The Gronwall Form of the Schrodinger Equation for ^1S Helium

C. W. David*

Department of Chemistry

University of Connecticut

Storrs, Connecticut 06269-3060

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Abstract

The Gronwall form of the ^1S Helium atom's electron's Schrödinger Equation is re-derived in a straight forward manner, and the derivation is validated with a Maple program.

*Electronic address: `Carl.David@uconn.edu`

I. INTRODUCTION

In 1937, Bartlett [1] published a piece of work by T. H. Gronwall (then deceased) titled "The Helium Wave Equation" in which a new and unique form of the Schrödinger equation for the 2-electron atom/ion problem was investigated. In that paper, Gronwall/Bartlett refers to a previous paper [2] in which Gronwall actually carried out a complicated derivation of his form of the Helium Schrödinger equation. Parenthetically, in this latter paper, Gronwall's reference 7 refers to a paper which does not (to my knowledge) exist. Would that we had the "direct and very short calculation" which resulted in the desired equation.

In this paper, an elementary (and possibly pedestrian) derivation proceeding directly from Hyllerass' [3–5] formulation is presented. For those persons who, in the future, might use the Gronwall form of the Schrödinger equation for the electrons of ^1S Helium, this paper serves as a second validation of this peculiar form.

II.

We start with Gronwall's definitions for x_1, x_2 and x_3:

$$4x_1 = r_1^2 + r_2^2 - r_{12}^2 = 2r_1r_2\cos\vartheta \tag{1}$$

from which we obtain

$$x_1 = \frac{1}{2}r_1r_2\cos\vartheta \tag{2}$$

and

$$4x_2 = r_1^2 - r_2^2 \tag{3}$$

and

$$4x_3 = \sqrt{(r_1+r_2+r_{12})(r_1+r_2-r_{12})(r_2+r_{12}-r_1)(r_{12}+r_1-r_2)} = 2r_1r_2\sin\vartheta \tag{4}$$

This is such a strange definition that we note that the term:

$$16x_3^2 = (r_1+r_2+r_{12})(r_1+r_2-r_{12})(r_2+r_{12}-r_1)(r_{12}+r_1-r_2)$$

expands to

$$16x_3^2 = -r_1^4 + 2r_1^2r_2^2 + 2r_1^2r_{12}^2 - r_2^4 + 2r_2^2r_{12}^2 - r_{12}^4 = 4r_1^2r_2^2\sin^2\vartheta$$

while

$$16x_1^2 = \left(r_1^2 + r_2^2 - r_{12}^2\right)^2 = +r_1^4 + r_2^4 + r_{12}^4 + 2r_1^2r_2^2 - 2r_1^2r_{12}^2 - 2r_2^2r_{12}^2 = 4r_1^2r_2^2\cos^2\vartheta$$

so, adding these two obtains

$$16(x_1^2 + x_3^2) = 4r_1^2r_2^2(\sin^2\vartheta + \cos^2\vartheta) \tag{5}$$

Amazing. It turns out that this is Heron's formula, a piece of trigonometry which appears to have fallen out of common knowledge.

From Equation 4 we obtain

$$x_3^2 = \frac{1}{4}r_1^2r_2^2\sin^2\vartheta$$

We knew from Equation 5 that

$$x_1^2 + x_3^2 = \frac{1}{4}r_1^2r_2^2$$

and

$$x_2^2 = \frac{r_1^4 - 2r_1^2r_2^2 + r_2^4}{16}$$

so

$$x_1^2 + x_3^2 + x_2^2 = \frac{r_1^4}{16} + \frac{r_2^4}{16} - 2\frac{r_1^2r_2^2}{16} + \frac{1}{4}r_1^2r_2^2 = \frac{r_1^4}{16} + \frac{r_2^4}{16} + 2\frac{r_1^2r_2^2}{16} \tag{6}$$

i.e., we can define a hyper-radius as

$$r^2 = x_1^2 + x_3^2 + x_2^2 = \frac{(r_1^2 + r_2^2)^2}{16} = \frac{r_1^4 + r_2^4 + 2r_1^2r_2^2}{16}$$

i.e.,

$$r = \frac{r1^2 + r2^2}{4} \tag{7}$$

We have

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

the law of cosines, so

$$r_{12}^2 = 4r - 4x_1 = 4(r - x_1)$$

so

$$r_{12} = 2\sqrt{r - x_1}$$

Further

$$r_1 = \sqrt{2\left(\sqrt{x_1^2 + x_2^2 + x_3^2} + x_2\right)} = \sqrt{2(r + x_2)}$$

and

$$r_2 = \sqrt{2\left(\sqrt{x_1^2 + x_2^2 + x_3^2} - x_2\right)} = \sqrt{2(r - x_2)}$$

We seek the differential equation (Gronwall/Bartlett's equation 1)

$$\frac{\partial^2\psi}{\partial x_1^2} + \frac{\partial^2\psi}{\partial x_2^2} + \frac{\partial^2\psi}{\partial x_3^2} + \frac{1}{x_3}\frac{\partial\psi}{\partial x_3} + \frac{1}{r}\left(\frac{E}{4} + \frac{1}{\sqrt{2(r+x_2)}} + \frac{1}{\sqrt{2(r-x_2)}} - \frac{1}{2Z\sqrt{(r-x_1)}}\right)\psi = 0$$

which we obtain from the $\{r_1, r_2, \vartheta\}$ form (Equation 7 in reference [2])due to Hylleraas rather than the form $\{r_1, r_2, r_{12}\}$:

$$\begin{aligned}
&\frac{\partial^2\psi}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial\psi}{\partial r_1} + 2\hat{r}_1\cdot\hat{r}_{12}\frac{\partial^2\psi}{\partial r_1\partial r_{12}} \\
+&\frac{\partial^2\psi}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial\psi}{\partial r_2} + 2\hat{r}_2\cdot\hat{r}_{12}\frac{\partial^2\psi}{\partial r_2\partial r_{12}} \\
&+\frac{4}{r_{12}}\frac{\partial\psi}{\partial r_{12}} + 2\frac{\partial^2\psi}{\partial r_{12}^2} \\
+&\left(\frac{E}{4} + \frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{Zr_{12}}\right)\psi = 0
\end{aligned}$$

i.e., we use the Laplacian in one of its other manifestations:

$$\nabla_1^2 + \nabla_2^2 =$$

$$\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial z_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial y_2^2} + \frac{\partial^2}{\partial z_2^2} = \tag{8}$$

$$\frac{1}{r_1^2}\frac{\partial\left(r_1^2\frac{\partial}{\partial r_1}\right)}{\partial r_1} + \frac{1}{r_2^2}\frac{\partial\left(r_2^2\frac{\partial}{\partial r_2}\right)}{\partial r_2} + \left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right)\left(\frac{1}{\sin\vartheta}\right)\frac{\partial\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right)}{\partial\vartheta} \tag{9}$$

III. BEGINNING

The chain rule yields

$$\frac{\partial}{\partial r_1} = \left(\frac{\partial x_1}{\partial r_1}\right)_{r_2,\vartheta}\frac{\partial}{\partial x_1} + \left(\frac{\partial x_2}{\partial r_1}\right)_{r_2,\vartheta}\frac{\partial}{\partial x_2} + \left(\frac{\partial x_3}{\partial r_1}\right)_{r_2,\vartheta}\frac{\partial}{\partial x_3}$$

Since

$$x_1 = \frac{1}{2}r_1 r_2\cos\vartheta$$

$$x_2 = \frac{1}{4}\left(r_1^2 - r_2^2\right)$$

and

$$x_3 = \frac{1}{2} r_1 r_2 \sin\vartheta$$

we have

$$\left(\frac{\partial x_1}{\partial r_1}\right)_{r_2,\vartheta} = \frac{1}{2} r_2 \cos\vartheta$$

We assemble a table of all the required partial derivatives in Table 1.

We then have

$$\frac{\partial}{\partial r_1} = \frac{1}{2} r_2 \cos\vartheta \frac{\partial}{\partial x_1} + \frac{1}{2} r_1 \frac{\partial}{\partial x_2} + \frac{1}{2} r_2 \sin\vartheta \frac{\partial}{\partial x_3} \tag{10}$$

Next, we need $\frac{\partial}{\partial r_2}$.

$$\frac{\partial}{\partial r_2} = \left(\frac{\partial x_1}{\partial r_2}\right)_{r_1,\vartheta} \frac{\partial}{\partial x_1} + \left(\frac{\partial x_2}{\partial r_2}\right)_{r_1,\vartheta} \frac{\partial}{\partial x_2} + \left(\frac{\partial x_3}{\partial r_2}\right)_{r_1,\vartheta} \frac{\partial}{\partial x_3}$$

i.e.,

$$\frac{\partial}{\partial r_2} = \frac{1}{2} r_1 \cos\vartheta \frac{\partial}{\partial x_1} - \frac{1}{2} r_2 \frac{\partial}{\partial x_2} + \frac{1}{2} r_1 \sin\vartheta \frac{\partial}{\partial x_3} \tag{11}$$

Finally, we need $\frac{\partial}{\partial\vartheta}$ which is

$$\frac{\partial}{\partial\vartheta} = \left(\frac{\partial x_1}{\partial\vartheta}\right)_{r_1,r_2} \frac{\partial}{\partial x_1} + \left(\frac{\partial x_2}{\partial\vartheta}\right)_{r_1,r_2} \frac{\partial}{\partial x_2} + \left(\frac{\partial x_3}{\partial\vartheta}\right)_{r_1,r_2} \frac{\partial}{\partial x_3}$$

which is

$$\frac{\partial}{\partial\vartheta} = -\frac{1}{2} r_1 r_2 \sin\vartheta \frac{\partial}{\partial x_1} + \frac{1}{2} r_1 r_2 \cos\vartheta \frac{\partial}{\partial x_3} \tag{12}$$

IV. CONTINUING FROM PRELIMINARIES, THE r_1 TERM

We form using Equation 10,

$$r_1^2 \frac{\partial}{\partial r_1} = r_1^2 \left(\frac{1}{2} r_2 \cos\vartheta \frac{\partial}{\partial x_1} + \frac{1}{2} r_1 \frac{\partial}{\partial x_2} + \frac{1}{2} r_2 \sin\vartheta \frac{\partial}{\partial x_3} \right)$$

and ask, what is $\frac{1}{r_1^2} \frac{\partial \left(r_1^2 \frac{\partial}{\partial r_1} \right)}{\partial r_1}$ which becomes, after some manipulation

$$\frac{1}{r_1^2} \frac{\partial \left(r_1^2 \frac{\partial}{\partial r_1} \right)}{\partial r_1} = \frac{2}{r_1} \left(\frac{1}{2} r_2 \cos\vartheta \frac{\partial}{\partial x_1} + \frac{1}{2} r_1 \frac{\partial}{\partial x_2} + \frac{1}{2} r_2 \sin\vartheta \frac{\partial}{\partial x_3} \right)$$
$$+ \frac{1}{4} r_2^2 \cos^2\vartheta \frac{\partial^2}{\partial x_1^2} + \frac{1}{4} r_2 r_1 \cos\vartheta \frac{\partial^2}{\partial x_1 \partial x_2} + \frac{1}{4} r_2^2 \cos\vartheta \sin\vartheta \frac{\partial^2}{\partial x_1 \partial x_3} +$$
$$\frac{1}{2} \frac{\partial}{\partial x_2} +$$

$$\frac{1}{4}r_1 r_2 \cos\vartheta \frac{\partial^2}{\partial x_2 \partial x_1} + \frac{1}{4}r_1^2 \frac{\partial^2}{\partial x_2^2} + \frac{1}{4}r_1 r_2 \sin\vartheta \frac{\partial^2}{\partial x_2 \partial x_3} +$$
$$\frac{1}{4}r_2^2 \sin\vartheta\cos\vartheta \frac{\partial^2}{\partial x_3 \partial x_1} + \frac{1}{4}r_2 r_1 \sin\vartheta \frac{\partial^2}{\partial x_3 \partial x_2} + \frac{1}{4}r_2^2 \sin^2\vartheta \frac{\partial^2}{\partial x_3^2} \tag{13}$$

V. THE r_2 TERM

We form using Equation 11,

$$r_2^2 \frac{\partial}{\partial r_2} = r_2^2 \left(\frac{1}{2}r_1 \cos\vartheta \frac{\partial}{\partial x_1} - \frac{1}{2}r_2 \frac{\partial}{\partial x_2} + \frac{1}{2}r_1 \sin\vartheta \frac{\partial}{\partial x_3} \right)$$

and obtain $\frac{1}{r_2^2}\frac{\partial\left(r_2^2\frac{\partial}{\partial r_2}\right)}{\partial r_2}$ i.e.,

$$\frac{1}{r_2^2}\frac{\left(\partial r_2^2 \frac{\partial}{\partial r_2}\right)}{\partial r_2} = \frac{2}{r_2}\left(\frac{1}{2}r_1 \cos\vartheta \frac{\partial}{\partial x_1} - \frac{1}{2}r_2 \frac{\partial}{\partial x_2} + \frac{1}{2}r_2 \sin\vartheta \frac{\partial}{\partial x_3} \right)$$
$$+ \left(\frac{1}{4}r_1^2 \cos^2\vartheta \frac{\partial^2}{\partial x_1^2} - \frac{1}{4}r_2 r_1 \cos\vartheta \frac{\partial^2}{\partial x_2 x_1} + \frac{1}{4}r_1^2 \sin\vartheta\cos\vartheta \frac{\partial^2}{\partial x_1 x_3} \right.$$
$$- \frac{1}{2}\frac{\partial}{\partial x_2}$$
$$- \frac{1}{4}r_1 r_2 \cos\vartheta \frac{\partial^2}{\partial x_2 x_1} + \frac{1}{4}r_2^2 \frac{\partial^2}{\partial x_2^2} - \frac{1}{4}r_1 r_2 \sin\vartheta \frac{\partial^2}{\partial x_2 x_3}$$
$$\left. + \frac{1}{4}r_1^2 \sin\vartheta\cos\vartheta \frac{\partial^2}{\partial x_1 x_3} - \frac{1}{4}r_2 r_1 \sin\vartheta \frac{\partial^2}{\partial x_2 x_3} + \frac{1}{4}r_1^2 \sin^2\vartheta \frac{\partial^2}{\partial x_3^2} \right) \tag{14}$$

VI. THE ϑ TERM

Finally, we have using Equation 12,

$$\frac{1}{\sin\vartheta}\frac{\partial \sin\vartheta \frac{\partial}{\partial\vartheta}}{\partial\vartheta} =$$
$$-r_1 r_2 \cos\vartheta \frac{\partial}{\partial x_1} + \frac{1}{4}r_1^2 r_2^2 \sin^2\vartheta \frac{\partial^2}{\partial x_1^2} - \frac{1}{4}r_1^2 r_2^2 \sin\vartheta\cos\vartheta \frac{\partial^2}{\partial x_1 x_3}$$
$$+\frac{1}{2}r_1 r_2 \left(\frac{\cos^2\vartheta - \sin^2\vartheta}{\sin\vartheta} \right) \frac{\partial}{\partial x_3} - \frac{1}{4}r_1^2 r_2^2 \cos\vartheta\sin\vartheta \frac{\partial^2}{\partial x_1 x_3} + \frac{1}{4}r_1^2 r_2^2 \cos^2\vartheta \frac{\partial^2}{\partial x_3^2} \tag{15}$$

VII. COMBINING TERMS

Adding the three terms (Equations 13, 14, and 15) appropriately we have (marking some terms which will cancel):

$$
\begin{aligned}
&\frac{1}{r_1^2}\frac{\partial\left(r_1^2\frac{\partial}{\partial r_1}\right)}{\partial r_1}+\frac{1}{r_2^2}\frac{\partial\left(r_2^2\frac{\partial}{\partial r_2}\right)}{\partial r_2}+\left(\frac{1}{r_1^2}+\frac{1}{r_2^2}\right)\left(\frac{1}{\sin\vartheta}\frac{\partial\sin\vartheta\frac{\partial}{\partial\vartheta}}{\partial\vartheta}\right)= \\
&\frac{2}{r_1}\left(\frac{1}{2}r_2\cos\vartheta\frac{\partial}{\partial x_1}+\frac{1}{2}r_1\frac{\partial}{\partial x_2}+\frac{1}{2}r_2\sin\vartheta\frac{\partial}{\partial x_3}\right)+ \\
&\frac{1}{4}r_2^2\cos^2\vartheta\frac{\partial^2}{\partial x_1\partial x_1}+\overbrace{\underbrace{\frac{1}{4}r_2r_1\cos\vartheta\frac{\partial^2}{\partial x_1\partial x_2}}}+\frac{1}{2}r_2\cos\vartheta\frac{1}{2}r_2\sin\vartheta\frac{\partial^2}{\partial x_1\partial x_3}+ \\
&\underbrace{\frac{1}{2}\frac{\partial}{\partial x_2}}+ \\
&\overbrace{\frac{1}{4}r_1r_2\cos\vartheta\frac{\partial^2}{\partial x_2\partial x_1}}+\frac{1}{4}r_1^2\frac{\partial^2}{\partial x_2^2}+\overline{\frac{1}{4}r_1r_2\sin\vartheta\frac{\partial^2}{\partial x_2\partial x_3}}+ \\
&\frac{1}{4}r_2^2\sin\vartheta\cos\vartheta\frac{\partial^2}{\partial x_3\partial x_1}+\underline{\frac{1}{4}r_2r_1\sin\vartheta\frac{\partial^2}{\partial x_3\partial x_2}}+\frac{1}{4}r_2^2\sin^2\vartheta\frac{\partial^2}{\partial x_3^2}+ \\
&\frac{2}{r_2}\left(\frac{1}{2}r_1\cos\vartheta\frac{\partial}{\partial x_1}-\frac{1}{2}r_2\frac{\partial}{\partial x_2}+\frac{1}{2}r_1\sin\vartheta\frac{\partial}{\partial x_3}\right) \\
&+\Bigg(\frac{1}{4}r_1^2\cos^2\vartheta\frac{\partial^2}{\partial x_1^2}-\overbrace{\underbrace{\frac{1}{4}r_2r_1\cos\vartheta\frac{\partial^2}{\partial x_2x_1}}}+\frac{1}{4}r_1^2\sin\vartheta\cos\vartheta\frac{\partial^2}{\partial x_1x_3} \\
&-\underbrace{\frac{1}{2}\frac{\partial}{\partial x_2}} \\
&-\overbrace{\frac{1}{4}r_1r_2\cos\vartheta\frac{\partial^2}{\partial x_2x_1}}+\frac{1}{4}r_2^2\frac{\partial^2}{\partial x_2^2}-\overline{\frac{1}{4}r_1r_2\sin\vartheta\frac{\partial^2}{\partial x_2x_3}} \\
&+\frac{1}{4}r_1^2\sin\vartheta\cos\vartheta\frac{\partial^2}{\partial x_1x_3}-\underline{\frac{1}{4}r_2r_1\sin\vartheta\frac{\partial^2}{\partial x_2x_3}}+\frac{1}{4}r_1^2\sin^2\vartheta\frac{\partial^2}{\partial x_3^2}\Bigg)+ \\
&\left(\frac{1}{r_1^2}+\frac{1}{r_2^2}\right)\Bigg(-r_1r_2\cos\vartheta\frac{\partial}{\partial x_1}+\frac{1}{4}r_1^2r_2^2\sin^2\vartheta\frac{\partial^2}{\partial x_1^2}-\frac{1}{4}r_1^2r_2^2\sin\vartheta\cos\vartheta\frac{\partial^2}{\partial x_1x_3} \\
&+\frac{1}{2}r_1r_2\left(\frac{\cos^2\vartheta-\sin^2\vartheta}{\sin\vartheta}\right)\frac{\partial}{\partial x_3}-\frac{1}{4}r_1^2r_2^2\cos\vartheta\sin\vartheta\frac{\partial^2}{\partial x_1x_3}+\frac{1}{4}r_1^2r_2^2\cos^2\vartheta\frac{\partial^2}{\partial x_3^2}\Bigg)
\end{aligned}
\tag{16}
$$

which becomes upon doing the cancellations (penultimately)

$$
\begin{aligned}
&\frac{1}{r_1^2}\frac{\partial\left(r_1^2\frac{\partial}{\partial r_1}\right)}{\partial r_1}+\frac{1}{r_2^2}\frac{\partial\left(r_2^2\frac{\partial}{\partial r_2}\right)}{\partial r_2}+\left(\frac{1}{r_1^2}+\frac{1}{r_2^2}\right)\left(\frac{1}{\sin\vartheta}\frac{\partial\sin\vartheta\frac{\partial}{\partial\vartheta}}{\partial\vartheta}\right)= \\
&\frac{1}{4}\left(r_1^2+r_2^2\right)\left(\frac{\partial^2}{\partial x_1^2}++\frac{\partial^2}{\partial x_2^2}+\frac{\partial^2}{\partial x_3^3}\right) \\
&-\,+\left(\frac{r_2}{r_1}+\frac{r_1}{r_2}\right)\sin\vartheta\frac{\partial}{\partial x_3}
\end{aligned}
$$

$$+\frac{1}{2}\frac{r_2}{r_1}\left(\frac{\cos^2\vartheta-\sin^2\vartheta}{\sin\vartheta}\right)\frac{\partial}{\partial x_3}$$
$$+\frac{1}{2}\frac{r_1}{r_2}\left(\frac{\cos^2\vartheta-\sin^2\vartheta}{\sin\vartheta}\right)\frac{\partial}{\partial x_3} \quad (17)$$

or, collecting terms,

$$\frac{1}{r_1^2}\frac{\partial\left(r_1^2\frac{\partial}{\partial r_1}\right)}{\partial r_1}+\frac{1}{r_2^2}\frac{\partial\left(r_2^2\frac{\partial}{\partial r_2}\right)}{\partial r_2}+\left(\frac{1}{r_1^2}+\frac{1}{r_2^2}\right)\left(\frac{1}{\sin\vartheta}\frac{\partial\sin\vartheta\frac{\partial}{\partial\vartheta}}{\partial\vartheta}\right)=$$
$$\frac{1}{4}\left(r_1^2+r_2^2\right)\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_1^3}+\frac{\partial^2}{\partial x_2^2}\right)$$

$$- -$$

$$+\frac{(r_1^2+r_2^2)}{r_1r_2}\sin\vartheta\frac{\partial}{\partial x_3}+\frac{1}{2}\frac{r_1^2+r_2^2}{r_1r_2}\left(\frac{\cos^2\vartheta-\sin^2\vartheta}{\sin\vartheta}\right)\frac{\partial}{\partial x_3} \quad (18)$$

The coefficient of $\frac{\partial}{\partial x_3}$ in Equation 18 becomes

$$\frac{(r_1^2+r_2^2)}{r_1r_2}\sin\vartheta+\frac{1}{2}\frac{r_1^2+r_2^2}{r_1r_2}\left(\frac{\cos^2\vartheta-\sin^2\vartheta}{\sin\vartheta}\right)=\frac{(r_1^2+r_2^2)}{r_1r_2}\sin\vartheta+\frac{1}{2}\frac{r_1^2+r_2^2}{r_1r_2\sin\vartheta}-\frac{2}{2}\frac{r_1^2+r_2^2}{r_1r_2}\left(\frac{\sin^2\vartheta}{\sin\vartheta}\right)$$

which finally yields

$$\frac{r_1^2+r_2^2}{r_1r_2}\sin\vartheta-\frac{r_1^2+r_2^2}{r_1r_2}\sin\vartheta+\frac{1}{2}\frac{r_1^2+r_2^2}{r_1r_2\sin\vartheta}\rightarrow\frac{1}{2}\frac{r}{r_1r_2\sin\vartheta}\rightarrow\frac{1}{4}\frac{r}{x_3}$$

which leads to (Using Equation 7):

$$\frac{1}{r_1^2}\frac{\partial\left(r_1^2\frac{\partial}{\partial r_1}\right)}{\partial r_1}+\frac{1}{r_2^2}\frac{\partial\left(r_2^2\frac{\partial}{\partial r_2}\right)}{\partial r_2}+\left(\frac{1}{r_1^2}+\frac{1}{r_2^2}\right)\left(\frac{1}{\sin\vartheta}\frac{\partial\sin\vartheta\frac{\partial}{\partial\vartheta}}{\partial\vartheta}\right)=$$
$$\frac{(r_1^2+r_2^2)}{4}\left\{\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^3}+\frac{\partial^2}{\partial x_3^2}\right)+\frac{1}{x_3}\frac{\partial}{\partial x_3}\right\} \quad (19)$$

We then have

$$\left\{\left(\frac{\partial^2\psi}{\partial x_1^2}+\frac{\partial^2\psi}{\partial x_2^3}+\frac{\partial^2\psi}{\partial x_3^2}\right)+\frac{1}{x_3}\frac{\partial\psi}{\partial x_3}\right\}+\frac{1}{r}\left(\frac{E}{4}+\frac{1}{\sqrt{2(r+x_2)}}+\frac{1}{(\sqrt{2(r-x_2)}}-\frac{1}{2Z\sqrt{(r-x_1)}}\right)\psi=0 \quad (20)$$

VIII. DISCUSSION

The Schrödinger Equation for the ^1S state of Helium's two electrons has been written in many different forms, for various purposes. Bartlett [6] himself used Gronwall's formulation for a numerical approximation calculation of the Helium 2-electron wave function in the space $\{x_1, x_2, x_3\}$, achieving a reasonably constant local energy $(\frac{H_{op}\psi}{\psi})$; certainly a spectacular result for those times. The possibility of future calculations based on Gronwall's coordinate scheme suggests that independent validation of the form of the Laplacian in the his new scheme exist.

IX. MAPLE PROGRAM

The following Maple program is offered not for its sophistication but because it validates what is otherwise an enormous pencil and paper exercise subject to inevitable errors of transcription.

```
restart;
x1 :=(1/2)*r1*r2*cos(theta);
x2 :=(1/4)*(r1^2-r2^2);
x3 :=(1/2)*r1*r2*sin(theta);
t11 := diff(x1,r1);
t21 := diff(x2,r1);
t31 := diff(x3,r1);
t12 := diff(x1,r2);
t22 :=  diff(x2,r2);
t32 := diff(x3,r2);
t13 := diff(x1,theta);
t23 := diff(x2,theta);
t33 := diff(x3,theta);

unassign('x1');
unassign('x2');
unassign('x3');
```

```
term1 :=(t11*diff(g(x1,x2,x3),x1)+t21*diff(g(x1,x2,x3),x2)+t31*diff(g(x1,x2,x3),x3)):
term1a :=(2/r1)*term1+expand(r1^2*(t11*diff(term1,x1)+t21*diff(term1,x2)
+t31*diff(term1,x3)+diff(term1,r1))/r1^2);
term2 :=(t12*diff(g(x1,x2,x3),x1)+t22*diff(g(x1,x2,x3),x2)+t32*diff(g(x1,x2,x3),x3)):
term2a :=(2/r2)*term2+expand(r2^2*(t12*diff(term2,x1)+t22*diff(term2,x2)+t32*d
iff(term2,x3)+diff(term2,r2))/r2^2);
term3 :=(t13*diff(g(x1,x2,x3),x1)+t23*diff(g(x1,x2,x3),x2)+t33*diff(g(x1,x2,x3),x3));
term3a := expand((cos(theta)*term3+expand(sin(theta)*(t13*diff(term3,x1)+
t23*diff(term3,x2)+t33*diff(term3,x3)+diff(term3,theta))))/sin(theta));
term3a : = term3a*(1/r1^2+1/r2^2);
final_term := expand(term1a+term2a+term3a);

ans1 := expand(subs(sin(theta)^2=1-cos(theta)^2,final_term));
ans1 := expand(subs(r1^2=4*r-r2^2,ans1));
ans1 := normal(ans1);
ans1 := expand(subs(sin(theta)^2=(1-cos(theta)^2),ans1));
ans1 := normal(ans1) ;
ans1 := expand(subs(r1^2=4*r-r2^2,ans1));
ans1 := subs(sin(theta) = 2*x3/(r1*r2),ans1);
```

X. TABLES

$\left(\frac{\partial x_1}{\partial r_1}\right)_{r_2,\vartheta}$	$=$	$\frac{1}{2}r_2\cos\vartheta$
$\left(\frac{\partial x_2}{\partial r_1}\right)_{r_2,\vartheta}$	$=$	$\frac{1}{2}r_1$
$\left(\frac{\partial x_3}{\partial r_1}\right)_{r_2,\vartheta}$	$=$	$\frac{1}{2}r_2\sin\vartheta$
$\left(\frac{\partial x_1}{\partial \vartheta}\right)_{r_2,r_1}$	$=$	$-\frac{1}{2}r_1r_2\sin\vartheta$
$\left(\frac{\partial x_2}{\partial \vartheta}\right)_{r_2,r_1}$	$=$	0
$\left(\frac{\partial x_3}{\partial \vartheta}\right)_{r_2,r_1}$	$=$	$\frac{1}{2}r_1r_2\cos\vartheta$
$\left(\frac{\partial x_1}{\partial r_2}\right)_{r_2,\vartheta}$	$=$	$\frac{1}{2}r_1\cos\vartheta$
$\left(\frac{\partial x_2}{\partial r_2}\right)_{r_2,\vartheta}$	$=$	$-\frac{1}{2}r_2$
$\left(\frac{\partial x_3}{\partial r_2}\right)_{r_2,\vartheta}$	$=$	$\frac{1}{2}r_1\sin\vartheta$

TABLE I: Assembled Partial Derivatives

XI. REFERENCES

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