A New Pseudo-Solution of Hydrogen

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Abstract

The author has developed a simple technique for finding non-separable 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 is $J_0(2\sqrt{x+r})$ where J_0 is the Bessel function J_0, and the result can be easily verified using Mathematica (p. 11).

Introduction

An January 2023, I discovered a previously unknown solution to the simplest Schrödinger equation for the hydrogen atom.

It turns out that this function:

$$\Psi = J_0(2\sqrt{x+r}) \tag{1}$$

where J_0 is the ordinary Bessel function J_0, solves the simplest Schrödinger equation for hydrogen:

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

with E=0.

It does not, however, satisfy the global integrability condition required for it to be a valid wavefunction, i.e, it is not in L^2:

$$\int |\Psi|^2 < \infty \tag{3}$$

Therefore, it is only a pseudo-solution, since it satisfies the differential equation but is not a valid wavefunction.

A “proof by Mathematica” is on page 11, and a direct manual proof in included as an appendix.

This paper continues with an introduction to Schrödinger’s Equation for Hydrogen, then explains the solution technique used to discover (1) and concludes with a discussion of generalizations and further research.

Schrödinger’s 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 Ψ, which is a complex-valued function of particle positions that encodes a probability density function for the particle positions as $|\Psi|^2$ and a probability density function for the particle momenta as its Fourier transform $|\hat{\Psi}|^2$.

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 electron, 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 Ψ is the wavefunction, ∇^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[1] are assigned the value of 1, in order to eliminate the need for any physical constants in the equation. The unit of distance, in particular, is *Bohr radii*, approximately half an angstrom (Å$= 10^{-10}$ m). 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 restricting our attention to solutions that where the position and time dependence can be separated. 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:

$$-\frac{1}{2}\nabla^2\Psi - \frac{1}{r}\Psi = E\Psi \tag{4}$$

This equation is amenable to seperation of variables. Using spherical coordinates, we write Ψ as follows:

$$\Psi = R(r)Y(\theta,\psi) = R(r)P(\theta)F(\psi) \tag{5}$$

Substituting (5) into (4), and expanding the Laplacian ∇^2 in spherical coordinates, we obtain the following expansion[2]:

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

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

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[1] the reduced Planck constant, the elementary charge, the electron mass, and the Coulumb constant

[2] hyperphysics

Energy (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
	$(6-r)ye^{-r/3}$	
	$(6-r)ze^{-r/3}$	

energy would correspond to an electron and a proton at rest an (infinitely) large distance apart.

The classical solutions are separable and square integrable 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.

Solution Technique

The separation of variables step in (5) is an arbitrary assumption that discards all non-separable solutions. By making a different assumption, we can hope to find a non-seperable solution.

Let's assume that wavefunction Ψ satisfies a second-order ODE in some as yet unknown variable v:

$$a(v)\frac{\delta^2\Psi}{\delta v^2} + b(v)\frac{\delta\Psi}{\delta v} + c(v)\Psi = 0 \qquad (6)$$

We aim to parameterize our solution by a finite number of constants, so we further restrict our ODE by requiring its coefficients to be linear polynomials in v with constant coefficients:

$$
\begin{gathered}
(a_0 + a_1 v)\frac{\delta^2\Psi}{\delta v^2} + (b_0 + b_1 v)\frac{\delta\Psi}{\delta v} + (c_0 + c_1 v)\Psi = 0 \\
a_0, a_1, b_0, b_1, c_0, c_1 \in \mathbf{C}
\end{gathered}
\tag{7}
$$

Turning our attention to v, we (arbitrarily) select Cartesian coordinates, (arbitrarily) add the radius $r = \sqrt{x^2 + y^2 + z^2}$ to our list of coordinates, and (arbitrarily) restrict v to be a first degree polynomial in these coordinates, with constant coefficients:

$$
\begin{gathered}
v = v_1 x + v_2 y + v_3 z + v_4 r \\
v_1, v_2, v_3, v_4 \in \mathbf{C}
\end{gathered}
\tag{8}
$$

A constant term is excluded from v only because adding a constant to v would not meaningfully affect the solution. An ODE w.r.t. $x + 3$ has the same derivatives as an ODE w.r.t x, and the coefficients would only be shifted by constants, which could be absorbed into a_0, b_0, and c_0, so excluding a constant term in the polynomial for v simplifies the system with no further loss of generality.

Rearranging (7) like this:

$$
\frac{\delta^2\Psi}{\delta v^2} = -\frac{b_0 + b_1 v}{a_0 + a_1 v}\frac{\delta\Psi}{\delta v} - \frac{c_0 + c_1 v}{a_0 + a_1 v}\Psi \tag{9}
$$

substituting into (4) after expanding the Laplacian ∇^2 in Cartesian coordinates, using (8) for v, simplifying higher powers of r using $r^2 = x^2 + y^2 + z^2$, writing Ψ' for $\frac{d\Psi}{dv}$ and collecting all terms on one side of an equality with zero, we obtain a rational function in $x, y, z, r, \Psi, \Psi', E, a_0, a_1, b_0, b_1, c_0, c_1, v_1, v_2, v_3, v_4$ with a 228 term numerator and an 18 term denominator. We ignore the denominator. The numerator begins:

$$
r\Psi' x^3 v_1^3 b_1 + r\Psi' x y^2 v_1^3 b_1 + r\Psi' x z^2 v_1^3 b_1 + r\Psi' x^2 y v_1^2 v_2 b_1 + r\Psi' y^3 v_1^2 v_2 b_1 + \cdots \tag{10}
$$

We're looking for constants $E, a_0, a_1, b_0, b_1, c_0, c_1, v_1, v_2, v_3, v_4$ that will solve equation (10) for all values of x, y, z, r, Ψ, and Ψ', so we collect like terms in x, y, z, r, Ψ, and Ψ', organizing equation (10) like this:

$$
r\Psi' x^3 \left(v_1^3 b_1 + v_1 v_2^2 b_1 + v_1 v_3^2 b_1 + 3 v_1 v_4^2 b_1\right) + \cdots \tag{11}
$$

The expressions in parenthesis gives us a system of equations (only one is shown in (11)) involving the E, v_i, a_i, b_i and c_i variables that, if satisfied, will yield a solution to (4) in the form (7) and (8). Once duplicate equations are dropped, the system has 34 equations.

$$
\begin{aligned}
-2v_1v_4a_1+2v_1v_4b_0&=0\\
4v_1v_3v_4b_1&=0\\
4v_1v_3v_4c_1&=0\\
4v_1^2v_4b_1+4v_2^2v_4b_1+2v_3^2v_4b_1+2v_4^3b_1&=0\\
2v_1^2v_4c_1+4v_2^2v_4c_1+4v_3^2v_4c_1+2v_4^3c_1-4Ev_4a_1&=0\\
4v_1v_2v_4b_1&=0\\
4v_1v_2v_4c_1&=0\\
2v_1v_4c_0-2v_1a_1&=0\\
v_1^2v_3c_1+v_2^2v_3c_1+v_3^3c_1+3v_3v_4^2c_1-2Ev_3a_1&=0\\
-2v_3v_4a_1+2v_3v_4b_0&=0\\
v_1^2v_3b_1+v_2^2v_3b_1+v_3^3b_1+3v_3v_4^2b_1&=0\\
v_1^2v_4c_1+3v_2^2v_4c_1+v_3^2v_4c_1+v_4^3c_1-2Ev_4a_1&=0\\
v_1^2v_4b_1+3v_2^2v_4b_1+v_3^2v_4b_1+v_4^3b_1&=0\\
2v_3v_4c_0-2v_3a_1&=0\\
2v_1^2v_4b_1+4v_2^2v_4b_1+4v_3^2v_4b_1+2v_4^3b_1&=0\\
v_1^2v_2c_1+v_2^3c_1+v_2v_3^2c_1+3v_2v_4^2c_1-2Ev_2a_1&=0\\
-2v_2v_4a_1+2v_2v_4b_0&=0\\
v_1^3c_1+v_1v_2^2c_1+v_1v_3^2c_1+3v_1v_4^2c_1-2Ev_1a_1&=0\\
4v_2v_3v_4b_1&=0\\
4v_1^2v_4c_1+2v_2^2v_4c_1+4v_3^2v_4c_1+2v_4^3c_1-4Ev_4a_1&=0\\
v_1^2v_4b_1+v_2^2v_4b_1+3v_3^2v_4b_1+v_4^3b_1&=0\\
v_1^2v_4c_1+v_2^2v_4c_1+3v_3^2v_4c_1+v_4^3c_1-2Ev_4a_1&=0\\
4v_2v_3v_4c_1&=0\\
3v_1^2v_4c_1+v_2^2v_4c_1+v_3^2v_4c_1+v_4^3c_1-2Ev_4a_1&=0\\
3v_1^2v_4b_1+v_2^2v_4b_1+v_3^2v_4b_1+v_4^3b_1&=0\\
-2v_4^2a_1+v_1^2b_0+v_2^2b_0+v_3^2b_0+v_4^2b_0&=0\\
-2a_0&=0\\
v_1^3b_1+v_1v_2^2b_1+v_1v_3^2b_1+3v_1v_4^2b_1&=0\\
-2v_4a_0&=0\\
4v_1^2v_4c_1+4v_2^2v_4c_1+2v_3^2v_4c_1+2v_4^3c_1-4Ev_4a_1&=0\\
v_1^2v_2b_1+v_2^3b_1+v_2v_3^2b_1+3v_2v_4^2b_1&=0\\
2v_2v_4c_0-2v_2a_1&=0\\
v_1^2c_0+v_2^2c_0+v_3^2c_0+v_4^2c_0-2Ea_0-2v_4a_1&=0\\
4v_1^2v_4b_1+2v_2^2v_4b_1+4v_3^2v_4b_1+2v_4^3b_1&=0
\end{aligned}
\tag{12}
$$

The system (12) describes an algebraic variety in $\mathbf{C}^{11}$. We can better understand its structure by decomposing it into a union of its irreducible subvarieties. Numerous algorithms to do this have been proposed and/or implemented

[1, 3, 5, 7, 8, 9]. Due to the well-known correspondence between algebraic varieties and ideals in a polynomial ring, algorithms for the primary decomposition of ideals are well suited to decomposing an algebraic variety into its irreducible subvarieties.

I performed this step using Sage, by constructing an ideal consisting of the left hand sides of the equations in (12), and then calling a Sage method that uses Singular's implementation of the Shimoyama-Yokoyama algorithm[8] to compute the ideal's minimal associated prime ideals:

$$(c_1, c_0, b_1, b_0, a_1, a_0) \tag{13a}$$
$$(a_0, v_4, v_3, v_2, v_1) \tag{13b}$$
$$\left(v_1^2 + v_2^2 + v_3^2, a_1, a_0, v_4\right) \tag{13c}$$
$$\left(v_4 c_0 - b_0, E c_0 - v_4 c_1, -v_4^2 c_1 + E b_0, b_1, 2a_1 - b_0, a_0, v_3, v_2, v_1\right) \tag{13d}$$
$$\left(v_4 c_0 - b_0, v_1^2 + v_2^2 + v_3^2 - v_4^2, c_1, b_1, a_1 - b_0, a_0, E\right) \tag{13e}$$

Each of these five ideals corresponds to an algebraic variety described by setting all of the ideal generators equal to zero; the union of these five algebraic varieties is the algebraic variety described by (12). Every point on each of these varieties describes a set of constants that solve (12); each variety therefore describes a family of solutions.

Several of these varieties solve the system of equations, but do not lead to a meaningful solution to the differential equation (4). In brief,

(13a) sets all coefficients of the ODE to zero, so we discard it,

(13b) sets the variable v to zero, so we discard it,

(13c) sets the coefficient $(a_0 + a_1 v)$ of $\frac{d^2\Psi}{dv^2}$ in the ODE to zero, resulting in a first-order ODE, so we discard it, too,

(13d) corresponds to the classical solutions (see below), and

(13e) gives us our new solution (see below).

How to understand ideal (13d)? We form a system of equations that describe the corresponding variety by setting all of the ideal generators to zero. We can always multiply (7) by a constant without affecting our result, so we can set $a_1 = 1$ without loss of generality. 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 $v_4 = 1$. This simplifies the variety corresponding to ideal (13d) to the following system of equations:

$$\begin{array}{cc} a_0 = 0 & a_1 = 1 \\ b_0 = 2 & b_1 = 0 \\ c_0 = 2 & c_1 = 2E \\ v_4 = 1 & v_1 = v_2 = v_3 = 0 \end{array} \tag{14}$$

Substituting these values back into (7) and (8), we conclude that $\Psi(v)$ is a solution of (4) under these conditions:

$$\begin{gathered} v = r \\ v\Psi'' + 2\Psi' + 2(1 + Ev)\Psi = 0 \end{gathered} \tag{15}$$

This is the classical radial equation obtained by seperation of variables[3]. 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:

$$\frac{1}{R}\frac{d}{dr}\left[r^2\frac{dR}{dr}\right] + 2(Er^2 + r) = l(l+1) \tag{16}$$

where l is the orbital quantum number, which can be zero. Set $l = 0$, $v = r$ and $\Psi = R$ in (16) and expand out the derivative to obtain (15). The presence of this solution was expected and won't be commented on further.

Ideal (13e) was not expected, and contains our new solution. Again, we form a system of equations by setting all of the ideal generators to zero. Again, we can set $a_1 = 1$, by the same logic as above. Let's assume that our v_i coefficients are real (why?), so all of their squares must be positive, and since $v_4^2 - v_1^2 - v_2^2 - v_3^3 = 0$, v_4 must be non-zero. So we can normalize by setting $v_4 = 1$. That simplifies (13e) to this ideal:

$$\left(c_0 - 1, v_1^2 + v_2^2 + v_3^2 - 1, v_4 - 1, c_1, b_1, 1 - b_0, a_1 - 1, a_0, E\right) \tag{17}$$

This ideal corresponds to the following system of equations:

---

[3] See Pauling and Wilson or `http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hydrad.html`

$$
\begin{gathered}
E = 0 \\
a_0 = 0 \qquad a_1 = 1 \\
b_0 = 1 \qquad b_1 = 0 \\
c_0 = 1 \qquad c_1 = 0 \\
v_4 = 1 \qquad v_1^2 + v_2^2 + v_3^2 = 1
\end{gathered}
\tag{18}
$$

Substituting these values back into our ansatz, we conclude that $\Psi(v)$ is a solution of (4) under these conditions:

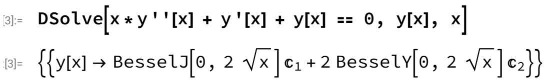
$$
\begin{gathered}
v\frac{\delta^2\Psi}{\delta v^2} + \frac{\delta\Psi}{\delta v} + \Psi = 0 \\
v = v_1 x + v_2 y + v_3 z + r \\
v_1^2 + v_2^2 + v_3^2 = 1
\end{gathered}
\tag{19}
$$

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) (note 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:

$$
v\Psi''(v) + \Psi'(v) + \Psi(v) = 0 \tag{20}
$$

Wolfram Mathematica[6] can now analyze this equation[4] and find a solution using the ordinary Bessel functions J_0 and Y_0:



```
[3]:= DSolve[x * y''[x] + y'[x] + y[x] == 0, y[x], x]
[3]= {{y[x] → BesselJ[0, 2 √x] ℂ1 + 2 BesselY[0, 2 √x] ℂ2}}
```

Therefore, setting

$$
\Psi = J_0(2\sqrt{x + r}) \tag{1}
$$

where x, y, z are Cartesian coordinates and $r = \sqrt{x^2 + y^2 + z^2}$, we conclude that (1) is an exact solution to (4), with $E = 0$.

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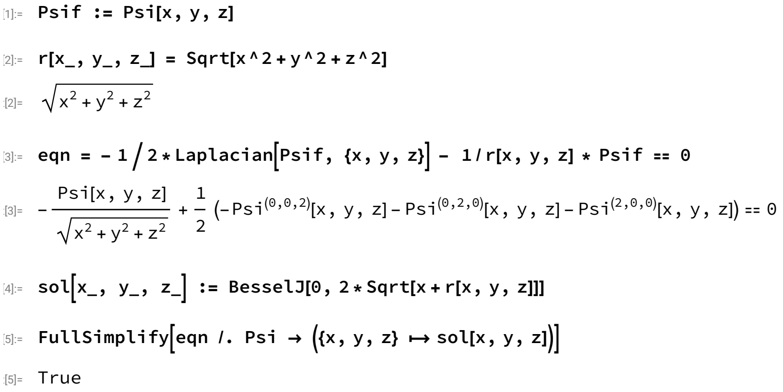
[4] I originally used Wolfram Alpha; the Wolfram Language Engine can also be used.

Verification

The result can be easily verified[5] using Mathematica, as follows:



```
[1]:= Psif := 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[Psif, {x, y, z}] - 1 / r[x, y, z] * Psif == 0
```

[3]= $-\frac{\text{Psi}[x, y, z]}{\sqrt{x^2+y^2+z^2}}+\frac{1}{2}\left(-\text{Psi}^{(0,0,2)}[x, y, z]-\text{Psi}^{(0,2,0)}[x, y, z]-\text{Psi}^{(2,0,0)}[x, y, z]\right) == 0$

```
[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
```

The Global Condition

As noted in the introduction, in order to be a valid wavefunction, (3) must also be satisfied. The physical intuition lying behind this requirement is that the square of the modulus $|\Psi|^2$ is a probability density function and its global integral must therefore be finite, as the total probability of the electron being somewhere is finite. [4, §1.4]

(1) does not satisfy (3). This can be easily seen by inspecting Bessel's original definition of J_0 [10, p. 19]:

$$J_0(z) = \frac{1}{2\pi}\int_0^{2\pi} \cos(z \sin\theta) d\theta \tag{21}$$

$J_0(z)$ is continuous everywhere on the real line and $J_0(0) = 1$. Also, $2\sqrt{x+r}$ is continuous everywhere in $\mathbb{R}^3$ and is zero along the negative x-axis. These facts imply that for any $\delta > 0$ there exists an $\epsilon > 0$ such that $J_0(2\sqrt{x+r}) > 1-\epsilon$ for any point within a distance of δ from the negative x-axis. (uniform continuity?)

This implies that for a small sphere S of radius δ, centered on a point along the negative x-axis,

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[5] A manual verification is presented in an appendix

$$\int_S \left|J_0(2\sqrt{x+r})\right|^2\ dV > \frac{4}{3}\pi\delta^3(1-\epsilon)$$

Since there are an infinite number of these small spheres (disjoint?),

$$\int_{\mathbb{R}^3} \left|J_0(2\sqrt{x+r})\right|^2\ dV = \infty$$

and $J_0(2\sqrt{x+r})$ is not square integrable[6].

Generalization

Any unit vector can be picked for (v_1, v_2, v_3), so the distance in any direction from the origin can be used in lieu of x, and any ordinary Bessel function can be used:

$$\Psi = F(2\sqrt{v_1 x + v_2 y + v_3 z + r}) \tag{22}$$

where

$$v_1^2 + v_2^2 + v_3^2 = 1$$

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

By linearity of (4), any finite linear combination of functions of the form (22) also solves (4).

The assumption that the v_i coefficients are real was arbitrary.

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.

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[6] Peter Ulrickson (Catholic University) pointed out to me that this argument also implies that Ψ is not in any L^p space except L^∞.

Use it to find ideal (13) 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.minimal_associated_primes()
```

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
eq_a_convertField       # the PDE modulo the ansatz
eq_a_reduceRing_n       # the expanded numerator
R                       # polynomial ring over integers
F                       # fraction field of R
eqns_RQQ                # system of equations to solve
```

Current Implementation Status

The algorithm presented above can be used to check any PDE to see if any of its solutions can be expressed using an ODE structured according to a specific ansatz. This technique is complementary to separation of variables, where we check a PDE to see if any of its solutions can be expressed as a product of factors, each depending on only a subset of the independent variables.

As my primary interest lies in quantum mechanics, I have investigated the PDEs that model hydrogen and helium.

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

For helium, the PDE is $\nabla_1^2\Psi + \nabla_2^2\Psi - \frac{2}{r_1} - \Psi\frac{2}{r_2} - \Psi\frac{1}{r_{12}}\Psi = E\Psi$, where $\Psi = \Psi(r_1, r_2, r_{12})$ and ∇_i is the Laplacian with respect to the i^{th} electron. Ψ is assumed to have no angular dependence, which has been known since at least the time of Hylleraas to be a valid assumption for the ground state.

In both cases, I use Hartree atomic units to render the equations dimensionless.

Conclusion

As we've seen, using a parameterized function space allows the use of algebraic geometry techniques to check a PDE to see if a solution exists in that function space. Doing so requires putting degree bounds on the various polynomials that form the ansatz, in contrast to separation of variables, which puts no degree bounds on the polynomials but requires the solution to be separable. As we've seen, even a fairly simple ansatz not only recovered a known separable solution, but also found a previously unknown solution that is not separable.

Currently, the primary barrier to successful execution of the algorithm is design limitations in the various software packages used to execute it. For example, no current Gröbner basis algorithms, to my knowledge, will fall back on using disk-based storage once RAM becomes exhausted. Run times of weeks or months can be expected when searching for truly unknown solutions to realistic problems, but no such calculation is possible if the machine "runs out of memory", even though an ample disk-based backing store may be available.

Any PDE can be explored using this technique. For studying a non-linear PDE such as Navier-Stokes, a different set of ansatzen formed from non-linear ODEs might be advisable.

No theoretical treatment is currently available to predict when these ansatzen might yield solutions. The discovery of a new result using such a simple ansatz suggests, however, that even very modest degree bounds can yield solutions.

The main thrust of the author's research, however, remains quantum mechanics and the hope of an ODE-based solution to helium. As of May 2023, the author continues to develop the software tools necessary to check helium ansatz 16.6, in the hopes of finding a solution to helium's ground state.

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/`

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Appendix: Manual Verification of the Result

For anybody wondering how Mathematica concludes that (1) solves (4), the claim is that $\Psi = J_0(2\sqrt{x+r}) = (J_0 \circ 2\sqrt{v})(x+r)$ satisfies:

$$\left(\frac{\delta^2}{\delta^2 x} + \frac{\delta^2}{\delta^2 y} + \frac{\delta^2}{\delta^2 z}\right)\Psi + \frac{2}{r}\Psi = 0 \tag{23}$$

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

$$\begin{aligned}
\frac{\delta \Psi}{\delta x} &= \frac{dv}{dx}\frac{d}{dv}\left(J_0 \circ 2\sqrt{v}\right) = \frac{dv}{dx} J_0'(2\sqrt{v})v^{-1/2} \\
\frac{\delta \Psi}{\delta y} &= \frac{dv}{dy}\frac{d}{dv}\left(J_0 \circ 2\sqrt{v}\right) = \frac{dv}{dy} J_0'(2\sqrt{v})v^{-1/2} \\
\frac{\delta \Psi}{\delta z} &= \frac{dv}{dz}\frac{d}{dv}\left(J_0 \circ 2\sqrt{v}\right) = \frac{dv}{dz} J_0'(2\sqrt{v})v^{-1/2}
\end{aligned} \tag{24}$$

Next we compute the partial second derivatives of Ψ:

$$\begin{aligned}
\frac{\delta^2 \Psi}{\delta x^2} &= \frac{d^2 v}{dx^2} J_0'(2\sqrt{v})v^{-1/2} + \left(\frac{dv}{dx}\right)^2 J_0''(2\sqrt{v})v^{-1} - \frac{1}{2}\left(\frac{dv}{dx}\right)^2 J_0'(2\sqrt{v})v^{-3/2} \\
\frac{\delta^2 \Psi}{\delta y^2} &= \frac{d^2 v}{dy^2} J_0'(2\sqrt{v})v^{-1/2} + \left(\frac{dv}{dy}\right)^2 J_0''(2\sqrt{v})v^{-1} - \frac{1}{2}\left(\frac{dv}{dy}\right)^2 J_0'(2\sqrt{v})v^{-3/2} \\
\frac{\delta^2 \Psi}{\delta z^2} &= \frac{d^2 v}{dz^2} J_0'(2\sqrt{v})v^{-1/2} + \left(\frac{dv}{dz}\right)^2 J_0''(2\sqrt{v})v^{-1} - \frac{1}{2}\left(\frac{dv}{dz}\right)^2 J_0'(2\sqrt{v})v^{-3/2}
\end{aligned} \tag{25}$$

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

$$\begin{aligned}
\frac{dv}{dx} &= \frac{d}{dx}(x+r) = 1 + \frac{x}{r} \\
\frac{dv}{dy} &= \frac{d}{dy}(x+r) = \frac{y}{r} \\
\frac{dv}{dz} &= \frac{d}{dz}(x+r) = \frac{z}{r}
\end{aligned} \tag{26}$$

$$\begin{aligned}\frac{d^2v}{dx^2} = \frac{d}{dx}\left(1+\frac{x}{r}\right) &= \frac{r - x(x/r)}{r^2} = \frac{r^2-x^2}{r^3} \\ \frac{d^2v}{dy^2} &= \frac{r^2-y^2}{r^3} \\ \frac{d^2v}{dz^2} &= \frac{r^2-z^2}{r^3}\end{aligned} \tag{27}$$

Substituting (26) and (27) into (25), and (25) into the LHS of (23), we obtain:

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

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

$$\begin{aligned}=&\frac{3r^2-x^2-y^2-z^2}{r^3}J_0'(2\sqrt{v})v^{-1/2} + (1+2\frac{x}{r}+\frac{x^2}{r^2}+\frac{y^2}{r^2}+\frac{z^2}{r^2})J_0''(2\sqrt{v})v^{-1} \\ &- \frac{1}{2}(1+2\frac{x}{r}+\frac{x^2}{r^2}+\frac{y^2}{r^2}+\frac{z^2}{r^2})J_0'(2\sqrt{v})v^{-3/2} + \frac{2}{r}J_0(2\sqrt{v})\end{aligned}$$

$$= \frac{2}{r}J_0'(2\sqrt{v})v^{-1/2} + (2+2\frac{x}{r})J_0''(2\sqrt{v})v^{-1} - \frac{1}{2}(2+2\frac{x}{r})J_0'(2\sqrt{v})v^{-3/2} + \frac{2}{r}J_0(2\sqrt{v})$$

$$= \frac{2}{r}J_0'(2\sqrt{v})v^{-1/2} + 2\frac{x+r}{r}J_0''(2\sqrt{v})v^{-1} - \frac{x+r}{r}J_0'(2\sqrt{v})v^{-3/2} + \frac{2}{r}J_0(2\sqrt{v})$$

Remembering that $v = x + r$,

$$= \frac{2}{r}J_0'(2\sqrt{v})v^{-1/2} + \frac{2}{r}J_0''(2\sqrt{v}) - \frac{1}{r}J_0'(2\sqrt{v})v^{-1/2} + \frac{2}{r}J_0(2\sqrt{v})$$

$$= \frac{2}{r}J_0''(2\sqrt{v}) + \frac{1}{r}J_0'(2\sqrt{v})v^{-1/2} + \frac{2}{r}J_0(2\sqrt{v})$$

$$= \frac{2}{r}J_0''(2\sqrt{v}) + \frac{2}{r \cdot 2\sqrt{v}}J_0'(2\sqrt{v}) + \frac{2}{r}J_0(2\sqrt{v})$$

$$= \frac{2}{r}\left(J_0''(2\sqrt{v}) + \frac{1}{2\sqrt{v}}J_0'(2\sqrt{v}) + J_0(2\sqrt{v})\right) \tag{28}$$

Assume for that moment that the Bessel function $J_0(x)$ satisfies Bessel's equation:

$$x^2 J_0''(x) + xJ_0'(x) + x^2 J_0(x) = 0 \tag{29}$$

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 (28) is zero, and establishes the proof of (23).

It remains to show that $J_0(x)$, defined by (21), actually satisfies (29).

The approach here largely follows [2, p. 92], with modern notation. For integer values of n, define $J_n(z)$ as follows:

$$J_n(z) = \frac{1}{2\pi}\int_0^{2\pi} \cos(n\theta - z\sin\theta)d\theta \qquad n \in \mathbb{Z} \tag{30}$$

Differentiating with respect to z, we obtain:

$$J_n'(z) = \frac{1}{2\pi}\int_0^{2\pi} \sin(n\theta - z\sin\theta)\sin\theta\, d\theta \tag{31}$$

Applying the trigonometric identity $2\sin\alpha\sin\beta = \cos(\alpha-\beta) - \cos(\alpha+\beta)$,

$$\begin{aligned} J_n'(z) = \frac{1}{2\pi}\int_0^{2\pi} \left[\frac{1}{2}\cos\left((n-1)\theta - z\sin\theta\right) - \frac{1}{2}\cos\left((n-1)\theta - z\sin\theta\right)\right] d\theta \\ = \frac{1}{2}J_{n-1}(z) - \frac{1}{2}J_{n+1}(z) \end{aligned} \tag{32}$$

Having found a relationship for the difference of $J_{n-1}(z)$ and $J_{n+1}(z)$, we now seek a relationship for their sum.

$$\begin{gathered} \frac{1}{2}J_{n-1}(z) + \frac{1}{2}J_{n+1}(z) \\ = \frac{1}{2\pi}\int_0^{2\pi} \left[\frac{1}{2}\cos\left((n-1)\theta - z\sin\theta\right) + \frac{1}{2}\cos\left((n+1)\theta - z\sin\theta\right)\right] d\theta \\ = \frac{1}{2\pi}\int_0^{2\pi} \cos(n\theta - z\sin\theta)\cos\theta\, d\theta \\ = \frac{n}{z}\cdot\frac{1}{2\pi}\int_0^{2\pi} \cos(n\theta - z\sin\theta)\, d\theta - \frac{1}{z}\cdot\frac{1}{2\pi}\int_0^{2\pi} \cos(n\theta - z\sin\theta)\,(n - z\cos\theta)\, d\theta \\ = \frac{n}{z}\cdot\frac{1}{2\pi}\int_0^{2\pi} \cos(n\theta - z\sin\theta)\, d\theta - \frac{1}{z}\cdot\frac{1}{2\pi}\Big[\sin(n\theta - z\sin\theta)\Big]_0^{2\pi} \\ = \frac{n}{z}J_n(z) \end{gathered} \tag{33}$$

where I used the fact that n is an integer to evaluate the bracketed expression as zero.

Now we use (32) and (33) to evaluate the LHS of (29):

$$\begin{gathered} x^2 J_0''(x) + xJ_0'(x) + x^2 J_0(x) \\ = \frac{1}{4}x^2 J_{-2}(x) - \frac{1}{2}x^2 J_0(x) + \frac{1}{4}x^2 J_2(x) + \frac{1}{2}xJ_{-1}(x) - \frac{1}{2}xJ_1(x) + x^2 J_0(x) \\ = \left[\frac{1}{4}x^2 J_{-2}(x) + \frac{1}{4}x^2 J_0(x)\right] + \left[\frac{1}{4}x^2 J_2(x) + \frac{1}{4}x^2 J_0(x)\right] + \frac{1}{2}xJ_{-1}(x) - \frac{1}{2}xJ_1(x) \\ = -\frac{1}{2}xJ_{-1}(x) + \frac{1}{2}xJ_1(x) + \frac{1}{2}xJ_{-1}(x) - \frac{1}{2}xJ_1(x) = 0 \end{gathered} \tag{34}$$

which proves that $J_0(x)$ satisfies (29).