A New Solution of Hydrogen

Brent Baccala

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Abstract

I show a previously unknown exact solution to the simplest time-independent Schrödinger equation for hydrogen. The solution involves a Bessel function, is not separable, and is not in L^2.

Theorem

Consider the following simple Schödinger equation for the hydrogen atom:

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

Let J_0 be the ordinary Bessel function J_0, and set

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

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

Then (2) is an exact solution to (1), with $E = 0$.

Verification

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

```
In[1]:= Psif := Psi[x, y, z]

In[2]:= r[x_, y_, z_] = Sqrt[x^2 + y^2 + z^2]
Out[2]= √(x² + y² + z²)

In[3]:= eqn = -1/2 * Laplacian[Psif, {x, y, z}] - 1/r[x, y, z] * Psif == 0
Out[3]= -Psi[x, y, z]/√(x² + y² + z²) + 1/2 (-Psi^(0,0,2)[x, y, z] - Psi^(0,2,0)[x, y, z] - Psi^(2,0,0)[x, y, z]) == 0

In[4]:= sol[x_, y_, z_] := BesselJ[0, 2 * Sqrt[x + r[x, y, z]]]

In[5]:= FullSimplify[eqn /. Psi → ({x, y, z} ↦ sol[x, y, z])]
Out[5]= True
```

Proof

The claim is that $\Psi = J_0(2\sqrt{x+r}) = (J_0 \circ 2\sqrt{v})(x+r)$ satisfies:

$$\left(\frac{\delta^2}{\delta^2 x} + \frac{\delta^2}{\delta^2 y} + \frac{\delta^2}{\delta^2 z}\right)\Psi + \frac{2}{r}\Psi = 0 \tag{3}$$

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

$$\begin{aligned}
\frac{\delta\Psi}{\delta x} &= \frac{dv}{dx}\frac{d}{dv}\left(J_0 \circ 2\sqrt{v}\right) = \frac{dv}{dx}J_0'(2\sqrt{v})v^{-1/2} \\
\frac{\delta\Psi}{\delta y} &= \frac{dv}{dy}\frac{d}{dv}\left(J_0 \circ 2\sqrt{v}\right) = \frac{dv}{dy}J_0'(2\sqrt{v})v^{-1/2} \\
\frac{\delta\Psi}{\delta z} &= \frac{dv}{dz}\frac{d}{dv}\left(J_0 \circ 2\sqrt{v}\right) = \frac{dv}{dz}J_0'(2\sqrt{v})v^{-1/2}
\end{aligned} \tag{4}$$

Next we compute the partial second derivatives of Ψ:

$$\begin{aligned}
\frac{\delta^2\Psi}{\delta x^2} &= \frac{d^2v}{dx^2}J_0'(2\sqrt{v})v^{-1/2} + \left(\frac{dv}{dx}\right)^2 J_0''(2\sqrt{v})v^{-1} - \frac{1}{2}\left(\frac{dv}{dx}\right)^2 J_0'(2\sqrt{v})v^{-3/2} \\
\frac{\delta^2\Psi}{\delta y^2} &= \frac{d^2v}{dy^2}J_0'(2\sqrt{v})v^{-1/2} + \left(\frac{dv}{dy}\right)^2 J_0''(2\sqrt{v})v^{-1} - \frac{1}{2}\left(\frac{dv}{dy}\right)^2 J_0'(2\sqrt{v})v^{-3/2} \\
\frac{\delta^2\Psi}{\delta z^2} &= \frac{d^2v}{dz^2}J_0'(2\sqrt{v})v^{-1/2} + \left(\frac{dv}{dz}\right)^2 J_0''(2\sqrt{v})v^{-1} - \frac{1}{2}\left(\frac{dv}{dz}\right)^2 J_0'(2\sqrt{v})v^{-3/2}
\end{aligned} \tag{5}$$

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

$$\begin{aligned}
\frac{dv}{dx} &= \frac{d}{dx}(x+r) = 1 + \frac{x}{r} \\
\frac{dv}{dy} &= \frac{d}{dy}(x+r) = \frac{y}{r} \\
\frac{dv}{dz} &= \frac{d}{dz}(x+r) = \frac{z}{r}
\end{aligned} \tag{6}$$

$$\begin{aligned}
\frac{d^2v}{dx^2} = \frac{d}{dx}\left(1 + \frac{x}{r}\right) &= \frac{r - x(x/r)}{r^2} = \frac{r^2 - x^2}{r^3} \\
\frac{d^2v}{dy^2} &= \frac{r^2 - y^2}{r^3} \\
\frac{d^2v}{dz^2} &= \frac{r^2 - z^2}{r^3}
\end{aligned} \tag{7}$$

Substituting (6) and (7) into (5), and (5) into the LHS of (3), 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 $v = x + r$,

$$\begin{aligned}
&= \frac{2}{r}J_0'(2\sqrt{v})v^{-1/2} + \frac{2}{r}J_0''(2\sqrt{v}) - \frac{1}{r}J_0'(2\sqrt{v})v^{-1/2} + \frac{2}{r}J_0(2\sqrt{v}) \\
&= \frac{2}{r}J_0''(2\sqrt{v}) + \frac{1}{r}J_0'(2\sqrt{v})v^{-1/2} + \frac{2}{r}J_0(2\sqrt{v}) \\
&= \frac{2}{r}J_0''(2\sqrt{v}) + \frac{2}{r\cdot 2\sqrt{v}}J_0'(2\sqrt{v}) + \frac{2}{r}J_0(2\sqrt{v}) \\
&= \frac{2}{r}\left(J_0''(2\sqrt{v}) + \frac{1}{2\sqrt{v}}J_0'(2\sqrt{v}) + J_0(2\sqrt{v})\right) \qquad (8)
\end{aligned}$$

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 (8) is zero, and establishes the proof of (3).

Generalization

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

$$\Psi = F(2\sqrt{a_1 x + a_2 y + a_3 z + r}) \tag{9}$$

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 (9) also solves (1).

Discovery

I found this solution roughly as follows.[1]

Use Cartesian coordinates. Let v be a linear polynomial in the coordinates and the root $r = \sqrt{x^2 + y^2 + z^2}$, with the following form (the v_i are constants):

$$v = v_0 r + v_1 x + v_2 y + v_3 z \tag{10}$$

Assume the solution to the input PDE (1) is a linear second-order ODE w.r.t. v with linear coefficeints, with the following form:

[1] I discovered an alternate form of this solution using a somewhat more complex ansatz on January 24, 2023. By January 26, I had established the solution in its current form. The original ansatz produced a rational function with a 1254 term numerator and a 36 term denominator, that gave rise to a system of 224 equations.

$$(d_0 + d_1 v)\frac{\delta^2\Psi}{\delta v^2} - (m_0 + m_1 v)\frac{\delta\Psi}{\delta v} - (n_0 + n_1 v)\Psi = 0 \tag{11}$$

or:

$$(d_0 + d_1 v)\frac{\delta^2\Psi}{\delta v^2} = (m_0 + m_1 v)\frac{\delta\Psi}{\delta v} + (n_0 + n_1 v)\Psi \tag{12}$$

Substituting (10) into (12), expanding derivatives in (1), substituting the RHS of (12) into (1) where the LHS of (12) appears, replacing all instances of r^2 with $x^2 + y^2 + z^2$, and canceling GCDs, we obtain a rational function with a 228 term numerator and an 18 term denominator. We ignore the denominator. The numerator begins:

$$-2r\Psi x^3 E d_1 v_1 - 3r\Psi x^3 n_1 v_0^2 v_1 - r\Psi x^3 n_1 v_1^3 - r\Psi x^3 n_1 v_1 v_2^2 - r\Psi x^3 n_1 v_1 v_3^2 - \cdots \tag{13}$$

We collect like terms in x, y, z, r, Ψ, and Ψ', organizing the numerator like this:

$$r\Psi x^3\left(-2Ed_1 v_1 - 3n_1 v_0^2 v_1 - n_1 v_1^3 - n_1 v_1 v_2^2 - n_1 v_1 v_3^2\right) - \cdots \tag{14}$$

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 (1) in the form (10) and (11). Once duplicate equations are dropped, the system has 34 equations.

Several solution techniques are available to solve a system of polynomial equations; I used a numerical approximation technique. A laptop computer finds the following approximate solution in less than three seconds:

```
(E, 1.2793593235207163e-32)
(d0, 1.4231937528298923e-43)
(d1, 1.0)
(m0, -1.0)
(m1, 5.0839108285704363e-42)
(n0, -1.0)
(n1, -8.795561312674161e-33)
(v0, 1.0)
(v1, 0.47255672374941904)
(v2, 0.5379975369878418)
(v3, 0.6980320859632679)
```
(15)

This is a *witness point*, a term common in the literature, an approximate solution accurate enough to recover an exact solution.

In this case, exactness recovery is simple and straightforward. E, d_0, m_1 and n_1 are all quite small, so we set them to zero, while d_1, m_0, n_0 and v_0 already have their exact values and:

$$0.4725567237^2 + 0.5379975369^2 + 0.6980320859^2 \approx 1.0000000000$$

so we add $v_1^2 + v_2^2 + v_3^2 = 1$ to our solution and conclude that our witness point lies approximately on the following algebraic variety:

$$\begin{gathered} E = 0 \\ d_0 = 0 \qquad d_1 = 1 \\ m_0 = -1 \qquad m_1 = 0 \\ n_0 = -1 \qquad n_1 = 0 \\ v_0 = 1 \qquad v_1^2 + v_2^2 + v_3^2 = 1 \end{gathered} \tag{16}$$

Substituting these values back into our ansatz, we conclude that $\Psi(v)$ is a solution of (1) under these conditions:

$$\begin{gathered} v\frac{\delta^2\Psi}{\delta v^2} + \frac{\delta\Psi}{\delta v} + \Psi = 0 \\ v = v_1 x + v_2 y + v_3 z + r \\ v_1^2 + v_2^2 + v_3^2 = 1 \end{gathered} \tag{17}$$

We now have to solve a second order ODE:

$$v\Psi''(v) + \Psi'(v) + \Psi(v) = 0 \tag{18}$$

Wolfram Mathematica[2] can now analyze this equation and determine that it is equivalent to the Bessel function (2).

```
In[3]:= DSolve[x * y''[x] + y'[x] + y[x] == 0, y[x], x]
Out[3]= {{y[x] → BesselJ[0, 2 √x] c1 + 2 BesselY[0, 2 √x] c2}}
```

[2] I originally used Wolfram Alpha

Software

The program used to find the witness point 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 the witness point (15) by running Sage as follows:

```
load('helium.sage')      # loads the script
prep_hydrogen(5)         # select PDE:hydrogen and ansatz:5
multi_init()             # form the equation
multi_expand()           # expand out the numerator and collect like terms into a matrix
random_numerical()       # run numerical optimizer
```

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

```
V, D, N, M               # trial forms of various polynomials
eq_a                     # PDE with ansatz substituted in and r^2 simplified
R                        # polynomial ring over integers
F                        # fraction field of R
F_eq_a                   # eq_a expanded out (in F)
F_eq_a_n                 # expanded numerator (in R)
F_eq_a_d                 # expanded denominator (in R)
eqns()                   # system of equations to solve
SciMin                   # solution from scipy.optimize.root
```

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/`