

# A New Solution of Hydrogen

Brent Baccala

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## Abstract

The author has developed a novel technique, based on differential algebra, for finding exact solutions of partial differential equations. As an illustration of the method, I derive a previously unknown exact solution to the simplest time-independent Schrödinger equation for hydrogen. The solution,  $J_0(2\sqrt{x+r})$ , involves a Bessel function, is not separable, and is not in  $L^2$ .

## Introduction

A short list of methods to find exact solutions to PDEs includes separation of variables, the method of characteristics, transform methods (including Fourier transforms), symmetry methods, Green's functions, Duhamel's principle, and the calculus of variations. The author has developed another exact solution technique based on differential algebra and has used it to find a new solution to one of the most well-studied equations in mathematical physics, the Schrödinger equation for hydrogen.

The Schrödinger equation is the quantum mechanical analog of Newton's second law. Both Newton's equation and Schrödinger's equation describe the time evolution of a system of particles interacting under the influence of forces. Newton's classical second law  $F = ma$  describes the time evolution of the position and velocity of each particle. Schrödinger's quantum mechanical formulation  $H\Psi = i\frac{\delta}{\delta t}\Psi$  describes the time evolution of the wavefunction  $\Psi$ , which is a complex-valued function of particle position that encodes a probability density function for the particle positions as  $|\Psi|^2$  and a probability density function for the particle momenta as  $|\hat{\Psi}|^2$ .

There is no one Schrödinger equation any more than there is one  $F = ma$ . Each physical system under consideration gives rise to a different collection of particles and interacting forces, and a different Hamiltonian operator  $H$ . Indeed, even the approximations we make strongly determine the form of the equation for a given system.

The Hamiltonian operator  $H$ , so named because of its connection to Hamiltonian mechanics, is most typically given in the form  $H = T - V$ , where  $T$  is the sum of the kinetic energy of all particles and  $V$  is the potential energy of the system, due to its forces.

$$H = T - V$$

One of the simplest Schrödinger equations is for the hydrogen atom, considering the electric force attraction between the nucleus and the electronic, and ignoring all other effects. It has the following form:

$$-\frac{1}{2}\nabla^2\Psi - \frac{1}{r}\Psi = i\frac{\delta}{\delta t}\Psi$$

where  $\Psi$  is the wavefunction,  $\nabla^2$  is the Laplacian, and  $r$  is the distance between the two particles. We use Hartree atomic units, a system of units in which four fundamental physical constants<sup>1</sup> are assigned the value of 1, in order to eliminate the need for any conversion constants in the equation. The unit of distance, in particular, is *Bohr radii*, approximately half an Angström, a Angström being  $10^{-10}$  meters. The first term,  $-\frac{1}{2}\nabla^2\Psi$ , is the kinetic energy operator, and the second term,  $-\frac{1}{r}\Psi$ , is the potential energy term.

We can further simplify the general, time-dependent Schrödinger equation by requiring that the position and momentum probability density functions each be time-independent. This restricts the solution to stable states of the hydrogen atom, settles the wavefunction up to a multiple of  $e^{itE}$ , where  $E$  is the state's energy in Hartrees (approximately 27 eV), and leads to the time-independent Schrödinger equation for hydrogen:

$$-\frac{1}{2}\nabla^2\Psi - \frac{1}{r}\Psi = E\Psi \tag{1}$$

This equation is amenable to separation of variables. Using spherical coordinates and writing  $\Psi$  as  $\Psi = R(r)Y(\theta, \psi) = R(r)P(\theta)F(\psi)$ , substituting into (1), we obtain the following expansion<sup>2</sup>:

$$\frac{1}{R} \frac{d}{dr} \left[ r^2 \frac{dR}{dr} \right] + 2(Er^2 + r) + \left[ \frac{1}{P \sin \theta} \frac{d}{d\theta} \left[ \sin \theta \frac{dP}{d\theta} \right] + \frac{1}{F \sin^2 \theta} \frac{d^2 F}{d\psi^2} \right] = 0$$

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<sup>1</sup>the reduced Planck constant, the elementary charge, the electron mass, and the Coulomb constant

<sup>2</sup>hyperphysics

| Energy<br>(Hartrees) | Wavefunction            | Shell |
|----------------------|-------------------------|-------|
| $-\frac{1}{2}$       | $e^{-r}$                | 1s    |
| $-\frac{1}{8}$       | $(2-r)e^{-r/2}$         | 2s    |
|                      | $xe^{-r/2}$             | 2p    |
|                      | $ye^{-r/2}$             |       |
|                      | $ze^{-r/2}$             |       |
| $-\frac{1}{18}$      | $(27-18r+2r^2)e^{-r/3}$ | 3s    |
|                      | $(6-r)xe^{-r/3}$        | 3p    |
|                      | $(6-r)ye^{-r/3}$        |       |
|                      | $(6-r)ze^{-r/3}$        |       |

The first part, dependant on  $r$ , is the *radical equation*, whose solutions are, in general. hypergeometric functions, but which, in the case of specific energy values, simplify to polynomials in  $r$  times an exponential of  $r$ . It is these solutions, combined with the solution of the second part of the equation (the colatitude equation, solved by the associated Laguerre polynomials, and the azimuthal equation), which have been known for a hundred years, and are hence referred to as the *classical solutions* to hydrogen.

The associated energy levels are negative because these are bound states. Zero energy would correspond to an electron and a proton at rest an (infinitely) large distance apart.

The classical solutions are separable, are in  $L^2$ , are in  $C^\infty$ , and are each paired with a negative energy value, of which  $-\frac{1}{2}$  is the lowest, and corresponds to the 1s or ground state.

Yet the existance of separable solutions leaves open the existance of non-separable solutions.

It is perhaps surprising that such a well-studied equation would have fairly simple, previously undiscovered, non-separable solutions.

I now describe the algorithm used to find the new solution of hydrogen.

## Solution Algorithm

Given a PDE defined by Ritt-type differential polynomials, attempt the following:

1. Select an ansatz that defines a differential space parameterized by constants (see next section)
2. Reduce the PDE modulo the differential ideal that characterizes the differential space (differential elimination step)
3. Construct a system of polynomial equations in the constants by collecting like terms in the remaining variables (projection step)
4. Construct the ideal  $I$  defined by that system of polynomial equations as generators
5. Are there any zero divisors in the differential space? (probably not) If not, take the radical of  $I$ .
6. Construct the primary decomposition (prime decomposition if  $I$  is radical)
7. Each ideal in the primary/prime decomposition corresponds to a variety in the space of constants, the union of which form the solution space of the PDE in the differential space.

## The Ansatz

Rather than attempt to derive differential equations that apply to all solutions of the PDE, we restrict our attention to an **ansatz**, which is a family of extensions to the differential ring used to define the PDE. These are the primary requirements for an **ansatz**:

- it must be formed from a finite sequence of linear ODE and algebraic extensions, and
- it must be expressed using differential polynomials, and
- it must be parametrized only by constants

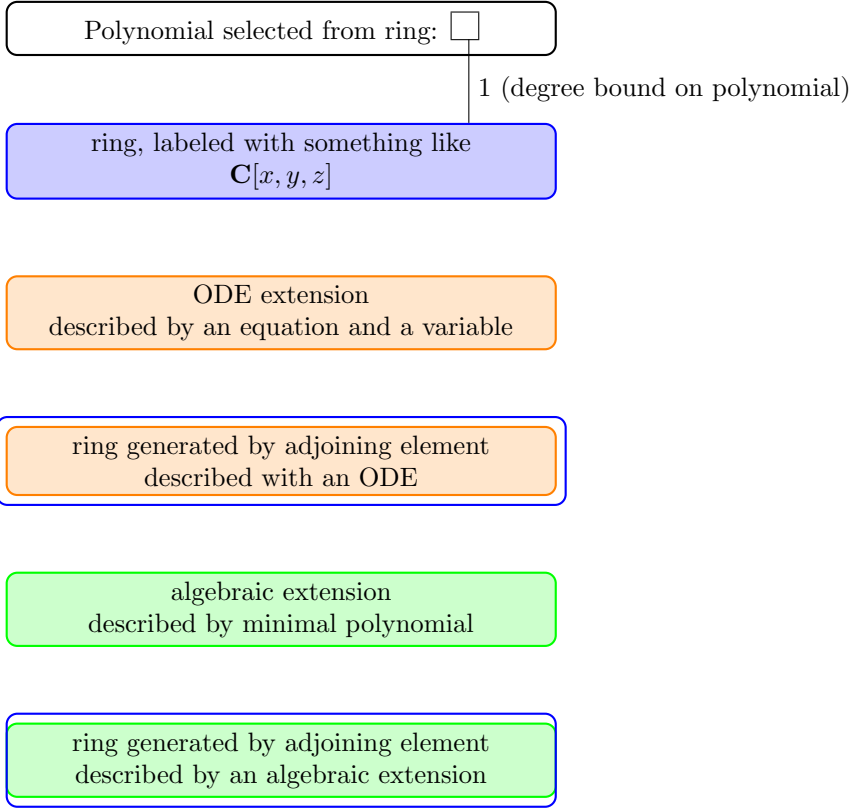
The first requirement arises because I am specifically looking for ODE based solutions, simply because our ODE theory and practice is far beyond our PDE theory and practice. One of the most fundamental questions to ask of a PDE, in my opinion, is can it be solved using ODEs? I further restrict to linear ODEs because their theory and practice is even more refined. Since algebraic extensions lead naturally to nonlinear ODE extensions, if I wish to include algebraic extensions with linear ODE, they must be included explicitly (and are).

The second requirement is natural within the context of differential algebra, but is even more important if we wish to systematize this algorithm using something like Rosenfeld-Gröbner to perform the differential reduction step.

The final requirement is meant to ensure that we can ultimately reduce this problem to a finite-dimensional space of constants, and as we use differential algebra throughout, we expect a system of polynomial equations in those constants, which will be amenable to the techniques of classical and modern algebraic geometry.

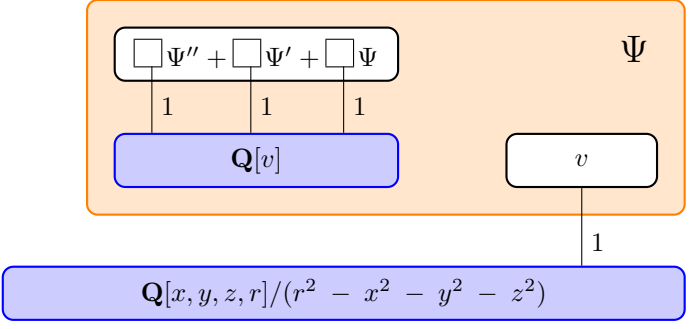
No algorithm is presently available to select an ansatz.

I've developed a graphical notation to describe an ansatz. Blue-purple boxes denote rings, orange boxes (whether shaded orange or not) denote ODE extensions, and green boxes denote algebraic extensions. A blue box drawn immediately around an orange or green box denote the ring formed by adjoining the element defined by the orange or green box. Polynomials are drawn as a square white box and are connected by a line to the ring to which they belong. A number next to the line indicates a degree bound on the polynomial, and two numbers separated by a slash denote a rational function. For example,  $2/2$  denotes a rational function with a second degree numerator and a second degree denominator.



**Ansatz 5**

Ansatz 5, used to find the new solution of hydrogen, is a second-order ODE with linear coefficients and a linear variable, i.e:



The structure of ansatz 5 can be described using differential polynomials and jet notation (subscripts indicate differentiation):

$$\begin{aligned}
\Psi_x &= \Psi'v_x & \Psi_y &= \Psi'v_y & \Psi_z &= \Psi'v_z \\
\Psi'_x &= \Psi''v_x & \Psi'_y &= \Psi''v_y & \Psi'_z &= \Psi''v_z \\
(a_0 + a_1v)\Psi'' + (b_0 + b_1v)\Psi' + (c_0 + c_1v)\Psi &= 0 \\
v &= v_1x + v_2y + v_3z + v_4r
\end{aligned} \tag{2}$$

Essentially we introduce a new derivation with respect to  $v$ . We're only interested in how  $\Psi$  differentiates with this new derivation, and that's what  $\Psi'$  and  $\Psi''$  tell us. We do not have to modify the original differential ring, except to add  $\Psi$ ,  $\Psi'$ , and  $\Psi''$  as new indeterminates. The first two lines of equations in (2) show how to evaluate the derivatives of  $\Psi$  and  $\Psi'$  with respect to the derivations in the differential ring (it's just the chain rule), and the third line shows how to eliminate  $\Psi''$  wherever it appears and replace it with an expression in  $\Psi$  and  $\Psi'$ . The final equation is there because  $v$ , too, must be degree bounded.

## Differential Reduction Step

I attempted to use the Rosenfeld-Gröbner algorithm to reduce equation (1) modulo (2), but it ultimately ran out of memory on a 96 GB computer after 30 hours. Instead, I used Sage to construct a polynomial ring modulo the ideal  $r^2 - x^2 - y^2 - z^2$  to handle the algebraic extension (present not in the ansatz proper, but in the original ring used to construct the PDE). Next I directed the software to expand the derivatives in (1) and substitute for  $\Psi''$  and  $v$  according to the ansatz. The result is a rational function with a 228 term numerator and an 18 term denominator. We ignore the denominator. The numerator begins:

$$-2r\Psi x^3 E d_1 v_1 - 3r\Psi x^3 n_1 v_0^2 v_1 - r\Psi x^3 n_1 v_1^3 - r\Psi x^3 n_1 v_1 v_2^2 - r\Psi x^3 n_1 v_1 v_3^2 - \dots \tag{3}$$

## Projection Step

Having reduced our PDE (14) by the differential ideal defined by (2), we now wish to project our solution onto the subspace of the constants. We're looking for constants that will solve equation (14) for all values of  $x$ ,  $y$ ,  $z$ ,  $r$ ,  $\Psi$ , and  $\Psi'$ , so we collect like terms in  $x$ ,  $y$ ,  $z$ ,  $r$ ,  $\Psi$ , and  $\Psi'$ , organizing the numerator like this:

$$r\Psi x^3 (-2E d_1 v_1 - 3n_1 v_0^2 v_1 - n_1 v_1^3 - n_1 v_1 v_2^2 - n_1 v_1 v_3^2) - \dots \tag{4}$$

The expressions in parenthesis gives us a system of equations (only one is shown) involving the  $v_i$ ,  $d_i$ ,  $m_i$  and  $n_i$  variables that, if satisfied, will yield a solution to (14) in the form (??) and (??). Once duplicate equations are dropped, the system has 34 equations.

$$\begin{aligned}
& -2 n_1 v_0^3 - 4 n_1 v_0 v_1^2 - 4 n_1 v_0 v_2^2 - 2 n_1 v_0 v_3^2 - 4 E d_1 v_0 \\
& -2 n_1 v_0^3 - 4 n_1 v_0 v_1^2 - 2 n_1 v_0 v_2^2 - 4 n_1 v_0 v_3^2 - 4 E d_1 v_0 \\
& -2 n_1 v_0^3 - 2 n_1 v_0 v_1^2 - 4 n_1 v_0 v_2^2 - 4 n_1 v_0 v_3^2 - 4 E d_1 v_0 \\
& \qquad -4 m_1 v_0 v_1 v_2 \\
& \qquad -4 m_1 v_0 v_1 v_3 \\
& \qquad -4 m_1 v_0 v_2 v_3 \\
& \qquad -4 n_1 v_0 v_1 v_2 \\
& \qquad -4 n_1 v_0 v_1 v_3 \\
& \qquad -4 n_1 v_0 v_2 v_3 \\
& \qquad -3 m_1 v_0^2 v_1 - m_1 v_1^3 - m_1 v_1 v_2^2 - m_1 v_1 v_3^2 \\
& \qquad -3 m_1 v_0^2 v_2 - m_1 v_1^2 v_2 - m_1 v_2^3 - m_1 v_2 v_3^2 \\
& \qquad -3 m_1 v_0^2 v_3 - m_1 v_1^2 v_3 - m_1 v_2^2 v_3 - m_1 v_3^3 \\
& \qquad -2 m_1 v_0^3 - 4 m_1 v_0 v_1^2 - 4 m_1 v_0 v_2^2 - 2 m_1 v_0 v_3^2 \\
& \qquad -2 m_1 v_0^3 - 4 m_1 v_0 v_1^2 - 2 m_1 v_0 v_2^2 - 4 m_1 v_0 v_3^2 \\
& -3 n_1 v_0^2 v_1 - n_1 v_1^3 - n_1 v_1 v_2^2 - n_1 v_1 v_3^2 - 2 E d_1 v_1 \\
& -3 n_1 v_0^2 v_2 - n_1 v_1^2 v_2 - n_1 v_2^3 - n_1 v_2 v_3^2 - 2 E d_1 v_2 \\
& -3 n_1 v_0^2 v_3 - n_1 v_1^2 v_3 - n_1 v_2^2 v_3 - n_1 v_3^3 - 2 E d_1 v_3 \\
& \qquad -2 m_1 v_0^3 - 2 m_1 v_0 v_1^2 - 4 m_1 v_0 v_2^2 - 4 m_1 v_0 v_3^2 \\
& - n_0 v_0^2 - n_0 v_1^2 - n_0 v_2^2 - n_0 v_3^2 - 2 E d_0 - 2 d_1 v_0 \\
& \qquad -2 n_0 v_0 v_1 - 2 d_1 v_1 \\
& \qquad -2 n_0 v_0 v_2 - 2 d_1 v_2 \\
& \qquad -2 n_0 v_0 v_3 - 2 d_1 v_3 \\
& \qquad -2 d_1 v_0 v_1 - 2 m_0 v_0 v_1 \\
& \qquad -2 d_1 v_0 v_2 - 2 m_0 v_0 v_2 \\
& \qquad -2 d_1 v_0 v_3 - 2 m_0 v_0 v_3 \\
& - n_1 v_0^3 - 3 n_1 v_0 v_1^2 - n_1 v_0 v_2^2 - n_1 v_0 v_3^2 - 2 E d_1 v_0 \\
& - n_1 v_0^3 - n_1 v_0 v_1^2 - 3 n_1 v_0 v_2^2 - n_1 v_0 v_3^2 - 2 E d_1 v_0 \\
& - n_1 v_0^3 - n_1 v_0 v_1^2 - n_1 v_0 v_2^2 - 3 n_1 v_0 v_3^2 - 2 E d_1 v_0 \\
& \qquad -2 d_1 v_0^2 - m_0 v_0^2 - m_0 v_1^2 - m_0 v_2^2 - m_0 v_3^2 \\
& \qquad -2 d_0 \\
& \qquad -2 d_0 v_0 \\
& \qquad -m_1 v_0^3 - 3 m_1 v_0 v_1^2 - m_1 v_0 v_2^2 - m_1 v_0 v_3^2 \\
& \qquad -m_1 v_0^3 - m_1 v_0 v_1^2 - 3 m_1 v_0 v_2^2 - m_1 v_0 v_3^2 \\
& \qquad -m_1 v_0^3 - m_1 v_0 v_1^2 - m_1 v_0 v_2^2 - 3 m_1 v_0 v_3^2
\end{aligned} \tag{5}$$



## Prime Decomposition

(5) is simple enough that we can form an ideal  $I$  in  $\mathbf{Q}[v_0, \dots, m_1, E]$  from (5), and Sage can calculate a Gröbner basis for the radical  $I$  in less than a second. While we could work with the Gröbner basis directly<sup>3</sup>, I find it more useful to study the primary decomposition, which Sage computes using the Shimoyama-Yokoyama algorithm<sup>4</sup> as implemented in Singular. Gröbner basis calculations are done as a subalgorithm of Shimoyama-Yokoyama.

Taking the radical of the ideal simplifies both the theory and the application, and can be justified because there are no nilpotent elements in our solution space, which is just 11-dimensional complex space  $\mathbf{C}^{11}$ . The primary decomposition of a radical ideal is also a prime decomposition, as the distinction between primary and prime ideals is only significant for non-radical ideals with nilpotent elements. Sage/Singular computes the following decomposition into prime ideals:

```
sage: I.radical().primary_decomposition()
```

$$(n_1, n_0, m_1, m_0, d_1, d_0) \tag{6a}$$

$$(v_3, v_2, v_1, v_0, d_0) \tag{6b}$$

$$(v_1^2 + v_2^2 + v_3^2, v_0, d_1, d_0) \tag{6c}$$

$$(v_3, v_2, v_1, m_1, m_0 - n_0 v_0, 2d_1 + n_0 v_0, d_0, En_0 - n_1 v_0) \tag{6d}$$

$$(v_0^2 - v_1^2 - v_2^2 - v_3^2, n_1, m_1, m_0 - n_0 v_0, d_1 + n_0 v_0, d_0, E) \tag{6e}$$

Several of these varieties solve the system of equations, but do not lead to a meaningful solution to the differential equation. In brief,

(6a) sets all coefficients of the ODE to zero, so we discard it,

(6b) sets the variable  $v$  to zero, so we discard it,

(6c) sets the coefficient of  $D^2\Psi$  in the ODE to zero, resulting in a first-order ODE, so we discard it, too,

(6d) corresponds to the classical solutions (see below), and

(6e) corresponds to our new solution (see below).

<sup>3</sup>A Gröbner basis of the solution ideal in lexicographic order  $E > d_i > m_i > n_i > v_i$  contains 65 polynomials.

<sup>4</sup>Localization and Primary Decomposition of Polynomial Ideals, *J. Symbolic Computation* (1996) **22**, 247–277

How to understand ideal (6d)?  $d_0$  is an ideal generator, so  $d_0 = 0$ , and we can always multiply our DE by a constant without affecting our result, so we can set  $d_1 = 1$ . Likewise, we can multiply our variable  $v$  by a constant and that will only change our coefficients by constants, and  $v_1 = v_2 = v_3 = 0$ , so we can normalize by setting  $v_0 = 1$ . This simplifies ideal (6d) to:

$$(v_3, v_2, v_1, v_0 - 1, n_0 + 2, m_1, m_0 + 2, d_1 - 1, d_0, 2E + n_1) \quad (7)$$

$$\begin{aligned} v &= r \\ v\Psi'' + 2\Psi' + 2(1 + Ev)\Psi &= 0 \end{aligned} \quad (8)$$

This is the classical radial equation obtained by separation of variables<sup>5</sup>. We use spherical coordinates, set  $\Psi = R(r)P(\theta)F(\psi)$ , and obtain the above equation for  $R(r)$ , though it is more commonly written in this form:

$$\frac{1}{R} \frac{d}{dr} \left[ r^2 \frac{dR}{dr} \right] + 2(Er^2 + r) = l(l + 1) \quad (9)$$

where  $l$  is the orbital quantum number, which can be zero. Set  $l = 0$ ,  $v = r$  and  $\Psi = R$  and expand out the derivative to obtain (8). Its presence here was expected and won't be commented on further.

Ideal (6e) was not expected, and contains our new solution. Does it contain any additional solutions?  $d_0$  is an ideal generator, so  $d_0 = 0$ , and we can set  $d_1 = 1$ , by the same logic as above. Our coordinates are in real space, so our  $v_i$  coefficients must be real (why?), so all of their squares must be positive, and since  $v_0^2 - v_1^2 - v_2^2 - v_3^2 = 0$ ,  $v_0$  must be non-zero. So we can normalize by setting  $v_0 = 1$ . That simplifies (6e) to this ideal:

$$(v_1^2 + v_2^2 + v_3^2 - 1, v_0 - 1, n_1, n_0 + 1, m_1, m_0 + 1, d_1 - 1, d_0, E) \quad (10)$$

This ideal corresponds to the following system of equations:

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<sup>5</sup>See Pauling and Wilson or <http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hydrad.html>

$$\begin{aligned}
E &= 0 \\
d_0 &= 0 & d_1 &= 1 \\
m_0 &= -1 & m_1 &= 0 \\
n_0 &= -1 & n_1 &= 0 \\
v_0 &= 1 & v_1^2 + v_2^2 + v_3^2 &= 1
\end{aligned} \tag{11}$$

Substituting these values back into our ansatz, we conclude that  $\Psi(v)$  is a solution of (14) under these conditions:

$$\begin{aligned}
v \frac{\delta^2 \Psi}{\delta v^2} + \frac{\delta \Psi}{\delta v} + \Psi &= 0 \\
v &= v_1 x + v_2 y + v_3 z + r \\
v_1^2 + v_2^2 + v_3^2 &= 1
\end{aligned} \tag{12}$$

The expression  $v_1 x + v_2 y + v_3 z$  is easily identified as a dot product between the coordinate  $(x, y, z)$  and the unit vector  $(v_1, v_2, v_3)$  (remembering that  $v_1^2 + v_2^2 + v_3^2 = 1$ ). The direction of this vector is arbitrary, so we can orient the  $x$ -axis in this direction and set  $(v_1, v_2, v_3) = (1, 0, 0)$  without loss of generality.

We now have to solve a second order ODE:

$$v \Psi''(v) + \Psi'(v) + \Psi(v) = 0 \tag{13}$$

Wolfram Mathematica<sup>6</sup> can now analyze this equation and determine that it is equivalent to the Bessel function (15).

```

[3]= DSolve[x * y''[x] + y'[x] + y[x] == 0, y[x], x]
[3]= {{y[x] -> BesselJ[0, 2 Sqrt[x]] c1 + 2 BesselY[0, 2 Sqrt[x]] c2}}

```

leading to...

## The Main Result

Consider the following simple Schödinger equation for the hydrogen atom:

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<sup>6</sup>I originally used Wolfram Alpha

$$-\frac{1}{2}\nabla^2\Psi - \frac{1}{r}\Psi = E\Psi \quad (14)$$

Let  $J_0$  be the ordinary Bessel function  $J_0$ , and set

$$\Psi = J_0(2\sqrt{x+r}) \quad (15)$$

where  $x, y, z$  are Cartesian coordinates and  $r = \sqrt{x^2 + y^2 + z^2}$ .

Then (15) is an exact solution to (14), with  $E = 0$ .

## Verification

The result can be easily verified using Mathematica<sup>7</sup>, as follows:

```

1]= Psi f := Psi[x, y, z]
2]= r[x_, y_, z_] = Sqrt[x^2 + y^2 + z^2]
2]= Sqrt[x^2 + y^2 + z^2]
3]= eqn = -1/2*Laplacian[Psi f, {x, y, z}] - 1/r[x, y, z]*Psi f == 0
3]= -Psi[x, y, z]/Sqrt[x^2 + y^2 + z^2] + 1/2*(-Psi^(0,0,2)[x, y, z] - Psi^(0,2,0)[x, y, z] - Psi^(2,0,0)[x, y, z]) == 0
4]= sol[x_, y_, z_] := BesselJ[0, 2*Sqrt[x+r[x, y, z]]]
5]= FullSimplify[eqn /. Psi -> (x, y, z) -> sol[x, y, z]]
5]= True

```

## Generalization

The choice of  $x$  is arbitrary, and any ordinary Bessel function can be used:

$$\Psi = F(2\sqrt{a_1x + a_2y + a_3z + r}) \quad (16)$$

where

$$a_1^2 + a_2^2 + a_3^2 = 1$$

and  $F$  is any linear combination of the Bessel functions  $J_0$  and  $Y_0$ .

Any finite linear combination of functions of the form (16) also solves (14).

<sup>7</sup>A manual verification is presented in an appendix

## Software

The program used to construct the system of equations is available here:  
<https://github.com/BrentBaccala/helium>

It's a Sage script that works fine with Sage 9.0 on Ubuntu 20.

Use it to find ideal (6) by running Sage as follows:

```
load('helium.sage')      # loads the script
prep_hydrogen(5)        # select PDE:hydrogen and ansatz:5
init()                  # finish setting everything up
I=ideal(eqns_RQQ)       # constuct ideal from equations
I.radical().primary_decomposition()
```

Here are some other convenient variables and functions in the script:

```
A, B, C, V              # trial forms of various polynomials
eq_a                    # the PDE in its original form
R                       # polynomial ring over integers
F                       # fraction field of R
F_eq_a                  # the PDE modulo the ansatz
F_eq_a_n                # expanded numerator (in R)
F_eq_a_d                # expanded denominator (in R)
eqns_RQQ                # system of equations to solve
```

## The Ansatzen

These are current and future ansatzen for the form of the ODE:

For hydrogen, the PDE is always  $\nabla^2\Psi - \frac{1}{r}\Psi = E\Psi$

For helium, the PDE is always  $\nabla_1^2\Psi + \nabla_2^2\Psi - \frac{2}{r_1} - \Psi\frac{2}{r_2} - \Psi\frac{1}{r_{12}}\Psi = E\Psi$

Ansatz 1: Exponential of a first degree polynomial times a first degree polynomial

Expected to find 1s and 2s levels of hydrogen,  $e^{-r}$  and  $(2-r)e^{r/2}$

$A, B \in \mathbf{C}[x, y, z, r]; \deg A \leq 1; \deg B \leq 1$

$\Psi = AF; F' = F; F_x = B_x F'; F_y = B_y F'; F_z = B_z F'$

or just:  $\Psi = AF; F_x = B_x F; F_y = B_y F; F_z = B_z F$

Example:  $B = -r; A = 1; E = -1/2 \Rightarrow e^{-r}$

Example:  $B = -r/2; A = r - 2; E = -1/8 \Rightarrow (2 - r)e^{-r/2}$

Ansatz 2: Logarithm of a first degree polynomial times a first degree polynomial

$A, B \in \mathbf{C}[x, y, z, r]; \deg A \leq 1; \deg B \leq 1$

$\Psi = AF; F' = 1/F; F_x = B_x F'; F_y = B_y F'; F_z = B_z F'$

or just:  $\Psi = AF; F_x = B_x/F; F_y = B_y/F; F_z = B_z/F$

Ansatz 3,4: Unused

Ansatz 5: Second-order ODE with linear coefficients and a linear variable

Expected to find 1s level of hydrogen,  $e^{-r}$

$A, B, C, V \in \mathbf{C}[x, y, z, r]; \deg A \leq 1; \deg B \leq 1; \deg C \leq 1; \deg V \leq 1$

$\Psi = F; AF'' + BF' + CF = 0; F_x = V_x F'; F_y = V_y F'; F_z = V_z F'$

Example:  $V = -r; A + C = -B; E = -1/2 (A, B, C \in \mathbf{C}) \Rightarrow e^{-r}$

Ansatz 6: Second-order ODE with linear coefficients and a first-degree rational function variable

Ansatz 7: Second-order ODE with second-degree coefficients and a second-degree rational function variable

Ansatz 8: (logically before ansatz 5) First-order ODE with linear coefficients and a linear polynomial variable

Ansatz 9: (logically before ansatz 8) First-order ODE with constant coefficients and a linear polynomial variable

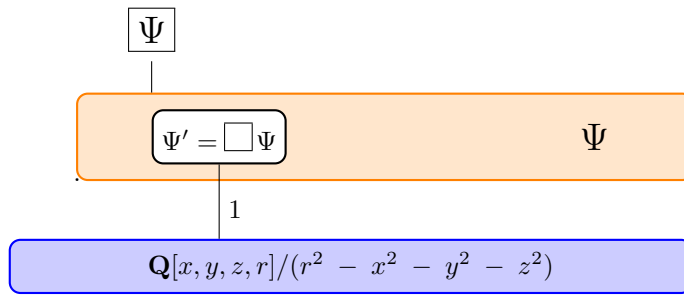
Ansatz 10: (logically before ansatz 7) Second-order ODE with second-degree coefficients and a second-degree polynomial variable

Ansatz 11: An second-degree algebraic extension with second-degree coefficients (involving  $E?$ ), followed by ansatz 7 (second-order ODE with second-degree coefficients and a second-degree rational function variable)

Ansatz 12: Two nested second-order ODEs with second-degree coefficients and a second-degree rational function variable (ansatz 7 twice)

Ansatz 13: Ansatz 11 twice

## Ansatz 1

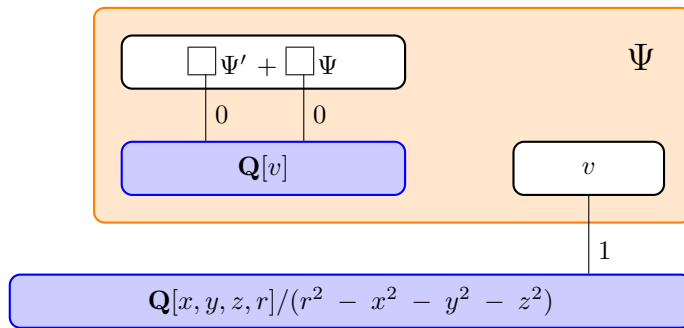


$$\Psi_x = \frac{\Psi'}{B_x} \quad \Psi_y = \frac{\Psi'}{B_y} \quad \Psi_z = \frac{\Psi'}{B_z}$$

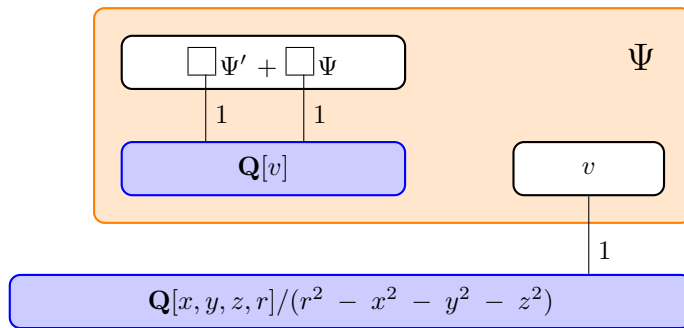
$$\Psi' = \Psi$$

$$B = b_0 + b_1x + b_2y + b_3z + b_4r$$

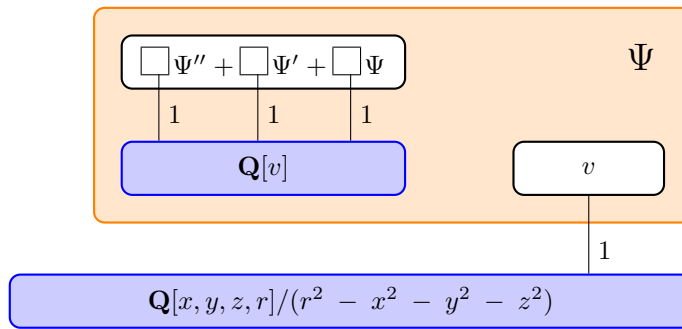
**Ansatz 9**



**Ansatz 8**

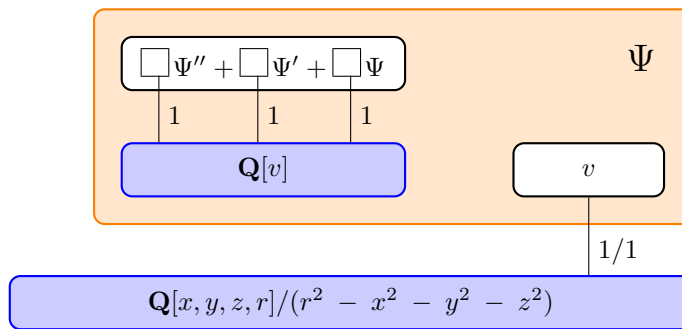


**Ansatz 5**

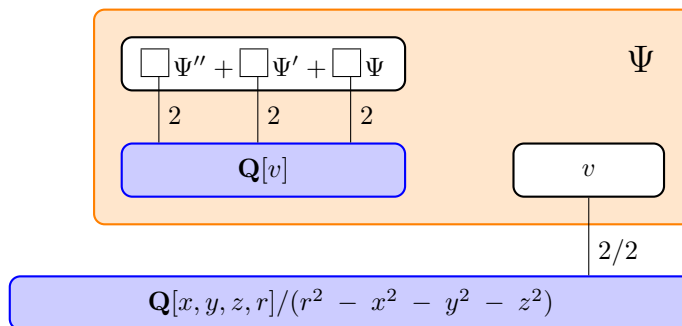


$$\begin{aligned}
 \Psi_x &= \Psi' v_x & \Psi_y &= \Psi' v_y & \Psi_z &= \Psi' v_z \\
 \Psi'_x &= \Psi'' v_x & \Psi'_y &= \Psi'' v_y & \Psi'_z &= \Psi'' v_z \\
 (a_0 + a_1 v) \Psi'' + (b_0 + b_1 v) \Psi' + (c_0 + c_1 v) \Psi &= 0 \\
 v &= v_1 x + v_2 y + v_3 z + v_4 r
 \end{aligned}$$

**Ansatz 6**

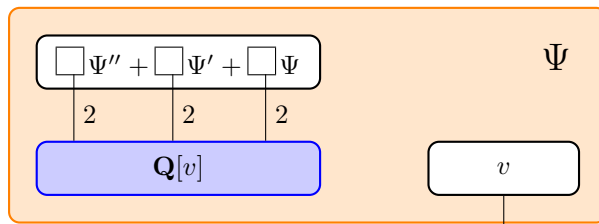


**Ansatz 7**



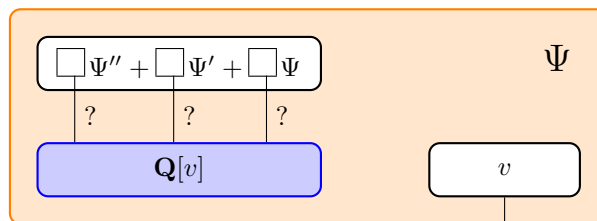
**Ansatz 10**



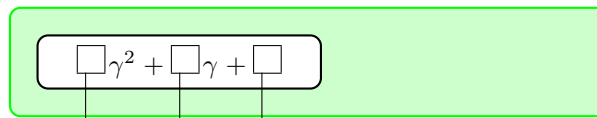


$$Q[x, y, z, r]/(r^2 - x^2 - y^2 - z^2)$$

**Ansatz 11**

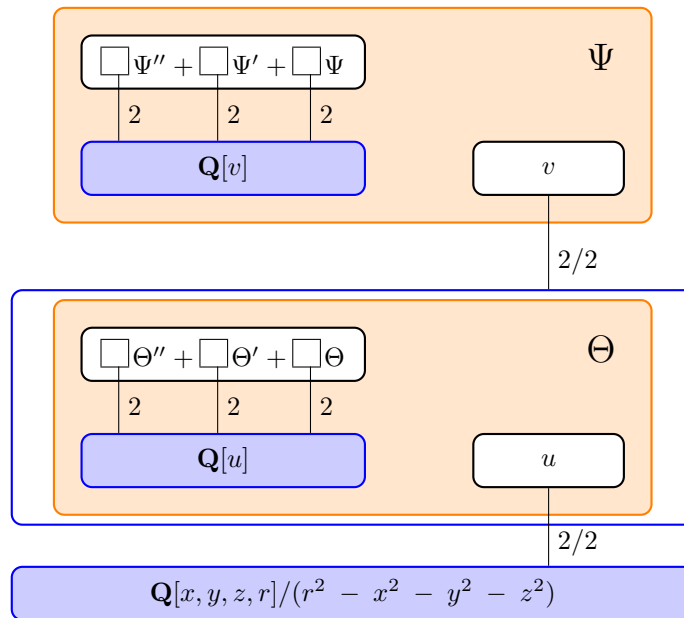


$$Q[x, y, z, r, \gamma]/(r^2 - x^2 - y^2 - z^2, \square \gamma^2 + \square \gamma + \square)$$

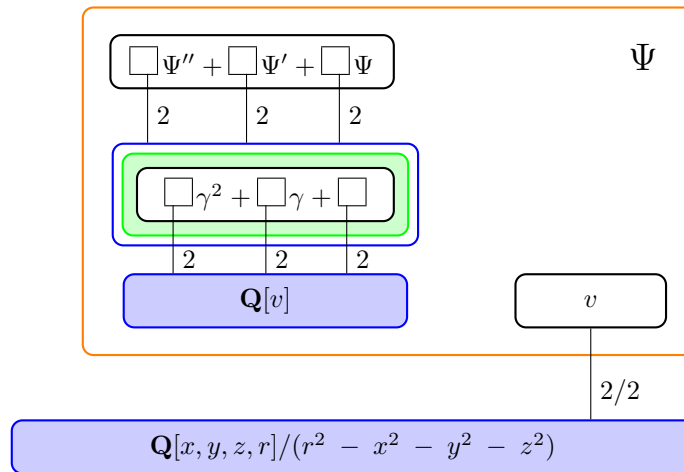


$$Q[x, y, z, r]/(r^2 - x^2 - y^2 - z^2)$$

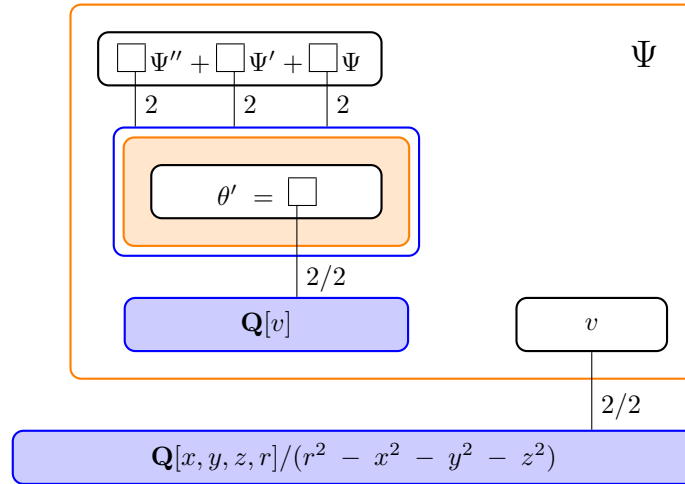
**Ansatz 12**



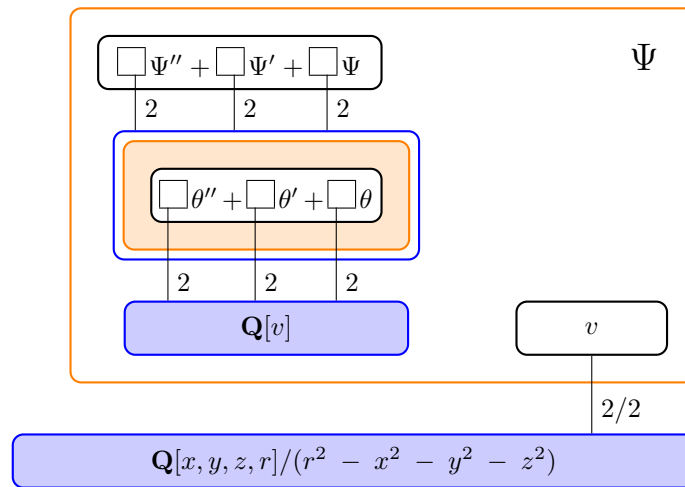
**Ansatz 13**



**Ansatz 14**



**Ansatz 15**



## Performance

|            |          |  |  |   |
|------------|----------|--|--|---|
| Ansatz 5   | Hydrogen | Differential Elimination<br>Sol of constant system | Rosenfeld-Groebner<br>Manual<br>Bertini<br>Singular radical<br>Singular prime decomp | memory exhaustion on 96 GB<br>quick<br>8.33 hours (laptop); only four<br>quick<br>quick |
| Ansatz 5.1 | Hydrogen | Differential Elimination<br>Sol of constant system | Manual<br>Singular radical<br>Singular prime decomp                                  | quick<br>quick<br>quick   |
| Ansatz 5.2 | Hydrogen | Differential Elimination<br>Sol of constant system | Manual<br>Singular radical<br>Singular prime decomp                                  | quick<br>quick<br>quick   |
| Ansatz 5.3 | Hydrogen | Differential Elimination<br>Sol of constant system | Manual<br>Singular radical<br>Singular prime decomp                                  | quick<br>5 minutes<br>quick   |
| Ansatz 6   | Helium   | Differential Elimination<br>Sol of constant system | Manual<br>Singular radical<br>Bertini  | 10 seconds<br>laptop crashed after about 1 w<br>laptop crashed after about 1 w          |
| Ansatz 11  | Hydrogen | Differential Elimination<br>Sol of constant system | Manual<br>Singular radical<br>Singular primary dec                                   | 18 hours (laptop)<br>oom, 96 GB, 39 hours, c200-1<br>oom, 96 GB, c200-1                 |

## Draft Status

This paper is still a draft and is being updated regularly.

## Contact

The author maintains a discussion page for this result on his personal blog at:

<https://www.freesoft.org/blogs/soapbox/a-new-solution-of-hydrogen/>

## Appendix: Manual Verification of the Result

For anybody wondering how Mathematica concludes that (15) solves (14), the claim is that  $\Psi = J_0(2\sqrt{x+r}) = (J_0 \circ 2\sqrt{v})(x+r)$  satisfies:

$$\left( \frac{\delta^2}{\delta^2 x} + \frac{\delta^2}{\delta^2 y} + \frac{\delta^2}{\delta^2 z} \right) \Psi + \frac{2}{r} \Psi = 0 \quad (17)$$

Letting  $v = x + r$ , we compute the first partial derivatives of  $\Psi$ :

$$\begin{aligned} \frac{\delta \Psi}{\delta x} &= \frac{dv}{dx} \frac{d}{dv} (J_0 \circ 2\sqrt{v}) = \frac{dv}{dx} J'_0(2\sqrt{v}) v^{-1/2} \\ \frac{\delta \Psi}{\delta y} &= \frac{dv}{dy} \frac{d}{dv} (J_0 \circ 2\sqrt{v}) = \frac{dv}{dy} J'_0(2\sqrt{v}) v^{-1/2} \\ \frac{\delta \Psi}{\delta z} &= \frac{dv}{dz} \frac{d}{dv} (J_0 \circ 2\sqrt{v}) = \frac{dv}{dz} J'_0(2\sqrt{v}) v^{-1/2} \end{aligned} \quad (18)$$

Next we compute the partial second derivatives of  $\Psi$ :

$$\begin{aligned} \frac{\delta^2 \Psi}{\delta x^2} &= \frac{d^2 v}{dx^2} J'_0(2\sqrt{v}) v^{-1/2} + \left( \frac{dv}{dx} \right)^2 J''_0(2\sqrt{v}) v^{-1} - \frac{1}{2} \left( \frac{dv}{dx} \right)^2 J'_0(2\sqrt{v}) v^{-3/2} \\ \frac{\delta^2 \Psi}{\delta y^2} &= \frac{d^2 v}{dy^2} J'_0(2\sqrt{v}) v^{-1/2} + \left( \frac{dv}{dy} \right)^2 J''_0(2\sqrt{v}) v^{-1} - \frac{1}{2} \left( \frac{dv}{dy} \right)^2 J'_0(2\sqrt{v}) v^{-3/2} \\ \frac{\delta^2 \Psi}{\delta z^2} &= \frac{d^2 v}{dz^2} J'_0(2\sqrt{v}) v^{-1/2} + \left( \frac{dv}{dz} \right)^2 J''_0(2\sqrt{v}) v^{-1} - \frac{1}{2} \left( \frac{dv}{dz} \right)^2 J'_0(2\sqrt{v}) v^{-3/2} \end{aligned} \quad (19)$$

We need to know the derivatives of  $v = r + x$  with respect to the coordinates:

$$\begin{aligned} \frac{dv}{dx} &= \frac{d}{dx}(x+r) = 1 + \frac{x}{r} \\ \frac{dv}{dy} &= \frac{d}{dy}(x+r) = \frac{y}{r} \\ \frac{dv}{dz} &= \frac{d}{dz}(x+r) = \frac{z}{r} \end{aligned} \quad (20)$$

$$\begin{aligned}
\frac{d^2v}{dx^2} &= \frac{d}{dx} \left(1 + \frac{x}{r}\right) = \frac{r - x(x/r)}{r^2} = \frac{r^2 - x^2}{r^3} \\
\frac{d^2v}{dy^2} &= \frac{r^2 - y^2}{r^3} \\
\frac{d^2v}{dz^2} &= \frac{r^2 - z^2}{r^3}
\end{aligned} \tag{21}$$

Substituting (20) and (21) into (19), and (19) into the LHS of (17), we obtain:

$$\begin{aligned}
&\frac{d^2v}{dx^2} J'_0(2\sqrt{v})v^{-1/2} + \left(\frac{dv}{dx}\right)^2 J''_0(2\sqrt{v})v^{-1} - \frac{1}{2} \left(\frac{dv}{dx}\right)^2 J'_0(2\sqrt{v})v^{-3/2} \\
&+ \frac{d^2v}{dy^2} J'_0(2\sqrt{v})v^{-1/2} + \left(\frac{dv}{dy}\right)^2 J''_0(2\sqrt{v})v^{-1} - \frac{1}{2} \left(\frac{dv}{dy}\right)^2 J'_0(2\sqrt{v})v^{-3/2} \\
&+ \frac{d^2v}{dz^2} J'_0(2\sqrt{v})v^{-1/2} + \left(\frac{dv}{dz}\right)^2 J''_0(2\sqrt{v})v^{-1} - \frac{1}{2} \left(\frac{dv}{dz}\right)^2 J'_0(2\sqrt{v})v^{-3/2} \\
&+ \frac{2}{r} J_0(2\sqrt{v}) \\
&= \frac{r^2 - x^2}{r^3} J'_0(2\sqrt{v})v^{-1/2} + \left(1 + \frac{x}{r}\right)^2 J''_0(2\sqrt{v})v^{-1} - \frac{1}{2} \left(1 + \frac{x}{r}\right)^2 J'_0(2\sqrt{v})v^{-3/2} \\
&+ \frac{r^2 - y^2}{r^3} J'_0(2\sqrt{v})v^{-1/2} + \left(\frac{y}{r}\right)^2 J''_0(2\sqrt{v})v^{-1} - \frac{1}{2} \left(\frac{y}{r}\right)^2 J'_0(2\sqrt{v})v^{-3/2} \\
&+ \frac{r^2 - z^2}{r^3} J'_0(2\sqrt{v})v^{-1/2} + \left(\frac{z}{r}\right)^2 J''_0(2\sqrt{v})v^{-1} - \frac{1}{2} \left(\frac{z}{r}\right)^2 J'_0(2\sqrt{v})v^{-3/2} \\
&+ \frac{2}{r} J_0(2\sqrt{v}) \\
&= \frac{3r^2 - x^2 - y^2 - z^2}{r^3} J'_0(2\sqrt{v})v^{-1/2} + \left(1 + 2\frac{x}{r} + \frac{x^2}{r^2} + \frac{y^2}{r^2} + \frac{z^2}{r^2}\right) J''_0(2\sqrt{v})v^{-1} \\
&- \frac{1}{2} \left(1 + 2\frac{x}{r} + \frac{x^2}{r^2} + \frac{y^2}{r^2} + \frac{z^2}{r^2}\right) J'_0(2\sqrt{v})v^{-3/2} + \frac{2}{r} J_0(2\sqrt{v}) \\
&= \frac{2}{r} J'_0(2\sqrt{v})v^{-1/2} + \left(2 + 2\frac{x}{r}\right) J''_0(2\sqrt{v})v^{-1} - \frac{1}{2} \left(2 + 2\frac{x}{r}\right) J'_0(2\sqrt{v})v^{-3/2} + \frac{2}{r} J_0(2\sqrt{v}) \\
&= \frac{2}{r} J'_0(2\sqrt{v})v^{-1/2} + 2\frac{x+r}{r} J''_0(2\sqrt{v})v^{-1} - \frac{x+r}{r} J'_0(2\sqrt{v})v^{-3/2} + \frac{2}{r} J_0(2\sqrt{v})
\end{aligned}$$

Remembering that  $v = x + r$ ,

$$\begin{aligned}
&= \frac{2}{r} J_0'(2\sqrt{v}) v^{-1/2} + \frac{2}{r} J_0''(2\sqrt{v}) - \frac{1}{r} J_0'(2\sqrt{v}) v^{-1/2} + \frac{2}{r} J_0(2\sqrt{v}) \\
&= \frac{2}{r} J_0''(2\sqrt{v}) + \frac{1}{r} J_0'(2\sqrt{v}) v^{-1/2} + \frac{2}{r} J_0(2\sqrt{v}) \\
&= \frac{2}{r} J_0''(2\sqrt{v}) + \frac{2}{r \cdot 2\sqrt{v}} J_0'(2\sqrt{v}) + \frac{2}{r} J_0(2\sqrt{v}) \\
&= \frac{2}{r} \left( J_0''(2\sqrt{v}) + \frac{1}{2\sqrt{v}} J_0'(2\sqrt{v}) + J_0(2\sqrt{v}) \right) \tag{22}
\end{aligned}$$

Now, the ordinary Bessel function  $J_0(x)$  satisfies:

$$x^2 J_0''(x) + x J_0'(x) + x^2 J_0(x) = 0$$

dividing through by  $x^2$  and changing variables, we get:

$$J_0''(2\sqrt{v}) + \frac{1}{2\sqrt{v}} J_0'(2\sqrt{v}) + J_0(2\sqrt{v}) = 0$$

which shows that (22) is zero, and establishes the proof of (17).