The Helium Wave Equation*

T. H. GRONWALL** Columbia University, New York, N. Y. (Received February 3, 1937)

This paper represents an attempt to solve the equation $\nabla^2 \psi + (1/2)\psi_z + (1/4r)(E-V)\psi = 0$, which is the Gronwall form of the wave equation for helium S states. The equation $\nabla^2 u + (1/z)u_z$ =0 is separable in polar coordinates (r, β, φ) , and has solutions $u_{mk} = r^{2m-k} \sin^k \beta v_{mk} (\sin^2 \beta) e^{ik\varphi}$ $=r^{2m-k}w_{mk}(\beta, \varphi)$, where the v_{mk} 's are Jacobi polynomials, and the w_{mk} 's form a complete orthogonal set of surface functions. The function ψ is expanded as $\psi = \sum \psi_{mk}(r^{\frac{1}{2}})w_{mk}$; resulting in an

infinite system of ordinary linear differential equations for the ψ_{mk} 's.

EDITOR'S INTRODUCTION

FTER persistent effort, the late T. H. Gronwall of Columbia University succeeded in putting the wave equation for helium S states into a remarkably simple form.¹ He then made an extensive study of the equation in order to learn something about the nature of the solutions. Many calculations had been made when death intervened, and the notes were left behind in an unordered state. Largely owing to the difficulty of arranging them, they were still unpublished in October, 1936, when they came into my hands through the courtesy of Dr. F. Bohnenblust. They have since proved very valuable for my own research, and so it is felt that the essential results should be published. Those results which are to be used in the following paper have been checked, but the unused results, such as the formulae for matrix elements in the Appendix, have not. (The derivation or verification is easy but tedious, and is hence left to any reader who may be sufficiently concerned.) For the sake of clarity and brevity, I have made several insertions, which are indicated by enclosure within curly brackets. Finally, it is a pleasure to express my appreciation of the opportunity to use freely the unpublished work of Gronwall, and to thank Professor E. Hille for permission to publish it.

WAVE EQUATION

The wave equation for S states of the helium atom may be written^{1, 2} in the form

$$\nabla^{2}\psi + \frac{1}{z}\frac{\partial\psi}{\partial z} + \frac{1}{r}\left(\frac{E}{4} + \frac{1}{[2(r+y)]^{\frac{1}{2}}} + \frac{1}{[2(r-y)]^{\frac{1}{2}}} - \frac{1}{2Z(r-x)^{\frac{1}{2}}}\right)\psi = 0, \tag{1}$$

where

$$4x = r_1^2 + r_2^2 - r_{12}^2 = 2r_1r_2 \cos \theta,$$

$$4y = r_1^2 - r_2^2,$$

$$4z = 4 \times \text{area of } \Delta \text{ with sides } r_1, r_2, r_{12} = 2r_1r_2 \sin \theta,$$

$$4r = 4(x^2 + y^2 + z^2)^{\frac{1}{2}} = r_1^2 + r_2^2.$$

Here r_1 and r_2 refer to the electron-nucleus distances, θ denotes the angle between the corresponding radius vectors, and r_{12} denotes the interelectronic distance. Since the range of θ is $0 \le \theta \le \pi$, the domain of x, y, and z is the upper half-space $z \ge 0$. {It may be noted that $\tan \theta = (z/x)$, so that θ is the angle in the xz plane from the x axis to the projection of the radius vector \mathbf{r} upon this plane. Also, if we let $\alpha = \tan^{-1} (r_2/r_1)$, it follows that 2α is the angle from the y axis to the radius vector. For $\cos 2\alpha$ = 2 cos² α - 1; cos $\alpha = [r_1/(r_1^2 + r_2^2)^{\frac{1}{2}}]$; and cos $2\alpha = [(r_1^2 - r_2^2)/(r_1^2 + r_2^2)] = (y/r)$.

^{*} Edited by J. H. Bartlett, Jr., University of Illinois, Urbana, Illinois. ** Dr. T. H. Gronwall died May 9, 1932. This paper together with other manuscripts was then transferred from the physics department of Columbia University where this work was done to the care of Dr. E. Hille of Princeton University. Γ. H. Gronwall, Annals of Mathematics 33, 279 (1932).

² The rational units of length and energy of Hylleraas are used. See Zeits. f. Physik 54, 347 (1929).

The variational problem corresponding to Eq. (1) is

$$\delta \int \left[\psi_x^2 + \psi_y^2 + \psi_z^2 - \frac{1}{r} \left(\frac{E}{4} + \frac{1}{[2(r+y)]^{\frac{1}{2}}} + \frac{1}{[2(r-y)]^{\frac{1}{2}}} - \frac{1}{2Z(r-x)^{\frac{1}{2}}} \right) \psi^2 \right] z \, dx \, dy \, dz = 0.$$

In order that this problem have a meaning, the integral must exist. Such a requirement is sufficient to exclude the so-called "second solutions" for hydrogen S states.³ We shall, therefore, adopt this as a necessary boundary condition on the (univalent) function ψ , which will also be required to be of class C^2 , except perhaps on the (+x) and y axes, where ψ might conceivably become infinite.

Introducing polar coordinates, with the z axis as the pole,

$$x = r \cos \varphi \sin \beta,$$

$$y = r \sin \varphi \sin \beta,$$

$$z = r \cos \beta,$$

we have

$$\delta \int_{0}^{\infty} \int_{0}^{2\pi} \int_{0}^{\pi/2} \left[\frac{1}{4} \psi_{s}^{2} + \frac{1}{s^{2} \sin^{2} \beta} \psi_{\varphi}^{2} + \frac{1}{s^{2}} \psi_{\beta}^{2} - \left(\frac{E}{4} + \frac{f}{s}\right) \psi^{2} \right] s^{5} ds \sin \beta \cos \beta d\beta d\varphi = 0,$$

where

$$f = [2(1 + \sin \varphi \sin \beta)]^{-\frac{1}{2}} + [2(1 - \sin \varphi \sin \beta]^{-\frac{1}{2}} - (1/2Z)[1 - \cos \varphi \sin \beta]^{-\frac{1}{2}}, \text{ and } r = s^2.$$

The corresponding differential equation is

$$\psi_{ss} + (5/s)\psi_s + (4/s^2\sin^2\beta)\psi_{\varphi\varphi} + (4/s^2)(\psi_{\beta\beta} + 2\cot 2\beta\psi_\beta) + [E + (4f/s)]\psi = 0.$$
(2)

BASIC ORTHOGONAL FUNCTIONS

To find an appropriate orthogonal system on the half-sphere, we consider the equation

$$u_{ss} + (5/s)u_s + (4/s^2 \sin^2 \beta)u_{\varphi\varphi} + (4/s^2)(u_{\beta\beta} + 2 \cot 2\beta u_{\beta}) = 0.$$
(3)

Substituting

$$u = s^{4m-2k} \sin^2 k \varphi g_{mk}(t), \quad t = \sin^2 \beta$$

where *m* and *k* are integers, $m \ge k \ge 0$, we find

$$\left[t(1-t)g'_{mk}\right]' + \left[\left(m-\frac{k}{2}\right)\left(m+1-\frac{k}{2}\right) - (k^2/4t)\right]g_{mk} = 0.$$

Now, writing $g_{mk}(t) = t^{k/2}v(m, k, t)$, the preceding equation gives

$$t(1-t)v_{tt} + [k+1-(k+2)t]v_t + (m+1)(m-k)v = 0.$$
(4)

{This equation may be recognized as the hypergeometric equation in the usual form.}

The only solution of (4) which is finite both at t=0 and t=1 is the Jacobi polynomial F(k-m, m+1, m)k+1, t), $m \ge k \ge 0$ (multiplied by a constant).

Now⁴

$$\int_{0}^{1} t^{k} F(k-m, m+1, k+1, t) F(k-m', m'+1, k+1, t) dt = (1/2m+1-k) [\Gamma(m-k+1)\Gamma(k+1)/\Gamma(m+1)]^{2} \delta_{mm'}.$$

³ The editor (J. H. B.) desires to thank Professor R. Courant for informing him of this. ⁴ This follows from Jordan, *Cours d'Analyse III*, 242, Eq. (45, 46) upon making $\alpha = \gamma = k+1$ and n = m-k.

We also have (Jordan⁴)

$$F(k-m, m+1, k+1, t) = [\Gamma(k+1)/\Gamma(m+1)]t^{-k}(d/dt)^{m-k}[t^m(1-t)^{m-k}].$$

Writing

$$v(m \ k \ t) = [\Gamma(m+1)/\Gamma(k+1)\Gamma(m-k+1)]F(k-m, m+1, k+1, t), \quad 0 \le k \le m,$$

we find

$$N_{mm'k} = \int_0^1 t^k v(m \ k \ t) v(m' \ k \ t) dt = (1/2m + 1 - k) \delta_{mm'}$$
(5)

and

From (6)

$$v(m \ k \ t) = \left[1/\Gamma(m-k+1)\right]t^{-k}(d/dt)^{m-k}\left[t^m(1-t)^{m-k}\right] = \sum_{\nu=0}^{m-k} (-)^{\nu} \frac{(m+\nu)!}{\nu!(k+\nu)!(m-k-\nu)!}t^{\nu}.$$
 (6)

$$\begin{cases} v(m \ k \ 0) = [m \ !/k \ !(m-k) \ !], \\ v(m \ k \ 1) = (-)^{m-k}, \end{cases}$$
(7)

and by (4)
$$\begin{cases} v_{\iota}(m \ k \ 0) = -\left[(m+1) \ !/(k+1) \ !(m-k-1) \ !\right], \\ v_{\iota}(m \ k \ 1) = (-)^{m-k}(m+1)(m-k). \end{cases}$$
(8)

EXPANSION IN TERMS OF ORTHOGONAL FUNCTIONS

The variational problem in terms of t may be written as

$$\delta \int_{0}^{\infty} \int_{0}^{2\pi} \int_{0}^{1} \left[(1/4) \psi_{s}^{2} + (1/s^{2}t) \psi_{\varphi}^{2} + \left[4t(1-t)/s^{2} \right] \psi_{t}^{2} - \left[(E/4) + (f/s) \right] \psi^{2} \right] s^{5} \, ds \, d\varphi \, dt = 0. \tag{9}$$

Expand

$$\psi = \sum_{mk} c_{mk} \psi_{mk}(s) g_{mk}(t) \, \frac{\cos}{\sin} \, k \varphi, \tag{10}$$

where the cosines belong to the *para* terms and the sines to the *ortho* terms. In the following treatment, we shall consider only the *para* terms.

Setting $\epsilon_k = 2$ for k = 0, and $\epsilon_k = 1$ for k > 0, we obtain

$$\begin{split} &\int_{0}^{2\pi} d\varphi \int_{0}^{1} dt \big[(1/4) \psi_{s}^{2} + (1/s^{2}t) \psi_{\varphi}^{2} + \big[4t(1-t)/s^{2} \big] \psi_{t}^{2} \big] \\ &= \sum_{mm'k} \pi \epsilon_{k} c_{mk} c_{m'k} \int_{0}^{1} dt \big[(1/4) \psi'_{mk} \psi'_{m'k} g_{mk} g_{m'k} + (1/s^{2}) \psi_{mk} \psi_{m'k} \big\{ (k^{2}/t) g_{mk} g_{m'k} + 4t(1-t) g'_{mk} g'_{m'k} \big\} \big] \\ &= \sum_{mm'k} \pi \epsilon_{k} c_{mk} c_{m'k} \int_{0}^{1} dt \big[(1/4) \psi'_{mk} \psi'_{m'k} g_{mk} g_{m'k} + (1/s^{2}) \psi_{mk} \psi_{m'k} (2m-k) (2m+2-k) g_{mk} g_{m'k} \big] \\ &= \sum_{mk} (\pi \epsilon_{k} c^{2}_{mk} / 2m + 1 - k) \big[(1/4) (\psi'_{mk})^{2} + (1/s^{2}) (2m-k) (2m+2-k) \psi^{2}_{mk} \big]. \end{split}$$

We have integrated by parts, used the differential equation for g_{mk} and Eq. (5).

The potential energy may be treated in like manner. Let us write

$$\int_{0}^{2\pi} d\varphi \int_{0}^{1} dt \psi^{2} [\{2(1+t^{\frac{1}{2}}\sin\varphi)\}^{-\frac{1}{2}} + \{2(1-t^{\frac{1}{2}}\sin\varphi)\}^{-\frac{1}{2}} - (1/2Z)\{1-t^{\frac{1}{2}}\cos\varphi\}^{-\frac{1}{2}}] = \sum_{mkm'k'} a(mkm'k')c_{mk}c_{m'k'}\psi_{mk}\psi_{m'k'}.$$

Then
$$a(mk \ m' \ k') = \int_0^{2\pi} d\varphi \int_0^1 dt [\{2(1+t^{\frac{1}{2}}\sin \varphi)\}^{-\frac{1}{2}} + \cdots]g_{mk}g_{m'k'}\cos k\varphi\cos k'\varphi.$$

To simplify, we observe that, n being an integer,

$$\int_{0}^{2\pi} (1+t^{\frac{1}{2}}\sin\varphi)^{-\frac{1}{2}}e^{in\varphi}d\varphi = e^{3n\pi i/2} \int_{0}^{2\pi} (1-t^{\frac{1}{2}}\cos\varphi)^{-\frac{1}{2}}e^{in\varphi}d\varphi$$
$$\int_{0}^{2\pi} (1-t^{\frac{1}{2}}\sin\varphi)^{-\frac{1}{2}}e^{in\varphi}d\varphi = e^{n\pi i/2} \int_{0}^{2\pi} (1-t^{\frac{1}{2}}\cos\varphi)^{-\frac{1}{2}}e^{in\varphi}d\varphi.$$

It follows that

and

$$a(mk, m'k') = (\sqrt{2} \cos(|k-k'|\pi/2) - (1/2Z))I(mk m'k'; |k-k'|) + (\sqrt{2} \cos((k+k')\pi/2) - (1/2Z))I(mk m'k'; k+k'),$$

where

Let

$$I(mk \; m'k'; n) = (1/2) \int_0^{2\pi} d\varphi \int_0^1 dt (1 - t^{\frac{1}{2}} \cos \varphi)^{-\frac{1}{2}} g_{mk} g_{m'k'} \cos n\varphi.$$

The variational problem is now, putting $c_{mk}^2 = (2m+1-k)/\pi\epsilon_k$,

$$\delta \int_{0}^{\infty} \{ \sum_{mk} [(1/4)(\psi'_{mk})^{2} + (1/s^{2})(2m-k)(2m+2-k)\psi^{2}_{mk} - (E/4)\psi^{2}_{mk}] - \sum_{mk} a(mk \ m'k')\psi_{mk}\psi_{m'k'}c_{mk}c_{m'k'} \} s^{5}ds = 0.$$

The corresponding Euler equations are, if we number the functions by setting $n = \frac{1}{2}m(m+1) + k$, and if we set $A(mk \ m'k') = 2\pi c_{mk}c_{m'k'}a(mk \ m'k')$,

$$(1/4)(s^{5}\psi_{n}')' - (2m-k)(2m+2-k)s^{3}\psi_{n} + (E/4)s^{5}\psi_{n} + \sum_{n'} [A(nn')/2\pi]s^{4}\psi_{n'} = 0.$$
(11)

{This is an infinite system of ordinary linear differential equations of the second order. We should like to find a solution which is finite everywhere.} Substitute $\psi_n = e^{-(\sqrt{-E})s} f_n(s)$, and let $\rho = 2(-E)^{\frac{1}{2}s}$, obtaining

$$\rho^{2} f_{n}^{\prime\prime} + (5\rho - \rho^{2}) f_{n}^{\prime} - 4(2m - k)(2m + 2 - k) f_{n} - (5/2)\rho f_{n} + \sum_{n'} \frac{A(nn')}{\pi(-E)^{\frac{1}{2}}} \rho f_{n'} = 0.$$
(12)

(The primes on f denote differentiation $re \rho$.)

$$b(nn') = A(nn')/\pi(-E)^{\frac{1}{2}}$$
 and set $f_n = \sum_{\nu=0}^{\infty} c_n^{(\nu)} \rho^{\nu}$. (13)

The recursion formula is then

$$(\nu - 4m + 2k)(\nu + 4 + 4m - 2k)c_n^{(\nu)} = (\nu + \frac{3}{2})c_n^{(\nu-1)} - \sum_{n'} b_{nn'}c_{n'}^{(\nu-1)}.$$
(14)

{Gronwall attempted to cut off the series (13) by setting $c_n^{(\nu)} = 0$. He calculated $A_{nn'}$ for n, n' = 0, 1, 2and solved the equations (14) for $\nu(-E)^{\frac{1}{2}}$. If this procedure were significant, then one might expect to obtain three eigenvalues of helium in this manner. However, it is not clear which three they would be, except that they would be of ¹S type. If it be assumed that they are the three lowest, and if one substitutes the experimentally observed values, then the resulting values of ν do not agree with one another. For this and other reasons, we therefore omit the reproduction of the calculations.

Gronwall also expanded the $c_n^{(\nu)}$ in factorial series of the form

$$c_n^{(\nu)} = \sum_{\mu=0}^{\infty} c_{n\mu} / \Gamma(\nu + \mu + \alpha),$$

and determined relations between the $c_{n\mu}$'s.

Appendix

1. Recursion formulae for the functions v(m k t)

$$tv(m, k, t) = -\left[(m+1)(m+1-k)/(2m+1-k)(2m+2-k)\right]v(m+1, k, t) \\ + \left\{\left[2m^2+2m(1-k)+k(k-1)\right]/(2m-k)(2m+2-k)\right\}v(m \ k \ t) \\ - \left[m(m-k)/(2m-k)(2m+1-k)\right]v(m-1, \ k, t), \right.$$
(15)
$$- \left[m(m-k)/(2m-k)(2m+1-k)\right]v(m-1, \ k, t), \\ t(1-t)v'(m, \ k, t) = \left[(m+1)(m-k)/(2m-k)(2m+2-k)\right]v(m \ k \ t) \\ - \left[k(m+1)(m-k)/(2m-k)(2m+1-k)\right]v(m-1, \ k, t), \\ tv'(m \ k \ t) + (m+1)v(m \ k \ t) + \left[(m+1)/(2m+2-k)\right]v'(m+1, \ k, t) - \left[(m+1-k)/(2m+2-k)\right]v'(m \ k \ t) = 0, \\ tv'(m \ k \ t) - (m-k)v(m \ k \ t) - \left[m/(2m-k)\right]v'(m \ k \ t) + \left[(m-k)/(2m-k)\right]v'(m-1, \ k, t) = 0, \\ v(m, \ k-1, \ t) = \left[(m+1)/(2m+2-k)\right]v(m+1, \ k, t) - \left[(m+1-k)/(2m+2-k)\right]v(m \ k \ t), \\ tv(m, \ k+1, \ t) = -\left[(m-k)/(2m-k)\right]v(m \ k \ t) + \left[m/2m-k\right]v(m-1, \ k, t) = 0, \\ tv(m, \ k+1, \ t) = -\left[(m-k)/(2m-k)\right]v(m \ k \ t) + \left[m/2m-k\right]v(m-1, \ k, t) = 0, \\ tv(m, \ k+1, \ t) = -\left[(m-k)/(2m-k)\right]v(m \ k \ t) + \left[m/2m-k\right]v(m-1, \ k, t) = 0, \\ tv(m, \ k+1, \ t) = -\left[(m-k)/(2m-k)\right]v(m \ k \ t) + \left[m/2m-k\right]v(m-1, \ k, t) = 0, \\ tv(m, \ k+1, \ t) = -\left[(m-k)/(2m-k)\right]v(m \ k \ t) + \left[m/2m-k\right]v(m-1, \ k, t) = 0, \\ tv(m, \ k+1, \ t) = -\left[(m-k)/(2m-k)\right]v(m \ k \ t) + \left[m/2m-k\right]v(m-1, \ k, t) = 0, \\ tv(m, \ k+1, \ t) = -\left[(m-k)/(2m-k)\right]v(m \ k \ t) + \left[m/2m-k\right]v(m-1, \ k, t) = 0, \\ tv(m, \ k+1, \ t) = -\left[(m-k)/(2m-k)\right]v(m \ k \ t) + \left[m/2m-k\right]v(m-1, \ k, t) = 0, \\ tv(m, \ k+1, \ t) = -\left[(m-k)/(2m-k)\right]v(m \ k \ t) + \left[m/2m-k\right]v(m-1, \ k, t) = 0, \\ tv(m, \ k+1, \ t) = -\left[(m-k)/(2m-k)\right]v(m \ k \ t) + \left[(m-k)/(2m-k)\right]v(m-1, \ k, t) = 0, \\ tv(m, \ k+1, \ t) = -\left[(m-k)/(2m-k)\right]v(m \ k \ t) + \left[(m-k)/(2m-k)\right]v(m-1, \ k, t) = 0, \\ tv(m, \ k+1, \ t) = -\left[(m-k)/(2m-k)\right]v(m \ k \ t) + \left[(m-k)/(2m-k)\right]v(m-1, \ k, t) = 0, \\ tv(m, \ k+1, \ t) = -\left[(m-k)/(2m-k)\right]v(m \ k \ t) + \left[(m-k)/(2m-k)\right]v(m-1, \ k, t) = 0, \\ tv(m, \ k+1, \ k+1, \ k) = -\left[(m-k)/(2m-k)\right]v(m \ k+1, \ k) = 0, \\ tv(m, \ k+1, \ k) = -\left[(m-k)/(2m-k)\right]v(m \ k+1, \ k) = 0, \\ tv(m, \ k+1, \ k) = -\left[(m-k)/(2m-k)\right]v(m \ k+1, \ k) = 0, \\ tv(m, \ k+1, \ k) = -\left[(m-k)/(2m-k)\right]v(m \ k+1, \ k) = 0, \\ tv(m, \ k+1, \ k) = 0, \\ tv(m, \ k+$$

$$(m, k+1, t) = -[(m-k)/(2m-k)]v(m k t) + [m/2m-k]v(m-1, k, t) = C_k v(m k t) + D_k v(m-1, k, t).$$
(20)

2. Expression for I(m, k m', k', n) in terms of the v's

Integrate with respect to φ .

$$(1-t^{\frac{1}{2}}\cos\varphi)^{-\frac{1}{2}} = \sum_{\nu=0}^{\infty} \frac{(2\nu)!}{2^{2\nu}\nu!\nu!} t^{\nu/2}\cos^{\nu}\varphi,$$

$$\frac{1}{2} \int_{0}^{2\pi} (1 - t^{\frac{1}{2}} \cos \varphi)^{-\frac{1}{2}} e^{in\varphi} d\varphi = \sum_{\mu=0}^{\infty} c_{\mu} t^{n/2+\mu},$$

$$c_{\mu} = \frac{\pi}{2^{3n+6\mu}} \frac{(2n+4\mu)!}{\mu!(n+\mu)!(n+2\mu)!} \cdot$$

 $\int_{0}^{2\pi} e^{in\varphi} \cos^{\nu} \varphi d\varphi = \frac{\pi}{2^{\nu-1}} \frac{\nu!}{\mu!(\nu-\mu)!} \delta_{\nu, n+2\mu}.$

where

We have

$$\frac{c_{\mu+1}}{c_{\mu}} = \frac{\left(\frac{2n+1}{4}+\mu\right)\left(\frac{2n+3}{4}+\mu\right)}{(1+\mu)(n+1+\mu)} \quad \text{and} \quad c_0 = \frac{\pi}{2^{3n}} \frac{(2n)!}{n!n!},$$

so that

$${}^{\frac{1}{2}} \int_{0}^{2\pi} (1-t^{\frac{1}{2}}\cos\varphi)^{-\frac{1}{2}} e^{in\varphi} d\varphi = t^{n/2} F_n(t),$$

$$F_n(t) = \frac{\pi}{2^{3n}} \frac{(2n)!}{n!n!} F\left(\frac{2n+1}{4}, -\frac{2n+3}{4}, -n+1, t\right).$$

where

This gives

 $I(m \ k, \ m' \ k'; \ n) = \int_0^1 t^{(n+k+k')/2} F_n(t) v(m \ k \ t) v(m' \ k' \ t) dt.$ (21)

For the problem at hand, we require the knowledge of I(m k, m' k'; n) only for n = k + k' and n = |k - k'|.

3. Formula for I(m, k, 0, 0, k)

By (21),
$$I(m, k, 0, 0, k) = \int_0^1 t^k F_k v(m \ k \ t) dt.$$

But $t^k F_k = [16/(2k+1)(2k+3)][t^{k+1}(1-t)F_k']'$ from the differential equation. Hence

$$(1/16)(2k+1)(2k+3)I(m \ k \ 0 \ 0 \ k) = \int_0^1 v[t^{k+1}(1-t)F_{k'}]'dt.$$

Integrate by parts and observe that

$$t^{k+1}(1-t) \frac{dF_k}{dt} \rightarrow 1/\sqrt{2} \text{ as } t \rightarrow 1$$

 $F_k \rightarrow \left[\Gamma(k+1) / \Gamma\left(\frac{k}{2} + \frac{1}{4}\right) \Gamma\left(\frac{k}{2} + \frac{3}{4}\right) \right] \log (1-t) \quad \text{as} \quad t \rightarrow 1.$

and

Then
$$\int_{0}^{1} v [t^{k+1}(1-t)F_{k'}]' dt = ((-)^{m-k}/\sqrt{2}) + \int_{0}^{1} F_{k} [t^{k+1}(1-t)v'(m \ k \ t)]' dt = ((-)^{m-k}/\sqrt{2}) - (m+1)(m-k) \int_{0}^{1} t^{k}F_{k}v(m \ k \ t) dt.$$

Therefore,
$$I(m \ k \ 0 \ 0 \ k) = [8\sqrt{2}(-)^{m-k}]/(4m-2k+1)(4m-2k+3).$$
(22)

Therefore,

4. Formula for $I(m \ k \ 1 \ 0 \ k)$

$$I(m \ k \ 1 \ 0 \ k) = \int_0^1 t^k F_k v(m \ k \ t) v(1 \ 0 \ t) dt = \int_0^1 t^k F_k v(m \ k \ t) (1 - 2t) dt = I(m \ k \ 0 \ 0 \ t) - 2 \int_0^1 t^{k+1} F_k v(m \ k \ t) dt.$$

But $tv(m \ k \ t) = Av(m+1, \ k \ t) + Bv(m \ k \ t) + Cv(m-1, \ k \ t)$, (Cf. Eq. (15)) and hence

$$I(m \ k \ 1 \ 0 \ k) = (1 - 2B)I(m \ k \ 0 \ 0 \ t) + AI(m + 1, \ k \ 0 \ 0 \ t) + CI(m - 1, \ k \ 0 \ 0 \ t).$$
(23)

5. Formulae for $I(m \ k, \ m' \ m'; \ n)$

First we may note that v(m' m' t) = 1. Then

$$\begin{split} I(m \ k \ m' \ m', \ k+m') &= \int_0^1 t^{k+m'} F_{k+m'} v(m \ k \ t) dt \\ t F_{k+1} &= \{4k \ F_k - (2k-1) \ F_{k-1}\} / (2k+1). \end{split}$$

Consider m' = 1. Then, applying formula (20)

$$\begin{split} \int_{0}^{1} t^{k+1} F_{k+1} v(m \ k \ t) dt &= (4k/2k+1) \int_{0}^{1} t^{k} F_{k} v(m \ k \ t) dt - \left[(2k-1)/(2k+1) \right] \int_{0}^{1} t^{k-1} F_{k-1} t v(m \ k \ t) dt \\ &= \left[4k/(2k+1) \right] I(m \ k \ 0 \ 0 \ k) - \left[(2k-1)/(2k+1) \right] \int t^{k-1} F_{k-1} \left[C_{k-1} v(m, \ k-1, \ t) + D_{k-1} v(m-1, \ k-1, \ t) \right] dt \end{split}$$

and

$$I(m \ k, 1 \ 1 \ k+1) = (4k/2k+1)I(m \ k \ 0 \ 0 \ k) - [(2k-1)/(2k+1)][C_{k-1}I(m, \ k-1, 0 \ 0, \ k-1) + D_{k-1}I(m-1, \ k-1, 0 \ 0 \ k-1)],$$
(24)

$$I(m \ m, \ m' \ m', \ m+m') = 8\sqrt{2}/(2n+1)(2n+3), \qquad n = m+m'.$$
⁽²⁵⁾

If I(m m, m' m', m - m') = J(m', n), n = m - m', then

$$\left(m' + \frac{2n+1}{4}\right)\left(m' + \frac{2n+3}{4}\right)J(m', n) = (1/\sqrt{2}) + m'(m'+n)J(m'-1, n),$$
(26)

so that the successive J's may be found. In particular, J

$$(0, n) = 8\sqrt{2}/(2n+1)(2n+3), \tag{27}$$

$$J(1, n) = [16/(2n+5)(2n+7)] \{ (1/\sqrt{2}) + 16(n+1)/\sqrt{2}(2n+1)(2n+3) \}.$$
(28)

6. Recursion formula for $I(m \ k \ m' \ k' \ n)$

One may derive the following:

$$(2n+1)/2m+1-k)[(m+1)I(m+1, k+1, m', k', n+1) - (m-k)I(n, k+1, m', k', n+1)] = 4nI(m, k, m', k', n) - [(2n-1)/(2m+1-k)][mI(m-1, k-1, m', k', n-1) - (m-k+1)I(m, k-1, m', k', n-1)].$$
(29)

{Gronwall actually computed only the first few I's. It might be useful to know their asymptotic properties in general (for large values of the indices) for the solution of the system (12).}