are given in terms of the B_1, B_2, and B_3 in equations (102). The a_L will be minimal as $L \to \pm\infty$ if ν is a solution of the implicit equation

$$\beta_0 = \left\{ \begin{array}{c} \dfrac{\alpha_{-1}\gamma_0}{\beta_{-1}-}\,\dfrac{\alpha_{-2}\gamma_{-1}}{\beta_{-2}-}\,\dfrac{\alpha_{-3}\gamma_{-2}}{\beta_{-3}-}\,\ldots \\ + \\ \dfrac{\alpha_0\gamma_1}{\beta_1-}\,\dfrac{\alpha_1\gamma_2}{\beta_2-}\,\dfrac{\alpha_2\gamma_3}{\beta_3-}\,\ldots \end{array} \right\} \tag{113}$$

Solutions to (113) exist and are periodic with period 1. Roots ν that are integer multiples of $1/2$ are usually spurious (there are some special exceptions). The only solutions ν for which the series (103) will actually solve the differential equation are those that map to the correct asymptotic values as $\omega \to 0$ or as $\omega x \to \infty$: see equation (121).

B. Convergence Properties

Convergence of the Coulomb wavefunction series solutions (103) to the generalized spheroidal wave equation (1) is similar to that of the Neumann series solutions (86) to the finite dipole wave equation (82). When ν is a solution to the continued fraction equation (113) the sequence of expansion coefficients $\{a_L : L = \ldots - 2, -1, 0, 1, 2 \ldots\}$ is minimal as $L \to \pm\infty$, but in the usual case that ν is not an integer the negative L part of the series cannot be truncated and both sequences of Coulomb wavefunctions $\{F_{L+\nu} : L = \ldots - 2, -1, 0, 1, 2 \ldots\}$ and $\{G_{L+\nu} : L = \ldots - 2, -1, 0, 1, 2 \ldots\}$ will be dominant either as $L \to +\infty$ or as $L \to -\infty$, or both. The solutions given by expansion (103), though independent, will both be seen to be irregular as $x \to x_0$.

Convergence properties of the solutions are illustrated by analysis of the limiting behavior of $a_L G_{L+\nu}(\eta, \omega x)$ as $L \to +\infty$. This behavior will be shared by the $L \to -\infty$ part of both series, and the positive L part of $\sum_L a_L F_{L+\nu}$ is obviously convergent. We will here consider only the case when $L^2 \gg |\eta\omega|$. From the recurrence relation (112) for the a_L, we obtain the limiting ratios

$$\lim_{L\to+\infty} \frac{a_L}{a_{L-1}} = \frac{\omega R_L}{2L^2} \left[x_0 L + C_1\right] \tag{114}$$

and

$$\lim_{L\to-\infty} \frac{a_L}{a_{L+1}} = \frac{\omega R_L}{2L^2} \left[x_0 L - C_1\right] \tag{115}$$

(the a_L being minimal as $L \to \pm\infty$), and from the recurrence relation (104) for the Coulomb wavefunctions

$$\lim_{L\to\infty} \frac{G_{L+\nu}(\eta, \omega x)}{G_{L+\nu-1}(\eta, \omega x)} \sim \frac{2L}{R_L} \left(\frac{1}{\omega x} + Q_{L-1}\right) \qquad (L \gg |\omega x|)$$

and

$$\lim_{L\to\infty} \frac{G_{L+\nu+1}(\eta, \omega x)}{G_{L+\nu-1}(\eta, \omega x)} = -1 \qquad (1 \ll L \ll |\omega x|) \quad ,$$

the $G_{L+\nu}$ being dominant solutions of recurrence relation (104). If $\eta\omega \ll L^2$ we immediately obtain

$$\lim_{L\to\infty} \frac{a_L G_{L+\nu}(\omega x)}{a_{L-1} G_{L+\nu-1}(\omega x)} = \frac{1}{x} \left(x_0 + C_1/L\right) \longrightarrow \begin{cases} x_0/x & \text{if} \quad x_0 \neq 0 \\ C_1/xL & \text{if} \quad x_0 = 0 \end{cases} \quad , \tag{116}$$

so that the series (103) is absolutely convergent for all $x > x_0$ and diverges at $x = x_0$ The $L < 0$ part of the series can be truncated when ν is an integer, and this will happen when $\eta = 0$ and A_{lm} is an eigenvalue of the ordinary spheroidal wave equation. If $\nu = l + m$ then the series $\sum_{L=0}^{\infty} a_L F_{L+l+m}(0, \omega x)$ will represent the regular ordinary spheroidal wavefunction.

Expressing, as it does, the limiting form of the ratio of successive terms in the series, expression (116) tells us not only that the series converges, but also says much about how rapid the convergence is. If for some $\epsilon > 0$ we wish to find an N such that

$$\left|\frac{a_N G_{N+\nu}(\eta, \omega x)}{a_0 G_\nu(\eta, \omega x)}\right| < \epsilon$$

then we can use (116) to estimate

$$\left|\frac{a_N G_{N+\nu}(\omega x)}{a_0 G_\nu(\omega x)}\right| = \epsilon \approx \left(\frac{x_0}{x}\right)^N \tag{117}$$

(assuming $|C_1| \ll N x_0$), from which

$$N \approx \frac{\log \epsilon}{\log(x_0/x)} \quad , \tag{118}$$

which again expresses the divergence of the series as $x \to x_0$. As an example, suppose one wished to compute the irregular ordinary spheroidal wavefunction (with $l = m = 0$) for $\omega = 1$ at $\lambda = 3$ to an accuracy of approximately seven decimal places. In this case $x_0 = 2$, $x = 4$, and $\epsilon = 10^{-7}$. Equation (118) then estimates $N \approx 23$. When actually computed, it turns out that $a_{23} = 1.51 \times 10^{-23}$ and $G_{23}(0,4) = 4.31 \times 10^{14}$. The product of the two, $a_{23}G_{23}(0,4) = 6.5 \times 10^{-9}$, is not unreasonably distant from the desired value 10^{-7}. Thus expression (118), though not exact, is a useful guide for computational purposes.

C. Solutions as $\omega \to 0$.

The solutions ν to equation (113) are periodic with period 1. As $\omega \to 0$ the differential equation (101) takes the limiting form

$$\lim_{\omega \to 0} \frac{d^2 h}{dz^2} + \left(1 - \frac{2\eta}{z} + \frac{C_2}{z^2}\right) h = 0 \tag{119}$$

and has solutions

$$\lim_{\omega \to 0} h_1(z) = F_{\nu_0}(\eta, z) \quad \text{and} \quad \lim_{\omega \to 0} h_2(z) = G_{\nu_0}(\eta, z) \ , \tag{120}$$

where

$$\nu_0 = -\frac{1}{2}\left[1 \pm \sqrt{1 - 4C_2}\right] \ . \tag{121}$$

If we normalize the a_L such that $a_{max} = a_0$, then the minimal solution sequence a_L to recurrence relation (112) has the property that $a_L \to 0$ as $\omega \to 0$ for all $L \neq 0$. The small ω form of expansion (103) will then be dominated by the single term $a_0 \boldsymbol{u}_\nu(\eta, \omega x)$. For larger ω the only solutions ν to equation (113) that can be used to generate the a_L and give a convergent series that actually solves the differential equation are those ν that are contiguous with the ν_0 as $\omega \to 0$. The values of ν_0 are the same as the values of the order ν_a of the asymptotic solutions (22) and (23) given in Sec. II.

D. Asymptotic Behavior

Two independent solutions to the generalized spheroidal wave equation

$$x(x - x_0)\frac{d^2 y}{dx^2} + (B_1 + B_2 x)\frac{dy}{dx} + \left[\omega^2 x(x - x_0) - 2\eta\omega(x - x_0) + B_3\right] y = 0$$

can now be written

$$\begin{aligned} y_+(x) &= x^{-B_2/2} \sum_{L=-\infty}^{\infty} a_L \left[G_{L+\nu}(\eta, z) + iF_{L+\nu}(\eta, z)\right] \\ y_-(x) &= x^{-B_2/2} \sum_{L=-\infty}^{\infty} a_L \left[G_{L+\nu}(\eta, z) - iF_{L+\nu}(\eta, z)\right] \ . \end{aligned} \tag{122}$$

The asymptotic form of y_+ and y_- can be expressed as

$$\lim_{x \to \infty} y_\pm(x) = x^{-B_2/2} \exp[\pm i(\omega x - \eta \ln(2\omega x) - \phi_\pm)] \ , \tag{123}$$

where ϕ_+ and ϕ_- are obtained from equations (109) and (122):

$$\phi_\pm = \pm i \ln\left[\sum_{L=-\infty}^{\infty} a_L \exp \mp i[(L + \nu)\tfrac{\pi}{2} - \sigma_L]\right] \ . \tag{124}$$

The σ_L are defined by equation (110). The asymptotic behavior of any combination of these solutions $Y(x) = A_{out}y_+(x)+A_{in}y_-(x)$ is therefore obtainable from the values of $Y(x)$ and $Y_{,x}(x)$ at any convenient x at which the matching coefficients A_{out} and A_{in} may be determined. Expressions (122), (123), and (124) are all analytic in ω and x, so there is no reason the phase of the x at which the matching is done need be the same as the phase of the asymptotic limit desired. This analyticity with the asymptotic form is the crucial property that makes a representation "truly useful," and the Coulomb wavefunction expansions (122) probably express it as well as is possible by anything short of an actual integral representation for the generalized spheroidal wavefunctions.

E. Values on the ω Branch Cut

The irregular generalized spheroidal wavefunctions have branch cuts in x that emanate from $x = 0$ and $x = x_0$. These may be treated in the usual manner using the known values of the indices k_1 and k_2 of equation (21). There is, however, a branch cut in the frequency ω that is an important consideration in some physical problems.[4] This branch cut starts at $\omega = 0$ and extends downward along the negative imaginary ω axis. The coulomb wavefunction expansions (122) allow the values of the irregular generalized spheroidal wavefunctions y_+ and y_- to be determined on each side of this cut. In terms of the regular and irregular confluent hypergeometric functions $M(a, b, 2iz)$ and $U(a, b, 2iz)$ as defined by Slater,[28] the Coulomb wavefunctions can be expressed as

$$G_{L+\nu}(\eta,z) \pm iF_{L+\nu}(\eta,z) \;=\; \frac{(-)^L(2z)^{L+\nu+1}e^{\pm iz}}{e^{-\pi\eta/2}e^{\pm i\pi(\nu+1/2)}}\left[\frac{\Gamma(L+\nu+1+i\eta)}{\Gamma(L+\nu+1-i\eta)}\right]^{\pm 1/2} U(L+\nu+1\pm i\eta, 2L+2\nu+2, \mp 2iz) \tag{125}$$

and

$$F_{L+\nu}(\eta,z) \;=\; \frac{[\Gamma(L+\nu+1+i\eta)\Gamma(L+\nu+1-i\eta)]^{1/2}}{2e^{\pi\eta/2}\Gamma(2L+2\nu+2)}(2z)^{L+\nu+1}e^{\pm iz}M(L+\nu+1\pm i\eta, 2L+2\nu+2, \mp 2iz) \tag{126}$$

Slater's equation 13.1.10 then gives the ω branch cut information:

$$\begin{aligned} U(L+\nu+1\pm i\eta, 2L+2\nu+2, \mp 2ize^{2n\pi i}) \;&=\; e^{-4n\pi i\nu}U(L+\nu+1\pm i\eta, 2L+2\nu+2, \mp 2iz) \\ &+\; \left(1-e^{-4n\pi i\nu}\right)\frac{\Gamma(-2L-2\nu-1)}{\Gamma(-L-\nu\pm i\eta)}M(L+\nu+1\pm i\eta, 2L+2\nu+2, \mp 2iz) \end{aligned} \tag{127}$$

Recall that $z = \omega x$. Equations (125) and (127) can be inserted into expansions (122), and the reflexion property of the gamma function eventually allows the final result:

$$y_\pm(\omega e^{2n\pi i}) = e^{-2n\pi i\nu}y_\pm(\omega) + \sin 2n\pi\nu\;\csc 2\pi\nu\;(e^{2\pi\eta} - e^{\mp 2\pi i\nu})[y_+(\omega) - y_-(\omega)] \quad . \tag{128}$$

Here $y_+(\omega) - y_-(\omega) = 2ix^{-B_2/2}\sum a_L F_{L+\nu}(\eta, \omega x)$. This expression is also valid in the limit when ν is an integer. It should be kept in mind that the expansion coefficients a_L and the phase parameter ν are implicit functions of ω. They appear, however, to be entire, and their values do not change across the ω branch cut.

F. An Alternate Normalization for the Coulomb Wavefunctions

There exist other normalizations for the Coulomb wavefunctions that should have definite computational advantages over the usual Coulomb wavefunctions discussed above. These are exemplified by a normalization first proposed by Gautschi,[6] who defined functions $f_{L+\nu}$ and $g_{L+\nu}$ by

$$f_{L+\nu}(\eta,z) = (2L+2\nu+1)e^{\pi\eta/2}\frac{\Gamma(L+\nu+1)}{[\Gamma(L+\nu+1+i\eta)\Gamma(L+\nu+1-i\eta)]^{\frac{1}{2}}}F_{L+\nu}(\eta,z) \qquad (129)$$

$$g_{L+\nu}(\eta,z) = (2L+2\nu+1)e^{\pi\eta/2}\frac{\Gamma(L+\nu+1)}{[\Gamma(L+\nu+1+i\eta)\Gamma(L+\nu+1-i\eta)]^{\frac{1}{2}}}G_{L+\nu}(\eta,z) \qquad (130)$$

The factor $(2L+2\nu+1)e^{\pi\eta/2}$ is not absolutely necessary, but it does no harm to retain it. The differential and recurrence relations obeyed by both $f_{L+\nu}$ and $g_{L+\nu}$ are

$$f_{L+\nu,z} = \frac{L+\nu+1}{2L+2\nu-1}f_{L+\nu-1} - Q_L f_{L+\nu} - \frac{L+\nu}{2L+2\nu+3}\left[1+\frac{\eta^2}{(L+\nu+1)^2}\right]f_{L+\nu+1} \qquad (131)$$

$$\frac{1}{z}f_{L+\nu} = \frac{1}{2L+2\nu-1}f_{L+\nu-1} - Q_L f_{L+\nu} + \frac{1}{2L+2\nu+3}\left[1+\frac{\eta^2}{(L+\nu+1)^2}\right]f_{L+\nu+1} \qquad (132)$$

where $Q_L = \eta/(L+\nu)(L+\nu+1)$ as in equation (106). Asymptotic forms for f and g may be expressed as

$$g_{L+\nu}(\eta,z) \pm i f_{L+\nu}(\eta,z) \overset{z\to\infty}{\longrightarrow} \exp\left[\pm i(z-\eta\ln 2z-(L+\nu)\tfrac{\pi}{2}+\sigma_L^{(\pm)})\right] \qquad (133)$$

where

$$\sigma_L^{(\pm)} = \mp i\ln\left[(2L+2\nu+1)e^{\pi\eta/2}\frac{\Gamma(L+\nu+1)}{\Gamma(L+\nu+1\mp i\eta)}\right] \quad .$$

If we write our solutions (122) to the generalized spheroidal wave equation as

$$y_\pm(x) = x^{-B_2/2}\sum_{L=-\infty}^{\infty} a_L\left[g_{L+\nu}(\eta,z) \pm i f_{L+\nu}(\eta,z)\right] \qquad (134)$$

then the asymptotic forms of y_+ and y_- are given by

$$\lim_{x\to\infty} y_\pm(x) = x^{-B_2/2}\exp[\pm i(\omega x - \eta\ln(2\omega x) - \tilde{\phi}_\pm)] \qquad (135)$$

where

$$\tilde{\phi}_\pm = \pm i\ln\left[\sum_{L=-\infty}^{\infty} a_L \exp\mp i[(L+\nu)\tfrac{\pi}{2} - \sigma_L^{(\pm)}]\right] \quad . \qquad (136)$$

The expansion coefficients a_L will satisfy the three-term recurrence relation

$$\alpha_L a_{L+1} + \beta_L a_L + \gamma_L a_{L-1} = 0 \quad , \qquad (137)$$

where now the recurrence coefficients are defined by

$$\alpha_L = -\frac{\omega}{2L+2\nu+1}[(L+\nu+1)(L+\nu+2)x_0 - (L+\nu+2)C_1 - C_3]$$
$$\beta_L = (L+\nu)(L+\nu+1) + C_2 + \omega Q_L[(L+\nu)(L+\nu+1)x_0 - C_1 - C_3]$$
$$\gamma_L = -\frac{\omega}{2L+2\nu+1}[(L+\nu)(L+\nu-1)x_0 + (L+\nu-1)C_1 - C_3][1+\eta^2/(L+\nu)^2] \quad .$$

The C_1, C_2, and C_3 are given in terms of the B_1, B_2, and B_3 in equations (102). The recurrence relations (131) and (132) for Gautschi's Coulomb wavefunctions should be compared with the corresponding relations (104) and (105) for the usual Coulomb wavefunctions, and the definitions of the α_L, β_L, and γ_L for equation (137) compared with the corresponding definitions for the α_L, β_L, and γ_L for equation (112). No square roots appear in any of the relations using Gautschi's normalization, a property that will greatly enhance the speed with which expansions (134) can be evaluated and, by eliminating spurious branch cuts associated with the unnecessary square roots, will probably enlarge the parameter regions for which the Coulomb wavefunction expansion is valid.

VII. SOLUTIONS BY EXPANSION IN SERIES OF CONFLUENT HYPERGEOMETRIC FUNCTIONS

One last set of representations for the generalized spheroidal wave functions may be obtained by expanding the solutions $y(x)$ to equation (1) in series of the confluent hypergeometric functions $\tilde{M}(a,b,z)$ and $U(a,b,z)$. Four new representations are obtained. The expansions for the solution that is regular as $x \to x_0$ are shown to be uniformly convergent both at $x = x_0$ and as $x \to \infty$. However, convergence of these series does not appear to be rapid, and the representations have not yet been implemented on a computer.

A. The Confluent Hypergeometric Function Expansion

Again start with equation (1):

$$x(x-x_0)\frac{d^2y}{dx^2} + (B_1 + B_2 x)\frac{dy}{dx} + \left[\omega^2 x(x-x_0) - 2\eta\omega(x-x_0) + B_3\right] y = 0 \quad .$$

Solutions can be expanded in the form

$$\begin{aligned} y_1(x) &= e^{+i\omega x} \sum_{L=-\infty}^{\infty} a_L \tilde{M}(\tfrac{1}{2}B_2 + i\eta, L + \nu_1, -2i\omega x) && (138)\\ y_2(x) &= e^{-i\omega x} \sum_{L=-\infty}^{\infty} b_L \tilde{M}(\tfrac{1}{2}B_2 - i\eta, L + \nu_2, +2i\omega x) && (139)\\ y_+(x) &= e^{+i\omega x} \sum_{L=-\infty}^{\infty} a_L U(\tfrac{1}{2}B_2 + i\eta, L + \nu_1, -2i\omega x) && (140)\\ y_-(x) &= e^{-i\omega x} \sum_{L=-\infty}^{\infty} b_L U(\tfrac{1}{2}B_2 - i\eta, L + \nu_2, +2i\omega x) \quad , && (141) \end{aligned}$$

where M and U are confluent hypergeometric functions. To demonstrate this substitute

$$y(x) = e^{+i\omega x} f(x) \ , \qquad z = -2i\omega x \ , \qquad \text{and} \qquad z_0 = -2i\omega x_0 \ , \tag{142}$$

then the differential equation for f in terms of z is

$$z(z-z_0)\frac{d^2 f}{dz^2} + (D_1 + D_2 z - z^2)\frac{df}{dz} + (D_3 + D_4 z)f = 0 \tag{143}$$

where

$$\begin{aligned} D_1 &= -2i\omega B_1 \\ D_2 &= B_2 - 2i\omega x_0 \\ D_3 &= B_3 + 2\eta\omega x_0 + i\omega B_1 \\ D_4 &= -\tfrac{1}{2}B_2 - i\eta \quad . \end{aligned} \tag{144}$$

The solutions $f(z)$ to equation (143) can be expanded in a series of the confluent hypergeometric functions $M_L(z)$ and $U_L(z)$, where M_L and U_L denote respectively the regular and irregular confluent hypergeometric functions

$$M_L(z) \equiv \tilde{M}(-D_4, L + \nu, -2i\omega x)$$

and

$$U_L(z) \equiv U(-D_4, L + \nu, -2i\omega x)$$

where $z = -2i\omega x$. $\tilde{M}(a,b,z)$ and $U(a,b,z)$ are defined by the integral representations

$$\tilde{M}(a,b,z) = \frac{1}{\Gamma(a)} \int_0^1 e^{zt} t^{a-1} (1-t)^{b-a-1} dt \qquad Re(b) > Re(a) > 0 \tag{145}$$

and

$$U(a,b,z) = \frac{1}{\Gamma(a)} \int_0^\infty e^{-zt} t^{a-1} (1+t)^{b-a-1} dt \qquad Re(a) > 0,\ Re(z) > 0 \quad . \tag{146}$$

Properties of these functions may be found in Slater.[28] The definition (145) that I use here for the regular confluent hypergeometric function $\tilde{M}(a,b,z)$ differs from the usual normalization of the Kummer series by a factor $\Gamma(b-a)/\Gamma(b)$:

$$\tilde{M}(a,b,z) = \frac{\Gamma(b-a)}{\Gamma(b)} \sum_{n=0}^{\infty} \frac{(a)_n z^n}{(b)_n n!} \quad ,$$

where $(a)_n$ denotes Pochammer's symbol: $(a)_n \equiv a(a+1)(a+2)\dots(a+n-1)$ and $(a)_0 \equiv 1$. Thus normalized $\tilde{M}(a,b,z)$ obeys the same differential and recurrence relations as does $U(a,b,z)$. Let $\mathcal{F}_L(z)$ denote any linear combination of the $M_L(z)$ and $U_L(z)$ defined above. Then $\mathcal{F}_L$ solves the confluent hypergeometric equation

$$z\mathcal{F}_{L,zz} + (L+\nu-z)\mathcal{F}_{L,z} + D_4\mathcal{F}_L = 0 \quad , \tag{147}$$

satisfies the differential relations

$$\begin{aligned} \mathcal{F}_{L,z} &= \mathcal{F}_L - \mathcal{F}_{L+1} & (148) \\ z\mathcal{F}_{L,z} &= (1-L-\nu)\mathcal{F}_L + (L+\nu-1+D_4)\mathcal{F}_{L-1} \quad , & (149) \end{aligned}$$

and obeys the recurrence relation

$$z\mathcal{F}_{L+1} - (L+\nu-1+z)\mathcal{F}_L + (L+\nu-1+D_4)\mathcal{F}_{L-1} = 0 \quad . \tag{150}$$

The $M_L(z)$ form the solution sequence to the recurrence relation (150) that is minimal as $L \to +\infty$, and the $U_L(z)$ form a solution that is dominant. The Wronskian of $M_L(z)$ and $U_L(z)$ is

$$M_L(z)U_{L,z}(z) - U_L(z)M_{L,z}(z) = \frac{\Gamma(L+\nu+D_4)}{\Gamma(-D_4)} z^{-L-\nu} e^z \quad . \tag{151}$$

The solutions $f(z)$ to equation (143) may now be expressed as

$$f(z) = \sum_{L=-\infty}^{\infty} a_L \mathcal{F}_L(z) \tag{152}$$

where ν must be chosen such that the coefficients a_L form a solution sequence minimal as $L \to \pm\infty$ of the recurrence relation

$$\alpha_L a_{L+1} + \beta_L a_L + \gamma_L a_{L-1} = 0 \tag{153}$$

where

$$\begin{aligned} \alpha_L &= -(L+\nu+D_4)(L+\nu+1-D_2+z_0) \\ \beta_L &= (L+\nu)(L+\nu-D_2+2z_0-1) + (D_4-1)z_0 + (D_1+D_2+D_3) \\ \gamma_L &= -(L+\nu-1)z_0 - D_1 \quad , \end{aligned} \tag{154}$$

or, in the current case where the D_i are given by equations (144),

$$\begin{aligned} \alpha_L &= -(L+\nu+1-B_2)(L+\nu-\tfrac{1}{2}B_2-i\eta) \\ \beta_L &= (L+\nu)(L+\nu-1-B_2-2i\omega x_0) + i\omega x_0(B_2-B_1/x_0) + B_2 + B_3 \\ \gamma_L &= +2i\omega x_0(L+\nu-1+B_1/x_0) \quad . \end{aligned}$$

The parameter ν must solve the implicit equation

$$\beta_0 = \left\{ \begin{array}{c} \dfrac{\alpha_{-1}\gamma_0}{\beta_{-1}-}\ \dfrac{\alpha_{-2}\gamma_{-1}}{\beta_{-2}-}\ \dfrac{\alpha_{-3}\gamma_{-2}}{\beta_{-3}-}\ \ldots \\ + \\ \dfrac{\alpha_0\gamma_1}{\beta_1-}\ \dfrac{\alpha_1\gamma_2}{\beta_2-}\ \dfrac{\alpha_2\gamma_3}{\beta_3-}\ \ldots \end{array} \right\} \tag{155}$$

The solutions ν to equation (155) are probably periodic. Experience with the Coulomb wave function expansion suggests that the correct values of ν will be those that are contiguous as $\omega \to 0$ with the $\omega = 0$ roots of (155), that is, the values ν_0 that make $\beta_0 = 0$ when $\omega = 0$:

$$\nu_0 = \tfrac{1}{2}\left[B_2 + 1 \pm \sqrt{B_2(B_2-2) - 4B_3 + 1}\right] \tag{156}$$

B. Convergence Properties

If the parameter ν is chosen to satisfy equation (155), then the a_L of equation (153) will be minimal as $L \to \infty$ and successive a_L will have the limiting ratios

$$\lim_{L\to+\infty} \frac{a_L}{a_{L-1}} = \frac{-2i\omega x_0}{L}\left[1 + \frac{1}{L}\left(B_2 + B_1/x_0 - \nu\right) + \mathcal{O}(L^{-2})\right] \tag{157}$$

and

$$\lim_{L\to-\infty} \frac{a_L}{a_{L+1}} = 1 + \frac{1}{L}\left(2 - \tfrac{1}{2}B_2 - i\eta\right) + \mathcal{O}(L^{-2}) \ . \tag{158}$$

Assume that both the $\boldsymbol{M}_L$ and the $\boldsymbol{U}_L$ are dominant solutions to recurrence relation (150) as $L \to -\infty$, and denote them again by $\mathcal{F}_L$. Successive $\mathcal{F}_L$ will have the limiting ratios

$$\lim_{L\to-\infty} \frac{\mathcal{F}_L}{\mathcal{F}_{L+1}} = 1 + \frac{1}{L}\left(\tfrac{1}{2}B_2 + i\eta\right) + \mathcal{O}(L^{-2}) \ . \tag{159}$$

As $L \to +\infty$ the $\boldsymbol{M}_L$ are minimal,

$$\lim_{L\to+\infty} \frac{\boldsymbol{M}_L}{\boldsymbol{M}_{L-1}} = 1 - \frac{1}{L}\left(\tfrac{1}{2}B_2 + i\eta\right) + \mathcal{O}(L^{-2}) \ , \tag{160}$$

while the $\boldsymbol{U}_L$ are dominant:

$$\lim_{L\to+\infty} \frac{\boldsymbol{U}_L}{\boldsymbol{U}_{L-1}} = \frac{L}{-2i\omega x}\left[1 + \frac{1}{L}\left(2\nu - 2\right) + \mathcal{O}(L^{-2})\right] \ . \tag{161}$$

From equations (158) and (159) we see that

$$\lim_{L\to-\infty} \frac{a_L\mathcal{F}_L}{a_{L+1}\mathcal{F}_{L+1}} = 1 + \frac{2}{L} + \mathcal{O}(L^{-2}) \tag{162}$$

so that the negative L part of series (152) is absolutely (albeit slowly) convergent for $\mathcal{F}_L$ either $\boldsymbol{M}_L$ or $\boldsymbol{U}_L$. From (157) and (160)

$$\lim_{L\to+\infty} \frac{a_L\boldsymbol{M}_L}{a_{L-1}\boldsymbol{M}_{L-1}} = \frac{-2i\omega x_0}{L}\left[1 + \frac{1}{L}\left(\tfrac{1}{2}B_2 + B_1/x_0 - i\eta\right) + \mathcal{O}(L^{-2})\right] \ , \tag{163}$$

and from (157) and (161)

$$\lim_{L\to+\infty} \frac{a_L\boldsymbol{U}_L}{a_{L-1}\boldsymbol{U}_{L-1}} = \frac{x_0}{x}\left[1 + \frac{1}{L}\left(B_2 + B_1/x_0 - \nu - 2i\omega x(\nu-2)\right) + \mathcal{O}(L^{-2})\right] \ . \tag{164}$$

Therefore $\sum a_L U_L$ converges for all x such that $|x| > |x_0|$, and $\sum a_L M_L$ converges, amusingly enough, for all x.

The preceding arguments may be repeated using in equation (142) the alternate substitutions

$$y(x) = e^{-i\omega x} f(x) \ , \qquad z = +2i\omega x \ , \qquad \text{and} \qquad z_0 = +2i\omega x_0 \ , \tag{165}$$

which yield two final representations for the generalized spheroidal wave functions:

$$y_2(x) = e^{-i\omega x} \sum_{L=-\infty}^{\infty} b_L \tilde{M}(\tfrac{1}{2}B_2 - i\eta, L + \nu, +2i\omega x) \tag{166}$$

and

$$y_-(x) = e^{-i\omega x} \sum_{L=-\infty}^{\infty} b_L U(\tfrac{1}{2}B_2 - i\eta, L + \nu, +2i\omega x) \tag{167}$$

where the expansion coefficients b_L are again a solution sequence minimal as $L \to \pm\infty$ of a three-term recurrence relation

$$\alpha_L b_{L+1} + \beta_L b_L + \gamma_L b_{L-1} = 0 \ \ , \tag{168}$$

with recurrence coefficients α_L, β_L, and γ_L given by

$$\begin{aligned}
\alpha_L &= -(L + \nu + 1 - B_2)(L + \nu - \tfrac{1}{2}B_2 + i\eta) \\
\beta_L &= (L + \nu)(L + \nu - 1 - B_2 + 2i\omega x_0) - i\omega x_0(B_2 - B_1/x_0) + B_2 + B_3 \\
\gamma_L &= -2i\omega x_0(L + \nu - 1 + B_1/x_0) \quad ,
\end{aligned}$$

which together with our first two confluent hypergeometric function solutions

$$y_1(x) = e^{+i\omega x} \sum_{L=-\infty}^{\infty} a_L \tilde{M}(\tfrac{1}{2}B_2 + i\eta, L + \nu, -2i\omega x) \tag{169}$$

and

$$y_+(x) = e^{+i\omega x} \sum_{L=-\infty}^{\infty} a_L U(\tfrac{1}{2}B_2 + i\eta, L + \nu, -2i\omega x) \tag{170}$$

constitute the last of our new representations for the generalized spheroidal wave functions. Note that the ν that solve equation (155) for the expansion coefficients b_L using the α, β, and γ of equation (168) will probably not be the same ν that solve the equation for the a_L using the α, β, and γ of equation (153). I have not written computer programs to generate any of these confluent hypergeometric function series, but equation (162) suggests that

$$\lim_{L\to-\infty} a_L \mathcal{F}_L \approx \mathcal{O}(L^{-2}) \ ,$$

so that roughly 10^N terms will be needed if the series (166), (167), (169), or (170) are to be summed to N figures accuracy. While one could hope that this is only a worst-case estimate and, at least for the series of the regular functions $\tilde{M}(\frac{1}{2}B_2 \pm i\eta, L + \nu, \mp 2i\omega x)$ and $|x| \approx 1$, that the series can in practice be made to converge much faster (perhaps with the help of a sequence accelerating algorithm), such speculation must be regarded as “wishful thinking” pending more detailed analysis.

C. Asymptotic Behavior

The limiting forms of the confluent hypergeometric functions for large values of the argument are

$$\lim_{|z|\to\infty} M_L(z) = e^{\mp i\pi D_4} z^{D_4} + \frac{\Gamma(L+\nu+D_4)}{\Gamma(-D_4)} e^z z^{-L-\nu-D_4} \left[1+\mathcal{O}(z^{-1})\right] \tag{171}$$

and

$$\lim_{|z|\to\infty} U_L(z) = z^{D_4} \tag{172}$$

The upper sign is taken in (171) if $-\pi/2 < arg(z) < 3\pi/2$, and the lower sign is taken if $-3\pi/2 < arg(z) \leq -\pi/2$. The factor $\Gamma(L+\nu+D_4)z^{-L-\nu-D_4}$ makes the large $|z|$ limit of the negative L part of series (166) and (169) difficult to evaluate. However, the series (167) and (170) involving the irregular functions $U_L(z)$ are relatively simple, and we may express the limiting forms of these solutions as

$$\begin{aligned} \lim_{|x|\to\infty} y_+(x) &= \lim_{|x|\to\infty} e^{+i\omega x} \sum_{L=-\infty}^{\infty} a_L U(\tfrac{1}{2}B_2 + i\eta, L+\nu, -2i\omega x) \\ &= (-2i\omega x)^{-B_2/2-i\eta} e^{+i\omega x} \sum_{L=-\infty}^{\infty} a_L \end{aligned} \tag{173}$$

and

$$\begin{aligned} \lim_{|x|\to\infty} y_-(x) &= \lim_{|x|\to\infty} e^{-i\omega x} \sum_{L=-\infty}^{\infty} b_L U(\tfrac{1}{2}B_2 - i\eta, L+\nu, +2i\omega x) \\ &= (+2i\omega x)^{-B_2/2+i\eta} e^{-i\omega x} \sum_{L=-\infty}^{\infty} b_L \quad . \end{aligned} \tag{174}$$

As noted before, these sums are only slowly convergent, and expansions (167) and (170) probably have no computational advantage over the Jaffé-type solutions discussed in Sec. IV. However, the convergence, no matter how slow, of the regular solution expansions (166) and (167) over the entire interval $[x_0 \leq x < \infty)$ may give them some unique analytic utility.

VIII. A CONFLUENT GENERALIZED SPHEROIDAL WAVE EQUATION

A. The Confluent Equation

When $x_0 = 0$ equation (1) becomes

$$x^2 y_{,xx} + (B_1 + B_2 x) y_{,x} + (\omega^2 x^2 - 2\eta\omega x + B_3) y = 0 \tag{175}$$

If $y(x) = x^{-B_2/2} h$ and $z = \omega x$ then the differential equation for $h(z)$ is

$$z^2 h_{,zz} + C_1 \omega h_{,z} + [z^2 - 2\eta z + C_2 + C_3 \omega / z] h = 0 \tag{176}$$

where $C_1 = B_1, \;\; C_2 = B_3 - \frac{1}{2}B_2\left(\frac{1}{2}B_2 - 1\right),$ and $C_3 = -\frac{1}{2}B_1 B_2$.

In the Sec. 6 we showed that h could be expanded as

$$h(x) = \sum_{L=-\infty}^{\infty} a_L \boldsymbol{u}_{L+\nu}(\eta, \omega x) \tag{177}$$

(where $\boldsymbol{u}_{L+\nu}$ is a Coulomb wavefunction), and that the expansion converges even in the present case when $x_0 = 0$. This property is intriguing, because as $x_0 \to 0$ the point $x = 0$ becomes a confluent singular point, and convergent expansions of solutions to differential equations near such points are generally difficult to obtain. Note that the point $x = 0$ is an irregular singular point only when $B_1 \neq 0$: when $B_1 = 0$ equations (175) is a simple confluent hypergeometric equation, equation (176) is the Coulomb wave equation, and the solutions $y(x)$ can be expressed as

$$y(x) = x^{-\frac{1}{2}B_2} \boldsymbol{u}_\nu(\eta, \omega x) \;\;, \;\; \text{where} \;\; \nu(\nu+1) = -C_2 = \frac{1}{2}B_2(\frac{1}{2}B_2 - 1) - B_3 \quad . \tag{178}$$

The solution regular at $x = 0$ is $\boldsymbol{u}_\nu = F_\nu(\eta, \omega x)$, and an irregular solution is given by $\boldsymbol{u}_\nu = G_\nu(\eta, \omega x)$.

However, when $B_1 \neq 0$ the point $x = 0$ is an irregular singular point and expansion (177) must be used for the two solutions, neither of which will converge at $x = 0$. When $x_0 \neq 0$ the solutions near $x = 0$ could be generated *via* the Jaffé expansion $\sum a_n[(x - x_0)/x]^n$. When $x_0 = 0$ the Jaffé expansion does not exist and another approach must be taken towards generating solutions good near that point. This can be done by exploiting the symmetry that exists between the point $x = 0$ and the point at ∞ : both are confluent singular points and with the substitutions

$$y(x) = e^{i\omega x + B_1/2x} x^{1 - B_2/2} f(\xi) \;, \qquad \xi = \frac{iB_1}{2x}$$

equation (175) becomes

$$\xi^2 f_{,\xi\xi} + \tilde{C}_1 \omega f_{,\xi} + [\xi^2 - 2\tilde{\eta}\xi + \tilde{C}_2 + \tilde{C}_3 \omega / \xi] f = 0 \tag{179}$$

where

$$\begin{aligned} &\tilde{C}_1 = C_1 = B_1, && \tilde{\eta} = -i(\tfrac{1}{2}B_2 - 1) \\ &\tilde{C}_2 = C_2 = B_3 - \tfrac{1}{2}B_2\left(\tfrac{1}{2}B_2 - 1\right) && \xi = iB_1/2x \\ &\tilde{C}_3 = -(1 + i\eta)B_1 \quad . && \end{aligned}$$

Hence solutions to equation (175) can also be written

$$y(x) = x^{1 - B_2/2} e^{i\omega x + B_1/2x} \sum_{L=-\infty}^{\infty} b_L \boldsymbol{u}_{L+\nu}(\tilde{\eta}, \xi) \quad . \tag{180}$$

Expansion (180) is uniformly convergent as $x \to 0$. The expansion coefficients a_L in expression (177) and the coefficients b_L in expression (180) are both defined by equations (112) and (113) using respectively the C_i of (176) and the $\tilde{C}_i$ of (179).

B. The Kerr Limit of Black Hole Rotation

An example of the confluent equation occurs at the Kerr limit of black hole rotation, where $b = 0$ and $a = 1/2$ in equations (15) and (19). If it were physically possible, the confluence of the event horizon at $x = x_0$ with the singularity at $x = 0$ would result in a naked singularity. The current theory of gravitation does not allow naked singularities to form,[42] but an understanding of the behaviour of the solutions to the wave equation (15) at the Kerr limit might allow some insight regarding the behaviour of solutions near that limit. At the Kerr limit equation (19) becomes

$$\begin{aligned} x^2 y_{,xx} &+ [2(1-s-i\omega)x - i(\omega-m)]y_{,x} \\ &+ [\omega^2 x^2 + 2(\omega+is)\omega x + \tfrac{3}{4}\omega^2 + (2s-1)i\omega - 2s - A_{lm}]y = 0 \quad , \end{aligned} \tag{181}$$

which is of the form (175). The substitutions $y = x^{s+i\omega-1}h(z)$ and $z = \omega x$ yield

$$z^2 h_{,zz} - i\omega(\omega-m)h_{,z} + [z^2 - 2\eta z + C_2 + i\omega(\omega-m)(1-s-i\omega)/z]h = 0 \tag{182}$$

where $C_2 = \frac{7}{4}\omega^2 - s(s+1) - A_{lm}$ and $\eta = -\omega - is$, which corresponds to equation (176). Similarly, the substitution $y = x^{s+i\omega}\exp i[\omega x - (\omega-m)/2x]f(\xi)$ with $\xi = (\omega-m)/2x$ gives

$$\xi^2 f_{,\xi\xi} - i\omega(\omega-m)f_{,\xi} + [\xi^2 - 2\tilde{\eta}\xi + C_2 + i\omega(\omega-m)(1+s-i\omega)/\xi]f = 0 \tag{183}$$

where $\tilde{\eta} = -\omega + is$. Two interesting limiting cases of equations (182) and (183) occur when $\omega \approx 0$ and when $\omega \approx m$. The occurrence of the product $i\omega(\omega-m)$ allows us to treat both cases in the same manner:

Let $C_1 = -i(\omega-m)$, $C_3 = i(\omega-m)(1-s-i\omega)$, $\tilde{C}_3 = i(\omega-m)(1+s-i\omega)$, and $\tilde{\eta} = -\omega + is$. Then expansions corresponding to (177) and (180) that are respectively convergent for x and $1/x$ bounded away from 0 are

$$y^{(\infty)}(x) = x^{s+i\omega-1} \sum_{L=-\infty}^{\infty} a_L \boldsymbol{u}_{L+\nu}(-\omega - is, \omega x) \tag{184}$$

$$y^{(0)}(x) = x^{s+i\omega} e^{i\omega x - i(\omega-m)/2x} \sum_{L=-\infty}^{\infty} b_L \boldsymbol{u}_{L+\nu}(-\omega + is, (\omega-m)/2x) \quad . \tag{185}$$

Again, $\boldsymbol{u}_{L+\nu}(\eta, z)$ denotes a Coulomb wavefunction. The ν in equation (184) is chosen to satisfy (113) and makes the a_L the minimal solution of

$$\alpha_L a_{L+1} + \beta_L a_L + \gamma_L a_{L-1} = 0 \quad , \tag{186}$$

where

$$\begin{aligned} \alpha_L &= -i\omega(\omega-m)R_{L+1}(\eta)(L+\nu+1+s+i\omega)/(2L+2\nu+3) \\ \beta_L &= (L+\nu)(L+\nu+1) + C_2 + i\omega(\omega-m)(s+i\omega)Q_L(\eta) \\ \gamma_L &= +i\omega(\omega-m)R_L(\eta)(L+\nu-s-i\omega)/(2L+2\nu-1) \quad . \end{aligned} \tag{187}$$

The ν and b_L of equation (185) are generated from

$$\tilde{\alpha}_L b_{L+1} + \tilde{\beta}_L b_L + \tilde{\gamma}_L b_{L-1} = 0 \quad , \tag{188}$$

where the $\tilde{\alpha}_L$, $\tilde{\beta}_L$, and $\tilde{\gamma}_L$ are the same as the α, β, and γ of equation (187) but with η replaced by $\tilde{\eta}$ and C_3 replaced by $\tilde{C}_3$ (*i.e.*, s is replaced by $-s$). As $\omega \to 0$ or as $\omega \to m$ only the a_0 and b_0 terms contribute to the sums in (184) and (185), so that limiting forms for $y^{(\infty)}$ and $y^{(0)}$ are (with $a_0 = b_0 = 1$)

$$\lim_{\omega\to 0,m} y^{(\infty)}(x) \sim x^{s+i\omega-1}\boldsymbol{u}_\nu(-\omega - is, \omega x) \tag{189}$$

$$\lim_{\omega\to 0,m} y^{(0)}(x) \sim x^{s+i\omega} e^{i\omega x - i(\omega-m)/2x}\boldsymbol{u}_\nu(-\omega + is, (\omega-m)/2x) \quad , \tag{190}$$

where $\nu(\nu+1) = -C_2(\omega = 0, m)$. Expressions (189) and (190) are valid for values of the rotation parameter such that $0 < b \ll 1$, not just $b = 0$. This generalization may be demonstrated by retaining b and interchanging w and $\omega - m$ when deriving the definitions (187) for the recurrence coefficients α_L, β_L, and γ_L.

The physically relevant field function is Teukolsky's $R_{lm}(r)$, which is related to $y(x)$ by equation (17):

$$R(r) = (r - r_-)^{k_-}(r - r_+)^{k_+} y(x) \quad ,$$

where $x = r - r_-$. Again, $r_\pm = (1 \pm b)/2$, $k_- = -s + i(\omega r_- - am)/b$, $k_+ = -s - i(\omega r_+ - am)/b$, and $a = \frac{1}{2}(1 - b^2)^{1/2}$. Taking the limit

$$\lim_{b \to 0}(r - r_-)^{k_-}(r - r+)^{k_+} = x^{-2s - i\omega} e^{i(\omega - m)/2x} \quad ,$$

we find the expansions for $R(r)$ that are respectively convergent away from $r = 1/2$ and away from $r = \infty$ are, with $x = r - 1/2$,

$$R_\pm^{(\infty)}(x) = x^{-s-1} e^{i(\omega - m)/2x} \sum_{L=-\infty}^{\infty} a_L [G_{L+\nu}(-\omega - is, \omega x) \pm i F_{L+\nu}(-\omega - is, \omega x)] \tag{191}$$

$$R_\pm^{(0)}(x) = x^{-s} e^{i\omega x} \sum_{L=-\infty}^{\infty} b_L [G_{L+\nu}(-\omega + is, (\omega - m)/2x) \pm i F_{L+\nu}(-\omega + is, (\omega - m)/2x)] \tag{192}$$

Equations (109) give the behaviour of the Coulomb wavefunctions for large magnitudes of the argument, and from them we obtain the desired behaviour of the two solutions near $x = 0$:

$$\lim_{x \to 0} R_+^{(0)}(x) \sim [(\omega - m)/2x]^{i\omega} e^{i(\omega - m)/2x} \tag{193}$$

$$\lim_{x \to 0} R_-^{(0)}(x) \sim x^{-2s}[(\omega - m)/2x]^{-i\omega} e^{-i(\omega - m)/2x} \quad . \tag{194}$$

With the sign convention ($e^{-i\omega t}$) of equation (13) it is $R_+^{(0)}(x)$ that describes the case of radiation going into the singularity.

A black hole rotates at the Kerr limit with angular velocity $d\phi/dt = 1$ in the normalized units used here, and a wave train with frequency $\omega = m$ at this limit corotates with the singularity. If $|\omega| \ll 1$ and $|\omega x| \ll 1$ expansion (192) is dominated by the b_0 term and may be approximated (with $b_0 = 1$) by

$$R_\pm^{(0)}(x) \approx x^{-s} e^{i\omega x}[G_\nu(-\omega + is, (\omega - m)/2x) \pm i F_\nu(-\omega + is, (\omega - m)/2x)] \tag{195}$$

where $\nu(\nu + 1) = -C_2(\omega)$. This result also holds for $|\omega - m| \ll 1$ and $|\omega x| \ll 1/2$. Similarly, if $|x/(\omega - m)| \gg 1$, then by equation (116) the a_0 term will dominate expansion (191) and $R_\pm^{(\infty)}$ may be approximated (with $a_0 = 1$) by

$$R_\pm^{(\infty)}(x) \approx x^{-s-1} e^{i(\omega - m)/2x}[G_\nu(-\omega - is, \omega x) \pm i F_\nu(-\omega - is, \omega x)] \quad . \tag{196}$$

These approximations may be used whenever the rotation parameter $b \ll 1$. A different approach to approximating the Teukolsky function R_{lm} near the Kerr limit may be found in Teukolsky and Press,[43] and has been used by Detweiler.[44]

C. Review of the Representations

In this study I have demonstrated ten analytic series representations for the solutions to the generalized spheroidal wave equation

$$x(x-x_0)\frac{d^2y}{dx^2} + (B_1 + B_2 x)\frac{dy}{dx} + \left[\omega^2 x(x-x_0) - 2\eta\omega(x-x_0) + B_3\right] y = 0$$

on the interval $[0 \le x < \infty)$. They are, together with the asymptotic form,

- The regular power series solutions of the Jaffé type (Sec. IV A):

$$y_1(x) = e^{+i\omega x} x^{-\frac{1}{2}B_2 - i\eta} \sum_{n=0}^{\infty} a_n^r \left(\frac{x-x_0}{x}\right)^n \tag{197}$$

  and

$$y_2(x) = e^{-i\omega x} x^{-\frac{1}{2}B_2 + i\eta} \sum_{n=0}^{\infty} b_n^r \left(\frac{x-x_0}{x}\right)^n \tag{198}$$

  cf. equations (39) and (49). These two expansions are proportional by a factor $e^{2i\omega x_0} a_0^r / b_0^r$ and represent the generalized spheroidal wave function that is regular at $x = x_0$. They converge for all x such that $|(x-x_0)/x| < 1$. The convergence is uniform only when ω is an eigenfrequency and the expansion coefficients form minimal solutions to their respective recurrence relations (40) and (50). When ω is not an eigenfrequency the convergence of these series is not uniform and the analytic forms of $y_1(x)$ and $y_2(x)$ as $x \to \infty$ cannot be deduced.

- The irregular confluent hypergeometric function solutions of Hylleraas type (Sec. IV C):

$$y_+(x) = e^{+i\omega x} \sum_{n=0}^{\infty} a_n^r (B_2 + B_1/x_0)_n U(\tfrac{1}{2}B_2 + i\eta + n, -B_1/x_0, -2i\omega x) \tag{199}$$

$$y_-(x) = e^{-i\omega x} \sum_{n=0}^{\infty} b_n^r (B_2 + B_1/x_0)_n U(\tfrac{1}{2}B_2 - i\eta + n, -B_1/x_0, +2i\omega x) \tag{200}$$

  cf. equations (73) and (74). These solutions are always independent and correspond, respectively, to the asymptotic forms $a_0^r x^{-\frac{1}{2}B_2} e^{+i(\omega x - \eta \ln x)}$ and $b_0^r x^{-\frac{1}{2}B_2} e^{-i(\omega x - \eta \ln x)}$. In general the expansions for y_+ and y_- do not converge as $x \to x_0$, and these solutions are usually irregular at that point. The exception occurs when ω is an eigenfrequency and either the a_n^r or the b_n^r (but never both) are minimal as $n \to \infty$. In this case these irregular Hylleraas solutions become regular eigensolutions proportional to the regular Jaffé solutions y_1 and y_2, equations (39) and (49).

- The irregular Coulomb wavefunction solutions of the generalized Stratton type (Sec. VI):

$$\begin{aligned} y_+(x) &= x^{-B_2/2} \sum_{L=-\infty}^{\infty} a_L \left[G_{L+\nu}(\eta,z) + iF_{L+\nu}(\eta,z)\right] \\ y_-(x) &= x^{-B_2/2} \sum_{L=-\infty}^{\infty} a_L \left[G_{L+\nu}(\eta,z) - iF_{L+\nu}(\eta,z)\right] \ . \end{aligned} \tag{201}$$

  cf. equations (122). The asymptotic forms of these expansions are given by equations (123):

$$\lim_{x\to\infty} y_\pm(x) = x^{-B_2/2} \exp[\pm i(\omega x - \eta \ln(2\omega x) - \phi_\pm)] \ , \tag{202}$$

  where the $\phi_\pm$ and the necessary σ_L are given by equations (124) and (110). The expansion coefficients a_L and the phase factor ν are defined by equations (112), (113), and (121).

- The asymptotic solutions in terms of Coulomb wavefunctions (Sec. II):

$$\lim_{x\to\infty} y_{\pm}(x) = x^{B_1/2x_0}(x-x_0)^{-\frac{1}{2}(B_2+B_1/x_0)}\left[G_{\nu_a}(\eta,\omega x) \pm iF_{\nu_a}(\eta,\omega x)\right]\left[1+\mathcal{O}(x^{-3})\right] \quad (203)$$

  cf. equations (22) and (23). The asymptotic phase parameter ν_a usually differs markedly from the Coulomb wavefunction phase parameter ν, and the asymptotic form can provide a check on the full expansion in the regions of large x for which both are valid.

- The confluent hypergeometric function expansions of Sec. VII:

$$\begin{aligned}
y_1(x) &= e^{+i\omega x}\sum_{L=-\infty}^{\infty} a_L\tilde{M}(\tfrac{1}{2}B_2+i\eta, L+\nu, -2i\omega x)\\
y_2(x) &= e^{-i\omega x}\sum_{L=-\infty}^{\infty} b_L\tilde{M}(\tfrac{1}{2}B_2-i\eta, L+\nu, +2i\omega x)\\
y_+(x) &= e^{+i\omega x}\sum_{L=-\infty}^{\infty} a_L U(\tfrac{1}{2}B_2+i\eta, L+\nu, -2i\omega x)\\
y_-(x) &= e^{-i\omega x}\sum_{L=-\infty}^{\infty} b_L U(\tfrac{1}{2}B_2-i\eta, L+\nu, +2i\omega x)
\end{aligned}$$

  cf. equations (166), (167), (169), and (170). The description of these solutions given in Sec. VII is brief enough (as befits the preliminary nature of their derivation) to make further discussion unnecessary.

D. Notes on the Computer Implementation

The expressions for which I have written FORTRAN subroutines to evaluate are those for the regular Jaffé solution

$$y_1(x) = e^{+i\omega x}x^{-\frac{1}{2}B_2-i\eta}\sum_{n=0}^{\infty} a_n^r\left(\frac{x-x_0}{x}\right)^n \quad , \quad (204)$$

the Coulomb wave function expansions (122)

$$y_{\pm}(x) = x^{-B_2/2}\sum_{L=-\infty}^{\infty} a_L\left[G_{L+\nu}(\eta,z) \pm iF_{L+\nu}(\eta,z)\right] \quad , \quad (205)$$

and the associated asymptotic forms (22) and (23)

$$\lim_{x\to\infty} y_{\pm}(x) = x^{B_1/2x_0}(x-x_0)^{-\frac{1}{2}(B_2+B_1/x_0)}\left[G_{\nu_a}(\eta,\omega x) \pm iF_{\nu_a}(\eta,\omega x)\right]\left[1+\mathcal{O}(x^{-3})\right] \quad . \quad (206)$$

The Jaffé solutions are regular and analytic as $x \to x_0$, but for general ω are divergent as $x \to \infty$. The Coulomb wavefunction expansions are analytic as $x \to \infty$, but diverge as $x \to x_0$. The combination of the two representations provides a powerful computational tool for analysis of physical systems described by generalized spheroidal wave equations. The parameter regions in which the Coulomb wavefunction expansion is valid often overlap the regions of validity of the Jaffé expansions, and frequently those of the asymptotic Coulomb wavefunction solutions as well, so the three different methods of solution can be used as checks against each other.

The regular Jaffé solution is a simple power series and coding it was straightforward. However, the Coulomb wavefunction expansions are irregular as $x \to x_0$, and usually have a branch cut associated with that point. Additional branch cuts arise in the continued fractions that define the expansion coefficients

a_L and the phase parameter ν. Some of these cuts no doubt are inherent to the fractions themselves, but others are spurious and are due to the square roots that occur in the recurrence relations both for the a_L and for the Coulomb wavefunctions. I showed in Sec. VI F how the square roots could be avoided by use of Gautschi's normalizations, but the current (July 1985) version of the program implements equation (122) with the usually defined Coulomb wavefunctions (equation (111)). The branch cuts are a genuine problem since the generalized spheroidal wavefunctions are functions of seven complex parameters: x, x_0, η, ω, B_1, B_2, and B_3. The Coulomb wavefunctions are computed using an analytic extension of Steed's algorithm,[45] and branch cuts in this subroutine alone restrict the product ωx to lie in the fourth quadrant of the complex ωx plane.

It probably is not possible with algorithms of this complexity to fully predict the ranges of the parameters for which they are valid, but fortunately there are enough self-consistency checks (computation of wronskians, independent sums of series for the derivatives, *etc.*) that the accuracy of the program that implements the Coulomb wavefunction expansion can be determined internally as it is run. Although one usually cannot predict *a priori* whether the program will run with a given set of arguments, the relative error of the calculation is accurately supplied at execution. External checks on the program's results, while comforting when they are obtainable, are not strictly necessary for reliable use.

The single precision version of the program typically returns five or six decimal places of accuracy on a 36-bit DEC20. (A double precision version using the COMPLEX*16 variable type available on VAX computers gives between twelve and sixteen places.) While I have found these algorithms to be quite powerful in the analysis of the perturbation response of Schwarzschild black holes,[4] the programs are not a complete panacea to the problem of generating generalized spheroidal wavefunctions, as there are values of the parameters for which it is not possible to find a value of the phase parameter ν that satisfies equation (113). However, I do believe that the elements of analyticity inherent to Jaffé's solutions and the Coulomb wavefunction expansion provide, in the regions where they are valid, a refreshing alternative to the usual recourse of brute force numerical integration of the generalized spheroidal wave equation.

The programs are fully portable and will be described in detail in a forthcoming article.[46] Future study should be in the direction of implementing Gautschi's normalization for the Coulomb wavefunctions (Sec. VI F), and the irregular Hylleraas solutions (Sec. IV C). Jen and Hu's high frequency approximation[41] for the ordinary spheroidal wavefunctions should be extended to the generalized functions. Further investigation should be made of the confluent hypergeometric function expansions discussed in Sec. VII.

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APPENDIX A. LAGUERRE POLYNOMIALS

The Laguerre polynomials used in this paper are the Laguerre polynomials defined by Slater,[28] and in Gradshteyn and Ryzhik.[29] They are generated by

$$\sum_{n=0}^{\infty} z^n L_n^\alpha(x) = (1-z)^{-\alpha-1} e^{xz/(z-1)} \qquad (|z| < 1)$$

obey the recurrence relation

$$(n+1)L_{n+1}^\alpha(z) - (2n+\alpha+1-z)L_n^\alpha(z) + (n+\alpha)L_{n-1}^\alpha(z) = 0$$

$$xL_0^\alpha(x) = -L_1^\alpha(x) + (\alpha+1)L_0^\alpha(x)$$

and satisfy the differential property

$$x\frac{d}{dx}L_n^\alpha(x) = -(n+1)L_{n+1}^\alpha(x) + (2n+\alpha+1)L_n^\alpha(x) - (n+\alpha)L_{n-1}^\alpha(x)$$

$$\frac{d}{dx}L_0^\alpha(x) = 0 \; .$$

Laguerre polynomials are solutions to the confluent hypergeometic equation

$$x\frac{d^2}{dx^2}L_n^\alpha(x) + (\alpha+1-x)\frac{d}{dx}L_n^\alpha(x) + nL_n^\alpha(x) = 0 \; ,$$

and $L_n^\alpha(x)$ is related to Kummer's function ${}_1F_1(a,b,x)$ by

$$L_n^\alpha(x) = \frac{\Gamma(\alpha+n+1)}{n!\Gamma(\alpha+1)}\, {}_1F_1(-n,\alpha+1,x)$$

There are several different normalizations of Laguerre polynomials currently in use. Three of them are listed below together with the names of the authors that have used them, and their relation to the Laguerre polynomials as normalized by Slater.

1. A. Messiah[47] and Morse and Feshbach[10]:
   L_n^m (Messiah, Morse and Feshbach) $= (n+m)!L_n^m$ (Slater)
2. E.C. Titchmarsh[48]:
   L_n^m (Titchmarsh) $= n!L_n^m$ (Slater)
3. E. Hylleraas[7]:
   L_n^m (Hylleraas) $= L_{n-m}^m$ (Slater)

APPENDIX B. AN INTEGRAL TRANSFORM

An outline of a proof of the validity of equation (62) is given using the standard theory of integral transforms.[49]

Start with equation (1):

$$x(x-x_0)\frac{d^2y}{dx^2}+(B_1+B_2x)\frac{dy}{dx}+\left[\omega^2x(x-x_0)-2\eta\omega(x-x_0)+B_3\right]y=0\ \ .$$

With the substitution $y(x)=e^{i\omega x}f(x)$ and the restriction $i\eta=B_2/2-1$ the differential equation for f is

$$\mathcal{L}_x\left\{f(x)\right\}=0 \tag{B1}$$

where the differential operator $\mathcal{L}_x$ is defined by

$$\mathcal{L}_x\equiv\left\{\begin{array}{c} x(x-x_0)\frac{d^2}{dx^2}+[B_1+B_2x+2i\omega x(x-x_0)]\frac{d}{dx} \\ +[2i\omega(B_2-1)(x-x_0)+i\omega x_0(B_2+B_1/x_0)+B_3] \end{array}\right\}\ .$$

With the further substitution $f(x)=x^{1+B_1/x_0}g(x)$, the differential equation for $g(x)$ is

$$\mathcal{M}_x\left\{g(x)\right\}=0$$

where the differential operator $\mathcal{M}_x$ is in turn defined by

$$\mathcal{M}_x\equiv\left\{\begin{array}{c} x(x-x_0)\frac{d^2}{dx^2}+[-B_1-2x_0+(2+B_2+2B_1/x_0)x+2i\omega x(x-x_0)]\frac{d}{dx} \\ +[(B_2+B_1/x_0)(2i\omega x-i\omega x_0+1+B_1/x_0)+B_3] \end{array}\right\}$$

so that $\mathcal{L}_x\{f\}=x^{1+B1/x_0}\mathcal{M}_x\{g\}$. The adjoint operator to $\mathcal{L}_x$ is

$$\bar{\mathcal{L}}_x=\left\{\begin{array}{c} x(x-x_0)\frac{d^2}{dx^2}+[-B_1-2x_0+(4-B_2)x-2i\omega x(x-x_0)]\frac{d}{dx} \\ +[2i\omega(B_2-3)x-i\omega x_0(B_2-B_1/x_0-4)+2-B_2+B_3] \end{array}\right\}\ .$$

The kernel

$$K(x,t)\equiv e^{2i\omega x(t-x_0)/x_0}(t-x_0)^{B_2+B_1/x_0-1}$$

has the property that $\mathcal{M}_x\left\{K(x,t)\right\}=\bar{\mathcal{L}}_t\left\{K(x,t)\right\}$. Hence if we write

$$\bar{f}(x)=x^{1+B_1/x_0}\int_c K(x,t)f(t)dt \tag{B2}$$

we can operate with $\mathcal{L}_x$ on $\bar{f}$ and find successively

$$\begin{aligned}
\mathcal{L}_x\left\{\bar{f}(x)\right\} &= \mathcal{L}_x\left\{x^{1+B_1/x_0}\int_c K(x,t)f(t)dt\right\} \\
&= x^{1+B_1/x_0}\int_c\left(\mathcal{M}_x\left\{K(x,t)\right\}\right)f(t)dt \\
&= x^{1+B_1/x_0}\int_c\left(\bar{\mathcal{L}}_t\left\{K(x,t)\right\}\right)f(t)dt \\
&= x^{1+B_1/x_0}\left[\int_c K(x,t)\mathcal{L}_t\left\{f(t)\right\}dt+\int_c\frac{d}{dt}P(x,t)\,dt\right]
\end{aligned}$$

where the bilinear concomitant $P(x,t)$ is given by

$$P(x,t)=\left\{\begin{array}{c} t(t-x_0)[f(t)\frac{d}{dt}K(x,t)-K(x,t)\frac{d}{dt}f(t)]\quad+ \\ [2i\omega t^2+(B_2+2B_1/x_0-2i\omega x_0)t-B_1-x_0]K(x,t)f(t) \end{array}\right\}\ .$$

Therefore two functions $\bar{f}(x)$ and $f(x)$ related by equation (B2) will both satisfy differential equation (B1) provided the contour c is chosen such that the integral converges and the value of $P(x,t)$ is the same at each end of the contour.

APPENDIX C. A SECOND SOLUTION BY EXPANSION IN IRREGULAR CONFLUENT HYPERGEOMETRIC FUNCTIONS

The validity of equation (70) is proven for arbitrary η, and convergence properties of the expansion are discussed. Start with equation (1):

$$x(x-x_0)\frac{d^2y}{dx^2} + (B_1 + B_2 x)\frac{dy}{dx} + \left[\omega^2 x(x-x_0) - 2\eta\omega(x-x_0) + B_3\right] y = 0$$

The substitution $y(x) = e^{+i\omega x} f(x)$ yields equation (56):

$$x(x-x_0)f_{,xx} + [B_1 + B_2 x + 2i\omega x(x-x_0)]f_{,x} + [(B_2 + 2i\eta)i\omega x + 2\eta\omega x_0 + i\omega B_1 + B_3]f = 0$$

which with the substitutions $z = -2i\omega x$ and $z_0 = -2i\omega x_0$ can be more suggestively written as

$$z(z-z_0)\frac{d^2 f}{dz^2} + (D_1 + D_2 z - z^2)\frac{df}{dz} + (D_3 + D_4 z)f = 0 \tag{C1}$$

where

$$\begin{aligned} D_1 &= -2i\omega B_1 \\ D_2 &= B_2 - 2i\omega x_0 \\ D_3 &= B_3 + 2\eta\omega x_0 + i\omega B_1 \\ D_4 &= -\tfrac{1}{2}B_2 - i\eta \ . \end{aligned} \tag{C2}$$

We expand f(z) as

$$f(z) = \sum_{n=0}^{\infty} b_n U(a+n, -B_1/x_0, z) \tag{C3}$$

where the $U(a+n, -B_1/x_0, z)$ are irregular solutions to the confluent hypergeometric equation

$$zU_{n,zz} - (B_1/x_0 + z)U_{n,z} - (a+n)U_n = 0 \ . \tag{C4}$$

I have denoted $U(a+n, -B_1/x_0, z)$ by U_n for notational convenience, and the parameter a is to be determined. The confluent hypergeometric functions used here are those defined by Slater.[28] They satisfy the differential property

$$zU_{n,z} = -(n+a)U_n + (n+a)(n+a+1+B_1/x_0)U_{n+1} \tag{C5}$$

and are a solution that is minimal as $n \to \infty$ of the recurrence relation

$$U_{n-1} - [2(n+a) + B_1/x_0 + z]U_n + (n+a)(n+a+1+B_1/x_0)U_{n+1} = 0 \ . \tag{C6}$$

Substituting (C3) into (C1) and using (C4), (C5), and (C6) we obtain

$$\begin{aligned} \sum_{n=0}^{\infty} b_n \{ &(n+a-B_2/2-i\eta)U_{n-1} \\ &+(n+a)(n+a+1+B_1/x_0)(n+a+B_2/2-i\eta+B_1/x_0)U_{n+1} \\ &- \left[2(n+a)^2 + (2B_1/x_0 - 2i\eta - 2i\omega x_0)(n+a) \right. \\ &\left. -(2\eta\omega x_0 + (B_2/2+i\eta)B_1/x_0 + i\omega B_1 + B_3)\right] U_n \} = 0 \end{aligned} \tag{C7}$$

The coefficient of U_{-1} must vanish if the series is to start at $n = 0$, so we must fix a to be $a = B_2/2 + i\eta$. Equation (C7) can then be re-indexed to yield

$$(\bar{\alpha}_0 b_1 + \bar{\beta}_0 b_0)U_0 + \sum_{n=1}^{\infty}(\bar{\alpha}_n b_{n+1} + \bar{\beta}_n b_n + \bar{\gamma}_n b_{n-1})U_n = 0 \tag{C8}$$

where

$$\begin{aligned}
\bar{\alpha}_n &= n+1 \\
\bar{\beta}_n &= -[2n^2 + 2(B_2 + B_1/x_0 + i\eta - i\omega x_0)n + (B_2 + B_1/x_0)(B_2/2 + i\eta - i\omega x_0) - B_3] \\
\bar{\gamma}_n &= (n + B_2/2 + i\eta - 1)(n + B_2/2 + i\eta + B_1/x_0)(n - 1 + B_2 + B_1/x_0)
\end{aligned}$$

Equation (C8) can hold only if the coefficient of each U_n vanishes. Letting $b_n = \Gamma(B_2 + B_1/x_0 + n)a_n$ in expansion (C3) and recurrence relation (C8), we can obtain as the recurrence relation for the a_n

$$\begin{aligned}
\alpha_0 a_1 \quad + \beta_0 a_0 \qquad &= 0 \\
\alpha_n a_{n+1} + \beta_n a_n + \gamma_n a_{n-1} &= 0 \quad n = 1, 2 \ldots
\end{aligned} \tag{C9}$$

where

$$\begin{aligned}
\alpha_n &= (n+1)(n + B_2 + B_1/x_0) \\
\beta_n &= \left\{ \begin{array}{l} -2n^2 - 2[B_2 + i(\eta - \omega x_0) + B_1/x_0]n \\ -[(B_2/2 + i\eta)(B_2 + B_1/x_0) - i\omega(B_1 + B_2 x_0) - B_3] \end{array} \right\} \\
\gamma_n &= (n - 1 + B_2/2 + i\eta)(n + B_2/2 + i\eta + B_1/x_0)
\end{aligned} \tag{C10}$$

which is the same recurrence relation as for the Jaffé coefficients, equation (41).

Convergence of series (C3) may be analyzed by considering the sequence of functions $\{\overline{U}_n,\ n = 0, 1, 2 \ldots\}$ defined by $\overline{U}_n = \Gamma(c+n)U(a, b, z)$, where $a = B_2/2 + i\eta$, $b = -B_1/x_0$, and $c = B_2 + B_1/x_0$. The $\overline{U}_n$ are a minimal solution to the recurrence relation

$$(n+a)(n+a+1-b)/(n+c)\overline{U}_{n+1} - (2n + 2a - b + z)\overline{U}_n + (n - 1 + c)\overline{U}_{n-1} = 0 \tag{C11}$$

which, after dividing by n and retaining terms to $O(1/n)$, takes the limiting form

$$[1 + (2a + 1 - b - c)/n]\overline{U}_{n+1} - [2 + (2a - b + z)/n]\overline{U}_n + [1 + (c-1)/n]\overline{U}_{n-1} + O(n^{-2}) \approx 0$$

Hence

$$\lim_{n\to\infty} \frac{\overline{U}_{n+1}}{\overline{U}_n} = 1 - \sqrt{-\frac{z}{n}} \ .$$

See the convergence discussion in Sec. 4a. Here $z = -2i\omega x$ and the branch of the square root is taken such that $Re(\sqrt{-z}) \geq 0$ (the $\overline{U}_n$ being a minimal solution to (C6)). We do not consider the case when z is positive real. Since

$$\lim_{n\to\infty} \frac{a_{n+1}}{a_n} = 1 \pm \sqrt{-2i\omega x_0/n}$$

(see equations (42) and (44)), our final result is that the limiting ratio of successive terms of series (C3) is given by

$$\lim_{n\to\infty} \frac{b_{n+1}U(a+n+1, b, -2i\omega x)}{b_n U(a+n, b, -2i\omega x)} = 1 - \frac{\sqrt{-2i\omega x} \pm \sqrt{-2i\omega x_0}}{\sqrt{n}} \ . \tag{C12}$$

The $(+)$ sign is obtained when ω is an eigenfrequency and the a_n are themselves a minimal solution to recurrence relation (C9). Then the series converges at $x = x_0$. When ω is not an eigenfrequency the a_n are dominant and the $(-)$ sign prevails in equation (C12). In this case the series converges for all $x > x_0$, but diverges when $x = x_0$. This is precisely the behaviour expected of a second solution.

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