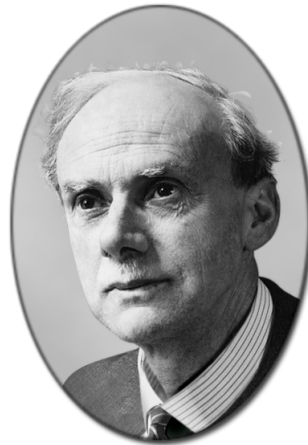


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DERIVATIONS FROM THE DIRAC EQUATION & NUMERICAL SOLUTIONS FOR  
HYDROGENIC ATOMS WITH NUCLEI OF FINITE SIZE

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Paul A.M. Dirac

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = mc^2\beta|\Psi\rangle - i\hbar\vec{\alpha}\cdot\vec{\nabla}|\Psi\rangle + V|\Psi\rangle$$

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# I A Brief Review of Quantum Mechanics

## I.1 Introduction

In 1926, Erwin Schrödinger published a landmark equation that governs the world of non-relativistic quantum mechanics.

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = -\frac{\hbar^2}{2m} \nabla^2 |\Psi\rangle + V(\vec{r}) |\Psi\rangle \quad (\text{I.1})$$

The Schrödinger Equation is a *quantum wave equation*. The solutions  $|\Psi\rangle$  are quantum *state vectors* which live in Hilbert space. In the position basis ( $\vec{r} = x\hat{x} + y\hat{y} + z\hat{z}$ ):

$$\langle \vec{r} | \Psi \rangle = \Psi(\vec{r}, t) \quad (\text{I.2})$$

The quantum state is now represented by a *position wavefunction*.

$$\Psi_n(\vec{r}, t) = \sum_n^{\infty} \alpha_n \psi_n(\vec{r}) e^{-iE_n t/\hbar} \quad (\text{I.3})$$

where  $\alpha_n$  are constant coefficients,  $\psi_n$  are *stationary states* and  $n$  is the principle quantum number.

There is an elegant connection between the Schrödinger Equation and classical mechanics, which comes in part from Schrödinger's original formulation. If there is a quantity,  $E$ , to represent the total energy of any system, we might write it as the sum of kinetic energy  $T$  and potential energy  $V$ . In a closed system,  $T$  and  $V$  are free to change, but  $E$  is invariant:

$$E = T + V \quad (\text{I.4})$$

The quantity which represents the total energy of the system is called the *Hamiltonian*.

In our macroscopic world, the possible energies of a Hamiltonian are continuous. A ball can be thrown into the air with 20 joules of kinetic energy, or 35.74, or however many one wishes, depending on the initial speed they give the ball; there are no restrictions on possible energy values in classical mechanics.

As Max Planck showed famously in 1900, though, this is not true for certain *quantum* systems. Energy can only be added or emitted in discrete chunks— *quanta*. This is a key feature of quantum mechanics:

**Not all quantum systems can have a continuous range of possible energies.**

Looking at Equation I.1 a little closer reveals that it shares the same form as Equation I.4. This relation can be clearly shown by comparing the  $\nabla^2 |\Psi\rangle$  term to the kinetic energy  $T$ . Like all measurable quantities in quantum mechanics,  $T$  becomes a *Hermitian operator*:

Classical Mechanics

$$T = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$

Quantum Mechanics

$$\hat{T} = \frac{\hat{p}^2}{2m}$$

where  $\hat{p}$  is a differential operator corresponding to momentum.

$$\hat{p} = -i\hbar\nabla$$

$$\hat{T} = \frac{(-i\hbar\nabla)^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2$$

This gives the Schrödinger Equation a very accessible interpretation in terms of energy: The kinetic energy plus the potential energy *is* the Hamiltonian– the total energy!

The Schrödinger Equation also functions as an *eigenvalue equation*. That is, the Hamiltonian becomes an operator which acts on the state-ket  $|\Psi\rangle$ , returning the same state-ket scaled by its *eigenvalue*<sup>1</sup>. The eigenvalues of the Hamiltonian operator are **the allowed energy values**.

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

## I.2 A Step Towards Relativity

To explain why Schrödinger’s equation does not apply to Einstein’s Special Theory of Relativity, it is often stated that it “does not treat space and time on equal footing.” This is exactly because of the difference in order between the spatial derivatives and the temporal derivative in Equation I.1; a truly relativistic quantum wave equation will match the order of derivatives in order to describe a single spacetime.

One solution is to use the *mass-energy formula* from special relativity, as opposed to the classical  $E = T + V$ :

Classical Mechanics

$$E = T + V$$

Special Relativity

$$E^2 = |\vec{p}|^2 c^2 + m_0^2 c^4$$

where  $|\vec{p}|^2$  is the squared magnitude of the object’s momentum,  $c$  is the cosmic speed limit, and  $m_0$  is the object’s *rest mass*, the mass which is measured in its *rest frame*. Plugging in our momentum operator yields:

$$\begin{aligned} -\hbar^2 \frac{\partial^2}{\partial t^2} &= -c^2 \hbar^2 \nabla^2 + m_0^2 c^4 \\ \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 &= \frac{m_0^2 c^2}{\hbar^2} \end{aligned} \tag{I.5}$$

The left side of Equation I.5 can be thought of as a *4D gradient*. This is called the *d’Alembertian* operator, and notice that it satisfies our search for a tool that will match the derivatives in time and space:

$$\square^2 \equiv \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2$$

When operating on a scalar wavefunction  $\phi$ , the resulting equation is the *Klein-Gordon Equation*:

$$\boxed{\square^2 \phi - \left(\frac{m_0 c}{\hbar}\right)^2 \phi = 0} \tag{I.6}$$

This appears to be an elegant (and suspiciously simple) transition from non-relativistic to relativistic quantum mechanics. Indeed, this was the first attempt at a unifying equation between quantum mechanics and special relativity. However, there remain issues with its structure and its solutions.

The energy eigenvalues obtained from Equation I.6 can be positive *and* negative. This is unsettling when compared to Schrödinger, where energies were one or the other, depending on if we are dealing with bound

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<sup>1</sup>The “eigen-” prefix meaning “same”.

or scattering states. One can hand-wave this away, but it also meant there was a chance the probability density of a given solution could be negative itself<sup>2</sup>. Another issue is that the Klein-Gordon equation only describes particles that of integral spin.

## II Derivations

### II.1 The Dirac Equation

The Dirac Equation was the answer to the uncomfortable implications of the Klein-Gordon Equation. Published in 1928 by Paul Dirac, it successfully describes the mechanics of *half-integer spin* particles, from which most visible matter is formed, and it indeed treats time and space as a single spacetime. It is one of the defining equations of *Quantum Electrodynamics*, the most successful quantum field theory.

Discovering the Dirac Equation required further manipulation of Equation L.6; Dirac wanted an equation *linear* in energy-momentum to hopefully solve the issue of negative energy solutions. For some solution  $|\Psi\rangle$ :

$$\boxed{i\hbar \frac{\partial}{\partial t} |\Psi\rangle = mc^2 \beta |\Psi\rangle - i\hbar \vec{\alpha} \cdot \vec{\nabla} |\Psi\rangle} \quad (\text{II.1})$$

The ‘trick’ was to effectively factor the Klein-Gordon Equation, and doing this meant introducing factors of  $\vec{\alpha}$  and  $\beta$ . To take the ‘square-root’ of the Klein-Gordon Hamiltonian, these factors needed to obey certain rules that real numbers, and even complex numbers couldn’t satisfy. Dirac knew immediately that these would instead need to be *matrices*. It was quickly found that the simplest choice ( $2 \times 2$ ) yields no solutions; in fact, the minimum size for viable *Dirac matrices* is  $4 \times 4$ .

There are an infinite number of  $4 \times 4$  matrices that could represent  $\vec{\alpha}$  and  $\beta$ ; they need only obey these rules:

$$\alpha_i^2 = \beta^2 = \mathbb{1} \quad \alpha_i \beta + \beta \alpha_i = 0 \quad (\text{II.2})$$

$$\alpha_i \alpha_j + \alpha_j \alpha_i = 0 \quad (\text{II.3})$$

where  $\alpha_i$  and  $\alpha_j$  are individual components of  $\vec{\alpha}$ . These are the only rules that need to be obeyed for the Dirac Equation to be physically correct<sup>3</sup>. A convenient form can be chosen:

$$\vec{\alpha} = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} \hat{x} + \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix} \hat{y} + \begin{pmatrix} 0 & \sigma_z \\ \sigma_z & 0 \end{pmatrix} \hat{z} \quad \beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} \quad (\text{II.4})$$

where  $\sigma_i$  are the *Pauli spin matrices* and notation be damned,  $\hat{x}$ ,  $\hat{y}$ , and  $\hat{z}$  are the unit basis vectors in Cartesian coordinates, **not** operators. It is easy to take for granted here the beauty of the Dirac Equation in this form; spin comes with it for free!

It is common to redefine

Equation II.1 is elegant in laying out the function of each term in the Dirac Hamiltonian. It may seem familiar!

- $i\hbar \frac{\partial}{\partial t} |\Psi\rangle$  is the *total energy* term, which also contains time dependence.
- $mc^2 \beta |\Psi\rangle$  is the *rest mass-energy* term.
- $-i\hbar \vec{\alpha} \cdot \vec{\nabla} |\Psi\rangle$  is the *kinetic* term.

<sup>2</sup>Emil Blomquist and Trotte Boman, “The Dirac Equation for a Particle in a Spherical Box Potential with Application in Bag Modeling,” *Royal Institute of Technology (KTH)*, 2015: 6.

<sup>3</sup>Tarun Biswas, *Quantum Mechanics: Concepts and Applications* (New York: 1999): 167.

Like the Schrödinger Equation, a term can be added to describe the spin-half particle in the presence of some electric potential:

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = mc^2 \beta |\Psi\rangle - i\hbar \vec{\alpha} \cdot \vec{\nabla} |\Psi\rangle + V |\Psi\rangle \quad (\text{II.5})$$

The potential term is what allows us flexibility in the situation we choose to examine. For example, setting  $V(x, y, z, t) = 0$  yields the solutions for a *free particle*, which is exactly what Equation II.1 describes. These are illuminating in their own right. In the case of the hydrogen atom, the solutions of which are the eigenstates and energy eigenvalues of the single electron orbiting its proton, the potential is slightly more exotic:

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r} \quad (\text{II.6})$$

where  $e$  is the elementary unit of charge and  $r$  is the coordinate in the *radial* direction.

We will be investigating numerical solutions to the Dirac Equation for the case of the *hydrogenic atom*. That is, an atom with a single electron (like hydrogen) and  $Z \geq 1$  protons.

The  $Z = 1$  case is, of course, equivalent to analyzing the energy levels of hydrogen itself, a system that has an analytical solution to which we can compare. For  $Z > 1$ , we turn to numerical solutions. A subtlety we are allowed to consider in a numerical solution is the *size of the nucleus*. The size of the nucleus would typically be considered negligible; i.e., the nucleus is considered a *point charge*. Realistically, there is nothing preventing the wavefunction of the electron from overlapping the nucleus; indeed, this can be neglected physically for very small nuclei— even if the electron did “enter” the nucleus, it would do so for a negligible amount of time. For completeness, we will consider this possible, as it may or may not affect results for very *large*  $Z$ .

To handle the messy calculations (the derivations are up to us), we will use a fourth-order Runge-Kutta method to solve a system of coupled, first-order ordinary differential equations. This method will be carried out in Python, code included.

## II.2 Converting to Spherical Coordinates

Equation II.1 assumes rectangular Minkowski coordinates. For our purposes, however, we can assume atoms are *spherically symmetric* in structure, motivating a change to spherical coordinates. Particularly, we will focus on the radial coordinate  $r$ , which measures distance from the center of the coordinate system (where the nucleus is.)

To perform this change requires significant algebraic manipulation. Along the way, we find that the *angular* part of the Hamiltonian  $\hat{H}_a$ , which depends on the coordinates  $\vartheta$  and  $\varphi$ , can be written as follows<sup>4</sup>:

$$\hat{H} = \hat{H}_a + \hat{H}_r \quad (\text{II.7})$$

$$\hat{H}_a = \hat{H}_r - \hat{H} \quad (\text{II.8})$$

$$\hat{H}_a = c(\vec{\alpha} \cdot \vec{p} - \alpha_r \hat{p}_r) \quad (\text{II.9})$$

We multiply this from the left by  $\alpha_r = \vec{\alpha} \cdot \vec{R}/R$ , noting that  $\alpha_r^2 = 1$ :

$$\alpha_r \hat{H}_a = c \left( R^{-1} (\vec{\alpha} \cdot \vec{R}) (\vec{\alpha} \cdot \vec{R}) - \alpha_r \alpha_r \hat{p}_r \right)$$

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<sup>4</sup>Tarun Biswas, *Quantum Mechanics: Concepts and Applications* (New York: 1999): 172–173.

$$\alpha_r \hat{H}_a = c \left( R^{-1} (\vec{\alpha} \cdot \vec{R}) (\vec{\alpha} \cdot \vec{R}) - \hat{p}_r \right) \quad (\text{II.10})$$

The form of  $(\vec{\alpha} \cdot \vec{A})(\vec{\alpha} \cdot \vec{B})$  is not trivial, and works out to:

$$(\vec{\alpha} \cdot \vec{A})(\vec{\alpha} \cdot \vec{B}) = \vec{A} \cdot \vec{B} + \vec{\sigma}' \cdot (\vec{A} \times \vec{B}) \quad (\text{II.11})$$

where  $\vec{\sigma}'$  is a 3-vector of  $4 \times 4$  matrices containing Pauli spin matrices along their diagonals:

$$\vec{\sigma}' = \begin{pmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{pmatrix} \hat{x} + \begin{pmatrix} \sigma_y & 0 \\ 0 & \sigma_y \end{pmatrix} \hat{y} + \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix} \hat{z} \quad (\text{II.12})$$

$$\sigma'_x = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad \sigma'_y = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix} \quad \sigma'_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (\text{II.13})$$

We note that  $\vec{R} \cdot \vec{p} = 0$  and  $\vec{R} \times \vec{p}$  is the *angular momentum*  $\vec{L}$ :

$$\alpha_r \hat{H}_a = icR^{-1} \left( \vec{\sigma}' \cdot \vec{L} + \hbar \right) - c\hat{p}_r \quad (\text{II.14})$$

Multiplying by  $\alpha_r$ :

$$\hat{H}_a = icR^{-1} \alpha_r \left( \vec{\sigma}' \cdot \vec{L} + \hbar \right) - c\alpha_r \hat{p}_r \quad (\text{II.15})$$

To neaten things up further, we will define a new operator  $\hbar \hat{K}'$  to contain the angular part of the expression (the part inside the parenthesis):

$$\hbar \hat{K}' = \vec{\sigma}' \cdot \vec{L} + \hbar \quad (\text{II.16})$$

From  $\hat{K}'$ ,  $\hat{K}$  is formed by:

$$\hat{K} = \beta \hat{K}'$$

$$\hat{H}_a = ic\hbar R^{-1} \alpha_r \beta \hat{K} - c\alpha_r \hat{p}_r \quad (\text{II.17})$$

Now that we have our angular part (and from it, the radial part), we can add the rest-frame and potential terms in order to construct the full Dirac Hamiltonian in spherical coordinates:

$$\hat{H}_s = mc^2 \beta + c\alpha_r \hat{p}_r + ic\hbar R^{-1} \alpha_r \beta \hat{K} + V(r, \varphi, \vartheta) \quad (\text{II.18})$$

Operating on the state vector  $|\Psi\rangle$  yields the energy eigenvalue equation:

$$E |\Psi\rangle = mc^2 \beta |\Psi\rangle + c\alpha_r \hat{p}_r |\Psi\rangle + ic\hbar R^{-1} \alpha_r \beta |\Psi\rangle + V(r, \varphi, \vartheta) |\Psi\rangle \quad (\text{II.19})$$

where  $k$  is the eigenvalue of the  $\hat{K}$  operator, and  $E$  is the energy eigenvalue itself. The radial form of the momentum operator  $\hat{p}_r$  is given by:

$$\hat{p}_r = \hat{p} \cdot \vec{R}/R \quad \rightarrow \quad \hat{p}_r = -i\hbar \left( \frac{\partial}{\partial r} + \frac{1}{r} \right) \quad (\text{II.20})$$

Finally, due to the symmetry of our problem, we will find that  $V$  is a function of the radial coordinate alone, and since the angular part of Equation II.19 is contained in that  $k$  eigenvalue, our solutions  $\langle r | \Psi \rangle$  will also only be functions of  $r$ :

$$E\Psi(r) = mc^2\beta\Psi(r) - i\hbar\alpha_r\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\Psi(r) + i\hbar kR^{-1}\alpha_r\beta\Psi(r) + V(r)\Psi(r) \quad (\text{II.21})$$

### II.3 Form of the Differential Equations

What has been derived is the Dirac Equation in the radial coordinate. In reality, due to the matrix nature of  $\alpha_r$  and  $\beta$ , we are really dealing with *multiple* equations.  $\alpha_r$  and  $\beta$  are at best  $4 \times 4$  matrices, so that means  $|\Psi\rangle$  must be some *4-component object* called a *Dirac spinor*, or *bispinor*.

We first write the Dirac Equation in all its gory, matrix-laden detail. We might wonder what form the “radial component” of  $\vec{\alpha}$  might take, but recall that any  $\alpha$  and  $\beta$  matrix must only obey the anticommutation relations of Equations II.2 and II.3 to be physically applicable. So again, we choose a convenient form<sup>5</sup>:

$$\alpha_r = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix} \quad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (\text{II.22})$$

$$\begin{aligned} E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} &= -i\hbar \left( \frac{d}{dr} + \frac{1}{r} \right) \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} + i\hbar kR^{-1} \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \\ &+ mc^2 \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} + V(r) \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \end{aligned}$$

In this form, the Dirac Equation looks amess, but there is another nice simplification that can be made. Notice that these 4-dimensional matrices can be reduced into 2-dimensional ones, letting the elements themselves be  $2 \times 2$  matrices<sup>6</sup>:

$$\begin{aligned} E \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} &= -i\hbar \left( \frac{d}{dr} + \frac{1}{r} \right) \begin{pmatrix} 0 & -\mathbb{i} \\ \mathbb{i} & 0 \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} + i\hbar kR^{-1} \begin{pmatrix} 0 & -\mathbb{i} \\ \mathbb{i} & 0 \end{pmatrix} \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} \\ &+ mc^2 \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} + V(r) \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} \quad (\text{II.23}) \end{aligned}$$

<sup>5</sup>Tarun Biswas, *Quantum Mechanics: Concepts and Applications* (New York: 1999): 173.

<sup>6</sup>Though the solution  $\Psi$  does have four components, it is **not a 4-vector**; the Dirac spinor can be considered *two separate* spinors, each with two components. This is why we can reduce the dimensionality of the Dirac spinors as well.



$$E \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = -i\hbar \left( \frac{d}{dr} + \frac{1}{r} \right) \begin{pmatrix} -i\psi_B \\ i\psi_A \end{pmatrix} + i\hbar k R^{-1} \begin{pmatrix} i\psi_B \\ i\psi_A \end{pmatrix} + mc^2 \begin{pmatrix} \psi_A \\ -\psi_B \end{pmatrix} + V(r) \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} \quad (\text{II.24})$$

$$\Psi(r) = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} \quad \psi_A = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \quad \psi_B = \begin{pmatrix} \psi_3 \\ \psi_4 \end{pmatrix} \quad (\text{II.25})$$

Equation II.24 produces two differential equations:

$$\frac{d\psi_A}{dr} - \frac{k-1}{r}\psi_A - \frac{mc^2 + E}{\hbar}\psi_B + \frac{V(r)}{\hbar}\psi_B = 0 \quad (\text{II.26})$$

$$\frac{d\psi_B}{dr} + \frac{k+1}{r}\psi_B - \frac{mc^2 - E}{\hbar}\psi_A - \frac{V(r)}{\hbar}\psi_A = 0 \quad (\text{II.27})$$

These equations are still completely general to any spherically symmetric (central) potential function we wish, and it is here we will pause to explore where the “hydrogenic” potential comes from.

## II.4 The Hydrogenic Potential

We will assume for simplicity that the nucleus of the atom is spherically symmetric with radius  $R$ , and its charge is distributed uniformly within it. Of course, the nucleus also contains neutrons with zero charge, however this assumption is more realistic than assuming the nucleus to be a point charge. The electric field generated by the nucleus,  $\vec{E}$ , is described in two regions. Outside of the nucleus ( $r > R$ ),  $\vec{E}$  is simply as if the nucleus were a point charge. Inside the nucleus ( $r < R$ ),  $\vec{E}$  is obtained by Gauss’ Law:

$$\oint \vec{E} \cdot d\vec{A} = \frac{q_{\text{enc}}}{\epsilon_0} \quad (\text{II.28})$$

$$E (4\pi r^2) = \frac{q_{\text{enc}}}{\epsilon_0} \quad (\text{II.29})$$

$\vec{E}$  does not vary over the surface area of the nucleus, so  $\oint dA = 4\pi r^2$ . The enclosed charge  $q_{\text{enc}}$  is a fraction of the total charge of the nucleus at the coordinate  $r$ :

$$q_{\text{enc}} = \frac{4/3\pi r^3}{4/3\pi R^3} Q$$

$$E (4\pi r^2) = \frac{Q r^3}{\epsilon_0 R^3} \quad (\text{II.30})$$

$$E = \frac{Q r}{4\pi\epsilon_0 R^3} \quad (\text{II.31})$$

$$\vec{E}(r) = \hat{r} \begin{cases} \frac{Q}{4\pi\epsilon_0 R^3} r & \text{if } r < R \\ \frac{Q}{4\pi\epsilon_0} \frac{1}{r^2} & \text{if } r > R \end{cases} \quad (\text{II.32})$$

The electric potential is obtained<sup>7</sup> by:

$$\Phi(r) = - \int \vec{E} \cdot d\hat{r} \quad (\text{II.33})$$

$$\Phi(r) = \begin{cases} \frac{3Q}{8\pi\epsilon_0 R} - \frac{Q}{8\pi\epsilon_0 R^3} r^2 & \text{if } r < R \\ \frac{Q}{4\pi\epsilon_0 r} & \text{if } r > R \end{cases} \quad (\text{II.34})$$

where  $Q$  is just an integer multiple of the charge of the proton ( $+e$ ).

$$Q = Ze \quad Z = 1, 2, 3 \dots$$

$Z$  is the *atomic number* of the atom we wish to find solutions for.

Equation II.34 gives the *electric potential*, but what the Dirac Equation takes in this case is *potential energy*. To obtain potential energy, we multiply our electric potential by the charge of the particle inside of the potential (the electron;  $-e$ ).

$$V(r) = \begin{cases} -\frac{3Ze^2}{8\pi\epsilon_0 R} + \frac{Ze^2}{8\pi\epsilon_0 R^3} r^2 & \text{if } r < R \\ -\frac{Ze^2}{4\pi\epsilon_0 r} & \text{if } r > R \end{cases} \quad (\text{II.35})$$

## II.5 Substitutions and Simplifications

It is often convenient when performing numerical techniques to render our differential equation in a *dimensionless* state. This will not only remove the need to worry about units, but will also allow results to be manageable in magnitude.

For example, in reality, the atomic scale is on the order of nanometers ( $10^{-9}m$ ) and our nucleus is measured in *femtometers* ( $10^{-15}m$ , a quadrillionth of one meter!). To avoid loss of accuracy, we will instead introduce a substitution to remove these units all together:

$$\rho = \delta r \quad (\text{II.36})$$

$r$  of course has units of  $m$ , and  $\delta$  has units of  $1/m$ , leaving us with the dimensionless quantity  $\rho$ , which becomes our new variable.

$\delta$  serves another purpose for substitution however:

$$\delta = \sqrt{\delta_A \delta_B} \quad (\text{II.37})$$

$$\delta_A = \frac{mc^2 + E}{c\hbar} \quad \delta_B = \frac{mc^2 - E}{c\hbar} \quad (\text{II.38})$$

If this seems unjust, check the units!

$$\delta_A : \quad \frac{J + J}{m/s \times Js} \rightarrow \frac{J}{m \times J} \rightarrow \frac{1}{m}$$

---

<sup>7</sup>The sign remains positive despite the negative in Equation II.33 because  $\vec{E}$  and  $d\hat{r}$  are at an angle of  $180^\circ$

$$\delta : \quad \sqrt{\frac{1}{m^2}} \rightarrow \frac{1}{m}$$

Plugging  $\delta_1$  and  $\delta_2$  into Equations II.26 and II.27:

$$\frac{d\psi_A}{dr} - \frac{k-1}{r}\psi_A - \left(\delta_A - \frac{V(r)}{c\hbar}\right)\psi_B = 0 \quad (\text{II.39})$$

$$\frac{d\psi_B}{dr} + \frac{k+1}{r}\psi_B - \left(\delta_B + \frac{V(r)}{c\hbar}\right)\psi_A = 0 \quad (\text{II.40})$$

Dividing by  $\delta$  itself will leave our differential equations almost entirely in terms of  $\rho$ , save the potential  $V(r)$ , which we will deal with next:

$$\frac{d\psi_A}{d\rho} - \frac{k-1}{\rho}\psi_A - \left(\frac{\delta_A}{\delta} - \frac{V(r)}{c\hbar\delta}\right)\psi_B = 0 \quad (\text{II.41})$$

$$\frac{d\psi_B}{d\rho} + \frac{k+1}{\rho}\psi_B - \left(\frac{\delta_B}{\delta} + \frac{V(r)}{c\hbar\delta}\right)\psi_A = 0 \quad (\text{II.42})$$

To render  $V(r)$  dimensionless, we will want to avoid absorbing the radius  $R$  into some constant  $\rho_0 = \delta R$ , as this will attach energy dependence to the radius; we want our nuclear radius to “depend” on nothing but the number of protons,  $Z$ . For each factor of  $R$ , then, we will multiply by  $\delta/\delta$  (effectively multiplying by 1), and make the usual substitution for the variable  $r$ .

$$V(\rho) = \begin{cases} -\frac{3Ze^2\delta}{8\pi\epsilon_0\delta R} + \frac{Ze^2\delta^3}{8\pi\epsilon_0\delta^3 R^3} \left(\frac{\rho}{\delta}\right)^2 & \text{if } \rho < \delta R \\ -\frac{Ze^2}{4\pi\epsilon_0} \left(\frac{\delta}{\rho}\right) & \text{if } \rho > \delta R \end{cases} \quad (\text{II.43})$$

$$V(\rho) = \begin{cases} -\frac{3Ze^2\delta}{8\pi\epsilon_0\delta R} + \frac{Ze^2\delta}{8\pi\epsilon_0\delta^3 R^3} \rho^2 & \text{if } \rho < \delta R \\ -\frac{Ze^2\delta}{4\pi\epsilon_0} \frac{1}{\rho} & \text{if } \rho > \delta R \end{cases} \quad (\text{II.44})$$

The remaining constants make quite a mess of the potential function, but there is another nice dimensionless quantity which falls out of it when inserted into Equations II.41 and II.42; notice that the potential  $V(\rho)$  will be divided by  $c\hbar\delta$ . This results in the *fine structure constant*:

$$\alpha \equiv \frac{e^2}{4\pi\epsilon_0 c\hbar} \approx \frac{1}{137} \quad (\text{II.45})$$

Notice, too, that the extra factors of  $\delta$  in  $V(\rho)$  cancel out. Factoring out the negative sign from  $V(\rho)$  and defining  $U(\rho) = V(\rho)/c\hbar\delta$ :

$$\frac{d\psi_A}{d\rho} - \frac{k-1}{\rho}\psi_A - \left(\frac{\delta_A}{\delta} + U(\rho)\right)\psi_B = 0 \quad (\text{II.46})$$

$$\frac{d\psi_B}{d\rho} + \frac{k+1}{\rho}\psi_B - \left(\frac{\delta_B}{\delta} - U(\rho)\right)\psi_A = 0 \quad (\text{II.47})$$

$$U(\rho) = \begin{cases} \frac{3Z\alpha}{2\delta R} - \frac{Z\alpha}{2\delta^3 R^3} \rho^2 & \text{if } \rho < \delta R \\ \frac{Z\alpha}{\rho} & \text{if } \rho > \delta R \end{cases} \quad (\text{II.48})$$

One final substitution will give us a dimensionless parameter to search over, related to the allowed energy values  $E' = E - mc^2$ . Since  $\delta_2$  is related directly to  $E'$ , we will choose:

$$\gamma = \frac{\delta_B}{\delta} \quad (\text{II.49})$$

And from Equation II.49, it can be shown:

$$\frac{1}{\gamma} = \frac{\delta_A}{\delta} \quad (\text{II.50})$$

$$E' = -\frac{2mc^2\gamma^2}{1+\gamma^2} \quad (\text{II.51})$$

$$\delta = \frac{2mc}{\hbar} \frac{\gamma^2}{1+\gamma^2} \quad (\text{II.52})$$

Therefore, our simplified differential equations in a dimensionless form, along with our dimensionless potential energy function, are given by:

$$\frac{d\psi_A}{d\rho} - \frac{k-1}{\rho}\psi_A - \left(\frac{1}{\gamma} + U(\rho)\right)\psi_B = 0 \quad (\text{II.53})$$

$$\frac{d\psi_B}{d\rho} + \frac{k+1}{\rho}\psi_B - \left(\gamma - U(\rho)\right)\psi_A = 0 \quad (\text{II.54})$$

## II.6 A Black Hole in the Hydrogenic Atom

In this state, there is a glaring issue with Equations II.53 and II.54, and when purely invested in deriving and obtaining a usable equation, it is easy to miss, because it is an issue with the relation to our differential equations and the régimes over which we are searching for solutions.

$$\frac{d\psi_A}{d\rho} = \frac{k-1}{\rho}\psi_A + \left(\frac{1}{\gamma} + U(\rho)\right)\psi_B \quad (\text{II.55})$$

$$\frac{d\psi_B}{d\rho} = -\frac{k+1}{\rho}\psi_B + \left(\gamma - U(\rho)\right)\psi_A \quad (\text{II.56})$$

There is a *singularity* at the center of our system, arising from the  $\pm \frac{k\mp 1}{\rho}\psi$  terms when  $\rho = 0$ .

This means there will be some constraints on the form of our solutions. Similar to an analytical solution of even the non-relativistic hydrogen atom (via the radial Schrödinger Equation), we will assume that solutions exist in the form:

$$\psi_A(\rho) = \rho^s \eta_A(\rho) \quad \psi_B(\rho) = \rho^s \eta_B(\rho) \quad (\text{II.57})$$

where  $\eta_A$  and  $\eta_B$  are *power series*:

$$\eta_A(\rho) = \sum_{i=0}^{\infty} a_i \rho^i \quad \eta_B(\rho) = \sum_{i=0}^{\infty} b_i \rho^i \quad (\text{II.58})$$

The derivatives of these solutions are then:

$$\frac{d\psi_A}{d\rho} = \frac{d\eta_A}{d\rho}\rho^s + s\rho^{s-1}\eta_A \quad \frac{d\psi_B}{d\rho} = \frac{d\eta_B}{d\rho}\rho^s + s\rho^{s-1}\eta_B \quad (\text{II.59})$$

If these are plugged into Equations [II.53](#) and [II.54](#):

$$\frac{d\eta_A}{d\rho}\rho^s + s\rho^{s-1}\eta_A - \frac{k-1}{\rho}\rho^s\eta_A - \left(\frac{1}{\gamma} - U(\rho)\right)\rho^s\eta_B = 0 \quad (\text{II.60})$$

$$\frac{d\eta_B}{d\rho}\rho^s + s\rho^{s-1}\eta_B + \frac{k+1}{\rho}\rho^s\eta_B - \left(\gamma + U(\rho)\right)\rho^s\eta_A = 0 \quad (\text{II.61})$$

Subtraction in the exponent is, of course, the same as dividing:

$$\frac{d\eta_A}{d\rho}\rho^s + \frac{s}{\rho}\rho^s\eta_A - \frac{k-1}{\rho}\rho^s\eta_A - \left(\frac{1}{\gamma} + U(\rho)\right)\rho^s\eta_B = 0 \quad (\text{II.62})$$

$$\frac{d\eta_B}{d\rho}\rho^s + \frac{s}{\rho}\rho^s\eta_B + \frac{k+1}{\rho}\rho^s\eta_B - \left(\gamma - U(\rho)\right)\rho^s\eta_A = 0 \quad (\text{II.63})$$

To remove the troublesome terms in Equation [II.62](#), we simply choose  $s = k - 1$  so that they cancel. Mending the issue in Equation [II.63](#) is more subtle. Choosing  $s = k - 1$  leaves a factor of  $2k$  behind, but that does not touch the  $\rho$  in the denominator. Consider  $\psi_B$ 's power series (Equation [II.58](#)):

$$\eta_B(\rho) = \sum_{i=0}^{\infty} b_i \rho^i$$

$$\eta_B(\rho) = b_0 + \sum_{i=1}^{\infty} b_i \rho^i$$

This sum is divided by  $\rho$  in Equation [II.63](#):

$$\frac{\eta_B(\rho)}{\rho} = \frac{b_0}{\rho} + \frac{b_1\rho}{\rho} + \frac{b_2\rho^2}{\rho} + \frac{b_3\rho^3}{\rho} + \dots$$

Notice that factors of  $\rho$  survive only for  $b_2$  and greater; when  $\rho = 0$ , these terms die off. We must also set  $b_0 = 0$  in order to avoid dividing by zero. This solves our singularity situation. However, the  $b_1$  term *still* survives(!) because the first order  $\rho$  was divided out:

$$\left. \frac{\eta_B(\rho)}{\rho} \right|_{\rho=0} = 0 + b_1 + b_2(0) + b_3(0)^2 + \dots$$

$$\left. \frac{\eta_B(\rho)}{\rho} \right|_{\rho=0} = b_1 \quad (\text{II.64})$$

So from Equation [II.63](#) (recalling  $s = k - 1$  and at  $\rho = 0$ ):

$$\left. \frac{d\eta_B}{d\rho} \right|_{\rho=0} = \left(\gamma - U(\rho)\right)\eta_A - 2kb_1 \quad (\text{II.65})$$

But from Equation II.58:

$$\begin{aligned}\left.\frac{d\eta_B}{d\rho}\right|_{\rho=0} &= \frac{d}{d\rho} \left[ b_1\rho + b_2\rho^2 + \dots \right]_{\rho=0} \\ \left.\frac{d\eta_B}{d\rho}\right|_{\rho=0} &= b_1\end{aligned}\tag{II.66}$$

Then, from Equations II.65 and II.66:

$$b_1 = \left( \gamma - U(\rho) \right) \eta_A - 2kb_1\tag{II.67}$$

$$b_1(1 + 2k) = \left( \gamma - U(\rho) \right) \eta_A\tag{II.68}$$

$$\frac{d\eta_B}{d\rho} = \frac{1}{1 + 2k} \left( \gamma - U(\rho) \right) \eta_A\tag{II.69}$$

Equation II.69 is therefore the differential equation of  $\eta_B$  when  $\rho = 0$ .

## II.7 Summary

We are nearly ready to start searching for solutions. When  $\rho = 0$ ,  $\eta_B = 0$  and our coupled ordinary differential equations come from Equations II.62 and II.69:

$$\frac{d\eta_A}{d\rho} = \left( \frac{1}{\gamma} + U(\rho) \right) \eta_B\tag{II.70}$$

$$\frac{d\eta_B}{d\rho} = \frac{1}{1 + 2k} \left( \gamma - U(\rho) \right) \eta_A\tag{II.71}$$

When  $\rho \neq 0$ , then  $\eta_B \neq 0$ :

$$\frac{d\eta_A}{d\rho} = \left( \frac{1}{\gamma} + U(\rho) \right) \eta_B\tag{II.72}$$

$$\frac{d\eta_B}{d\rho} = \left( \gamma - U(\rho) \right) \eta_A - \frac{2k}{\rho} \eta_B\tag{II.73}$$

The potential energy function, which divides our system into two régimes, is given by:

$$U(\rho) = \begin{cases} \frac{3Z\alpha}{2\delta R} - \frac{Z\alpha}{2\delta^3 R^3} \rho^2 & \text{if } \rho < \delta R \\ \frac{Z\alpha}{\rho} & \text{if } \rho > \delta R \end{cases}\tag{II.74}$$

In terms of our search parameter  $\gamma$ ,  $E'$  and  $\delta$  are given by:

$$E' = -\frac{2mc^2\gamma^2}{1 + \gamma^2}\tag{II.75}$$

$$\delta = \frac{2mc}{\hbar} \frac{\gamma^2}{1 + \gamma^2}\tag{II.76}$$

### III Numerical Methods

```
import numpy as np
import matplotlib.pyplot as plt
plt.style.use('dark_background') # Optional; enables 'dark mode' on graphs.
```

Listing 1: Imports

In Python, it is common to use built-in functions like `integrate.solve_ivp` from the `scipy` module to solve differential equations, among others in other modules. In fact, `solve_ivp` allows the user to choose between many solving techniques, including the *Runge-Kutta* method. While convenient, and certainly invaluable for many tasks, resorting to this can detract from a full understanding of what our code is doing, and I think it is important to explicitly write our own solver to ensure complete control.

Namely, we will be using a **fourth-order Runge-Kutta** method to solve our system of coupled differential equations. We will accomplish this by searching over many values of  $\gamma$  from some initial starting value to zero; recall that for bound states, the first allowed energy value is negative (for hydrogen, the ground state is  $\sim -13.6\text{eV}$ ), and the next is slightly more positive. Of course, the amount of energy levels we find will depend on the fineness of our  $\Delta\gamma$ , but we will address this later.

#### III.1 Defining Constants & Initial Conditions

```
hbar = 1.05457182E-34 # Planck's constant (Joule-seconds)
m = 9.1093837E-31 # Mass of electron (Kilograms)
c = 299792458 # Speed of light (Meters/second)
e = 1.60217663E-19 # Elementary charge unit (Coulombs)
alpha = 7.29735257E-3 # Fine structure constant (Dimensionless)
k = 1 # K-operator eigenvalue
Z = 1 # Atomic number
R = Radius(Z) # Nuclear radius (Meters)
```

One can tweak these values as they please, though their main purpose is to obtain accurate energy eigenvalues, and don't have much effect on the eigenstates themselves.

The variable `Z` is the value we will change the most, as it will allow us to analyze the eigenstates and energies of different elements. To make sure our code works, we will leave it as 1 for the hydrogen atom itself. Recall that we want the radius of our nucleus `R` to only vary with `Z`. Of course, we could manually change this value each time we change the atomic number, but to avoid this, I have implemented a function `Radius(Z)`:

```
def Radius(Z):
    if Z <= 30:
        # Nuclear charge radii values: /https://www-nds.iaea.org/radii
        radii = [0.8783, 1.9661, 2.5890, 2.6460, 2.4277, 2.4702, 2.5582, 2.6991, 2.8976, ... ]
        R = radii[Z-1]*1E-15 # Convert from femtometer values to meters
    else:
        # Approximate formula relates R to the cbrrt of Z.
        R = 2*0.8783*np.cbrt(Z)*1E-15
    return R
```

This function includes thirty approximate, experimental values of nuclear charge radii, so that for various elements we can be quite sure of our results. For  $Z > 30$ , a very rough approximate ‘function’ has been included, where:

$$R \propto R_0 \sqrt[3]{Z}$$

where  $R_0$  is the radius of a proton. This will allow a user to approximate nuclear radii of larger and larger elements.

Next, we define our initial conditions:

```
gamma_0 = 3.64230534E-3*Z+0.001      # Initial gamma value (Depends on Z)
dgamma = -0.00025                     # Gamma mesh width

rho_0 = 0                             # Rho initial value
drho = 0.001                          # Rho mesh width
etaA_0 = 1.0                          # etaA initial value
etaB_0 = 0.0                          # etaB initial value
psiA_0 = 1.0                          # psiA initial value
psiB_0 = 0.0                          # psiB initial value
etaPrev = 1                           # An initial value to check previous eta
n = 1                                 # Initial principal quantum number
l = k-1                               # Angular momentum quantum number
N = n + 1                             # Sum of principal and angular quantum numbers
```

`gamma` has been initialized as a very small, positive value that scales with  $Z$ , plus another small amount. This value was chosen since it corresponds to roughly the first energy eigenstate of hydrogen, known well to be  $-13.6\text{eV}$ . From Equation II.51:

$$\gamma_0 = \sqrt{\frac{-E'}{E' + 2mc^2}} \quad (\text{III.1})$$

$$\gamma_0 = \sqrt{\frac{-(-2.17 \times 10^{-18} J)}{(-2.17 \times 10^{-18} J) + 2(9.1 \times 10^{-31} kg)(2.9979 \times 10^8 m/s)^2}}$$

$$\gamma_0 = +0.0003647$$

The additional 0.001 added on ensures that the code can actually find the first eigenvalue on its own, rather than being given the value straight away.

We have also defined the initial conditions of our solutions; from Section II.6, we know that  $\eta_A(0) \neq 0$  and  $\eta_B(0) = 0$



## III.2 Potential & Differential Equation Functions

Since our potential  $U(\rho)$  is a piecewise function, it is very convenient to define it in its own function, which changes between cases depending on  $\rho$  by an *if statement*:

```
def Potential(rho,gamma):
    if rho >= Rp: # Outside the nucleus
        return (Z*alpha)/rho
    else: # Inside the nucleus
        return (3*Z*alpha)/(2*Rp) - ((Z*alpha)/(2*Rp*Rp*Rp))*rho*rho
```

$\gamma$  is taken as an input since  $R_p$  ( $R' = \delta R$ ) depends on  $\delta$ , which depends on  $\gamma$ .

Our differential equations will be defined in a similar way:

```
def dEta(rho,eta,gamma):
    # dEta[0] is d/drho(etaA) , dEta[1] is d/drho(etaB)
    # If rho == 0, then the -(2k/rho)*eta[1] term disappears from the second ODE, since b_0
    # = 0 in the power series solution.
    if rho == 0:
        return np.array([(1/gamma)*eta[1] + Potential(0,gamma)*eta[1],(gamma/(1+2*k))*eta[0]
        - (1/(1+2*k))*Potential(0,gamma)*eta[0]])
    else:
        return np.array([(1/gamma)*eta[1] + Potential(rho,gamma)*eta[1],(gamma)*eta[0] -
        Potential(rho,gamma)*eta[0] - (2*k/rho)*eta[1]])
```

From Section II.6, we saw that our differential equations, too, needed to be divided into two cases, when  $\rho = 0$  and when  $\rho \neq 0$ .

`dEta()` returns a `numpy` array `dEta[]`. The first element, `dEta[0]` corresponds to the  $d\eta_A/d\rho$  equation, and `dEta[1]` corresponds to the  $d\eta_B/d\rho$  equation.

Notice that one of the inputs `eta[]` is *also* an array; this is a 2-dimensional array that stores the solution values for  $\eta_A$  and  $\eta_B$  at a *single value* of  $\rho$ ; similarly, `eta[0]`  $\rightarrow \eta_A$  and `eta[1]`  $\rightarrow \eta_B$ .

If this is not convincing, compare each element of `dEta[]` to our differential equations:

$\rho = 0$ :

$$\frac{d\eta_A}{d\rho} = \frac{1}{\gamma}\eta_B + U(\rho)\eta_B \quad (\text{III.2})$$

$$\frac{d\eta_B}{d\rho} = \frac{\gamma}{1+2k}\eta_A - \frac{U(\rho)}{1+2k}\eta_A \quad (\text{III.3})$$

$\rho \neq 0$ :

$$\frac{d\eta_A}{d\rho} = \frac{1}{\gamma}\eta_B + U(\rho)\eta_B \quad (\text{III.4})$$

$$\frac{d\eta_B}{d\rho} = \gamma\eta_A - U(\rho)\eta_A - \frac{2k}{\rho}\eta_B \quad (\text{III.5})$$

### III.3 Calculating Energy Eigenvalues

```
def RungeKutta4(x, solution, dx, DiffEqs, gamma):
    # x: Independent variable
    # solution[:]: Dependent variable(s)
    # dx: Mesh width of independent variable
    # DiffEqs: Function which holds the coupled ODE's

    # Initial slope
    k1 = DiffEqs(x, solution, gamma)
    solAux = solution + (dx/2.0)*k1
    # Middle slopes
    k2 = DiffEqs(x+dx/2.0, solAux, gamma)
    solAux = solution + (dx/2.0)*k2
    k3 = DiffEqs(x+dx/2.0, solAux, gamma)
    solAux = solution + (dx/2.0)*k3
    # Final slope
    k4 = DiffEqs(x+dx, solAux, gamma)

    # Calculate solution & increment x
    solution = solution + (dx/6.)*k1 + (dx/3.)*k2 + (dx/3.)*k3 + (dx/6.)*k4
    x += dx
    return x, solution
```

Listing 2: Our RK4 function.

This form of RK4 generally requires four inputs; the only customization that was necessary was making sure that `gamma` was taken as an input as well.

The process of calculating each solution is straightforward:

1. For some `gamma`, call the RK4 function; this returns the solutions `eta[0]` and `eta[1]`, and increments `rho` by `drho`.
2. Store the values of `eta[]` as well as the incremented value of `rho` to respective arrays. These are the arrays that will eventually be plotted.
3. Continue solving and incrementing along `rho`. Eventually, accumulation of error will cause the solutions to diverge to  $\pm\infty$ ; we will think of this as the function growing a “tail”. Therefore, we will only continue solving while a solution<sup>8</sup> is under some large value.
4. If the solution has blown up, check to see if the sign has flipped. Visually, this manifests as the tail “wagging” the other direction. This corresponds to a node forming where the solution has reached zero. We can not be sure that the value of `gamma` we stop at, though, is the real eigenvalue; we only know for certain that we have *passed* it. We then call a function to perform a binary search between the current and previous `gamma` values, refining the search until a certain threshold of accuracy is reached.
5. If the solution blows up without crossing zero, then we increment to the next value of `gamma`, continuing the loop until we reach the end of the search.

---

<sup>8</sup>Either solution will do; here, I’ve decided to keep the `eta[0]` solution in check.

```

print("Starting search for Z =",Z)
for gamma in np.arange(gamma_0,0,dgamma):
    delta = (2*m*c/hbar)*(gamma/(1+gamma**2))    # Value of delta at current gamma search
    value
    Rp = R*delta

    rho = rho_0
    eta_check = np.array([etaA_0,etaB_0])    # Array to store test values of eta per gamma
    search

    # Search while eta doesn't blow up to large values
    while np.absolute(eta_check[0]) < 10:
        # Calculate eta and increment rho
        rho, eta_check = RungeKutta4(rho,eta_check,drho,dEta,gamma)

```

Listing 3: First part of solution calculation.

This creates a temporary array called `eta_check[]`. At each `rho`, its value is calculated, but not stored, as the only important element is the final one it calculates. When the calculation is over and the while loop is run out, the next part will check to see if this last element has flipped sign or not. This is what tells us if the tail has wagged.

As we decide to calculate more and more energy eigenvalues, an issue arises for larger and larger  $n$  values; that is, the separation between each eigenvalue shrinks, and eventually, no matter how small we set `dgamma`, the separation will shrink below our mesh width.

The binary search will help with this, though. We will define it as thus:

```

def BinarySearch(eta,gamma):
    global Rp
    global delta
    drhol = drho*0.01
    etaPrev1 = eta[0]
    gamma_upper = gamma-dgamma
    gamma_lower = gamma
    while np.absolute(gamma_upper - gamma_lower) > -dgamma*0.001:
        gamma_mid = (gamma_upper + gamma_lower)/2.0
        rhol = 0
        etal = np.array([etaA_0,etaB_0])
        delta = (2*m*c/hbar)*(gamma_mid/(1+gamma_mid**2))
        Rp = R*delta

        while np.absolute(etal[0])<10:
            # Compute solutions with finer gamma.
            rhol, etal = RungeKutta4(rhol,etal,drhol,dEta,gamma_mid)

        if etaPrev1*etal[0] < 0:
            gamma_upper = gamma_mid
        else:
            gamma_lower = gamma_mid
        print("Refining search...")
        #print("Gamma:",gamma_mid)
    return gamma_mid

```

Listing 4: Binary search function.

Notice how fine the parameters of this search are; `drho` shrinks by a factor of 100, and we are searching to an accuracy of `dgamma/1,000`.

```

# Check if "tail has wagged"
if eta_check[0]*etaPrev < 0:
    print("Tail has wagged.")
    etaPrev = eta_check[0]
    gammaFine = BinarySearch(eta_check, gamma)
    print("gamma =", gammaFine)
    print("Z =", Z)
    print("n =", n)
    print("l =", l)
    print("n' =", N)
    Ep = -(2*m*c**2)*(gammaFine**2/(1+gammaFine**2)) # (E') Allowed energy in Joules
    Ep = Ep*6.242E18 # Convert Joules to eV
    theoretical_Ep = -m*c*c*((Z**2)*alpha**2)/(2*N**2) - ((Z**4)*alpha**4)/(2*N**4)*((N
/np.absolute(k))-3/4) + ((Z**6*alpha**6)/(4*n**6))*(((3*n**3)/(2*k**3))*(1-(k/n)))+(3*n/k
)+(5/4))*6.242E18 # Theoretical allowed energy in eV
    n += 1
    N = n + 1
    print("Computed E':", Ep, "eV")
    print("Theoretical E' (6th order):", theoretical_Ep, "eV")
    print("Difference (6th order):", np.absolute(Ep - theoretical_Ep_2), "eV")
    print("Radius:", R*1E15, "fm")

```

Listing 5: Second part of solution calculation.

An energy eigenvalue solution is finally complete once the binary search computes the best value of `gamma`. This is then converted into the allowed energy value in Joules by Equation II.51, and then multiplied by a conversion factor to obtain the value in electron-volts.

We can compare this to a theoretical value of the allowed energy. Expanded in terms of the fine structure constant<sup>9</sup>:

$$E_n(Z) = mc^2 - mc^2 \frac{Z^2 \alpha^2}{2n^2} - mc^2 \frac{Z^4 \alpha^4}{2n^4} \left( \frac{n}{k} - \frac{3}{4} \right) - mc^2 \frac{Z^6 \alpha^6}{4n^6} \left[ \frac{3n^3}{2k^3} \left( 1 - \frac{k}{n} + \frac{2k^2}{n^2} \right) + \frac{5}{4} \right] \quad (\text{III.6})$$

Notice that the dependence on  $Z$  scales with the order of  $\alpha$ , just as in the Coulomb potential:

$$V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r} \quad \rightarrow \quad V(r) = -\frac{Z\alpha\hbar}{r}$$

The first term of Equation III.6 is, of course, the electron's rest mass-energy. The second gives the usual nonrelativistic energy levels, and the third corrects for fine-structure splitting. Were we only observing the hydrogen atom's energy levels, the fourth term would be an extremely minute correction. However, at large  $Z$ , it becomes non-negligible.

The rest energy dominates the value, so it is more interesting to subtract it out:

$$E'_n(Z) = E_n(Z) - mc^2$$

So for hydrogen ( $Z = 1$ ), the ground state ( $n = 1$  and  $k = 1$ ):

$$E'_1(1) = -m_e c^2 \left[ \frac{\alpha^2}{2} - \frac{\alpha^4}{8} - \frac{17\alpha^6}{16} \right] \quad (\text{III.7})$$

$$E'_1(1) = -13.606582 \text{ eV}$$

---

<sup>9</sup>See Appendix A for derivation.

### III.4 Constructing the Wavefunctions

Once the binary search has narrowed in on an accurate energy eigenvalue that we know corresponds to a solution to the Dirac Equation, we can solve the differential equations one more time, this time saving the solution at each `rho` value in order to plot it after.

First, we declare the arrays and our variables:

```
## DECLARING ARRAYS AND VARIABLES
rho_axis = np.array([rho_0])      # Array of rho values
etaA_axis = np.array([etaA_0])    # Array of etaA values
etaB_axis = np.array([etaB_0])    # Array of etaB values
psiA_axis = np.array([psiA_0])    # Array of psiA values
psiB_axis = np.array([psiB_0])    # Array of psiB values

rho = rho_0                       # Independent variable
eta = np.array([etaA_0, etaB_0])  # Dependant variable
```

Recall that the differential equations we are solving are in  $\eta_A$  and  $\eta_B$ . These are the power series which the wavefunctions  $\psi_A$  and  $\psi_B$  are in terms of. These are initialized here, and computed after since  $\psi = \rho^k \eta$ .

```
# Recompute wavefunctions with the correct gamma
while np.absolute(eta[0]) < 10:
    # Calculate eta and increment rho
    rho, eta = RungeKutta4(rho, eta, drho, dEta, gammaFine)

    # Append values to respective axes.
    rho_axis = np.append(rho_axis, rho)
    etaA_axis = np.append(etaA_axis, eta[0])
    etaB_axis = np.append(etaB_axis, eta[1])
```

Now, as RK4 calculates the solution at each point, that value is stored in its respective array.

```
# Since psiA = rho^(k-1) * eta1, we will multiply each etaA_axis[i]
# by its corresponding rho_axis[i]**(k-1). We will also take the
# absolute value of the solution to obtain the probability density.
# The same is done to obtain psiB if desired.
for i in range(len(etaA_axis)):
    etaA_axis[i] = (rho_axis[i]**(k-1)*etaA_axis[i])
    etaB_axis[i] = (rho_axis[i]**(k-1)*etaB_axis[i])
psiA_axis = etaA_axis
psiB_axis = etaB_axis
```

The wavefunctions have been recomputed as promised, but they still contain the “tail” they acquired during computation, so we must cut it off before plotting, as it is not really part of the wavefunction. This is accomplished by a backward-search over the `rho` and `psi` arrays, removing each element while the value of the array is above some small number *close* to zero.

```
# Backward search to remove the "tail"
while np.absolute(psiA_axis[psiA_axis.size - 1]) > 0.001 and psiA_axis.size > 1:
    rho_axis = rho_axis[:-1].copy()
    psiA_axis = psiA_axis[:-1].copy()
    psiB_axis = psiB_axis[:-1].copy()
```

The arrays `psiA_axis` and `psiB_axis` can then be plotted as one wishes against `rho_axis`.

## IV Results & Discussion

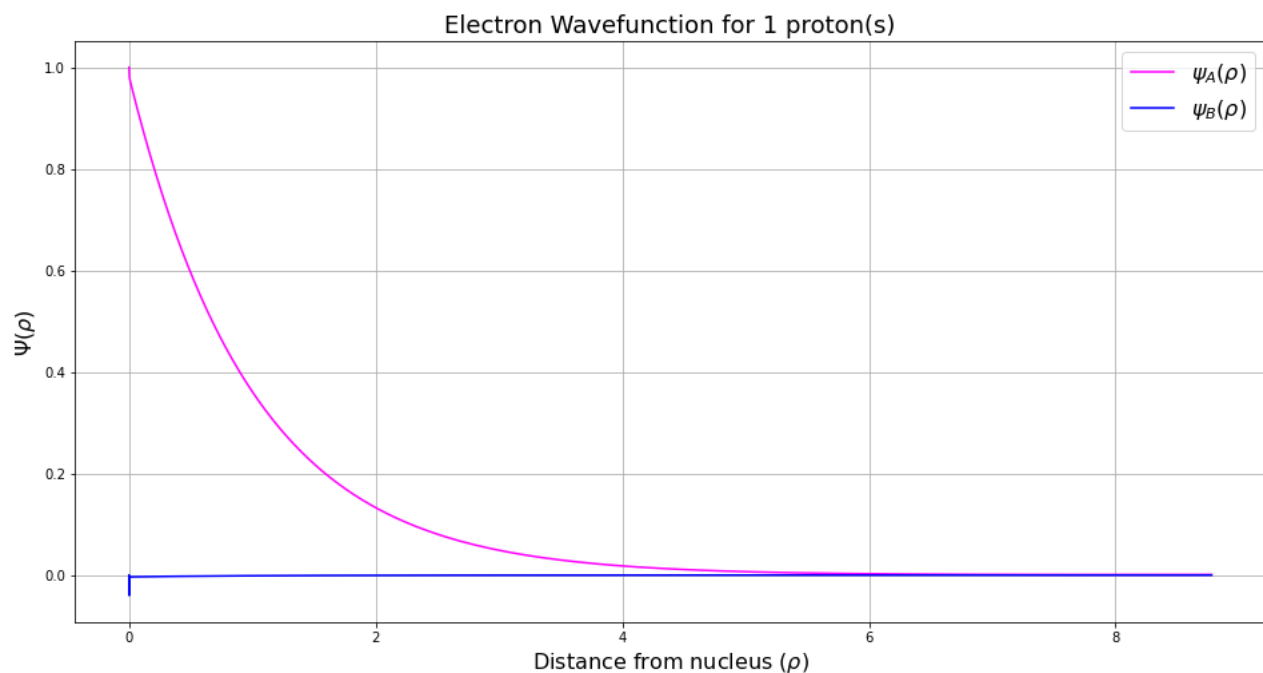
### IV.1 Hydrogen ( $Z = 1$ )

Hydrogen is, of course, the simplest case to which we can apply this method. As in later sections, we will examine the first three energy eigenvalues and eigenstates for  $k = 1$ , as well as the ground state of  $k = 2$  and  $k = 3$ .

#### Eigenstates for $k = 1$

This is the ground state of Hydrogen. Its energy eigenvalue is well-known, and as we have discussed, it is a good starting point to test the accuracy of our method.

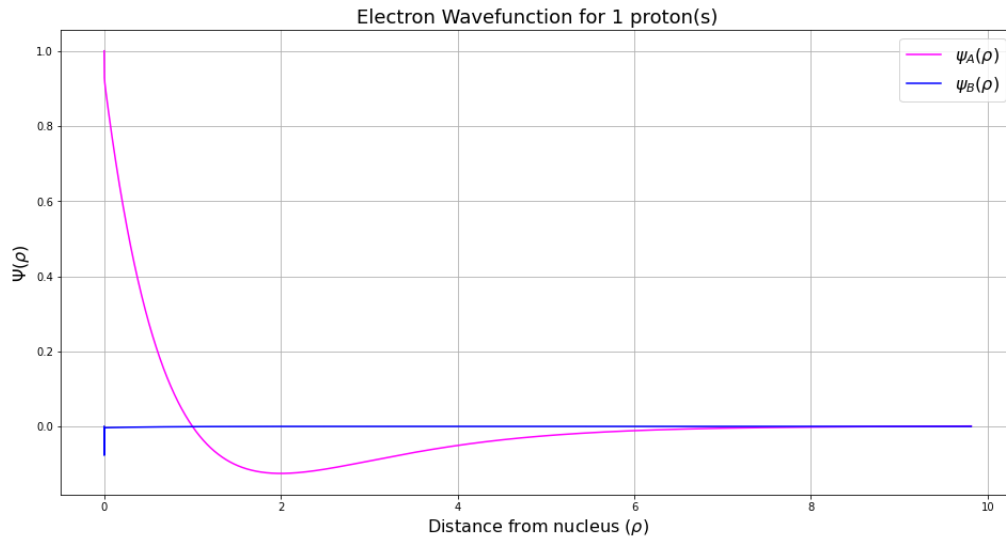
Running the code produces the following:



```
gamma = 0.003648897136874999
Z = 1
n = 1
l = 0
n' = 1
Computed E': -13.608229358223097 eV
Theoretical E' (6th order): -13.606582215700836 eV
Difference (6th order): 0.001647142522260836 eV
Radius: 0.8783 fm
```

The difference between the found energy and the theoretical energy is minute, but one might wonder if this is truly due to the finite size of the nucleus, or just an artifact of the numerical solution. To test this, we reduce the mesh width in `rho` to see if there is a change in the found value. Reducing by half, we find no noticeable change. So indeed, we can be confident that with a finite nucleus, there *is* change in the binding energy as compared to an assumption of a point-like nucleus.

The first excited state produces:

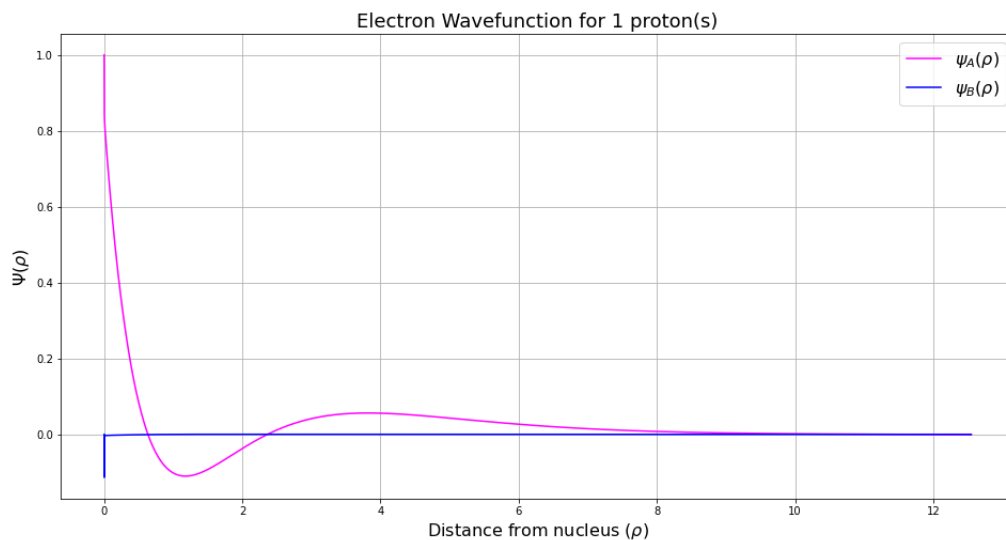


```
gamma = 0.0018241901056249973
Z = 1
n = 2
l = 0
n' = 2
Computed E': -3.4011274601886434 eV
Theoretical E' (6th order): -3.401634215880928 eV
Difference (6th order): 0.0005067556922844219 eV
Radius: 0.8783 fm
```

It is interesting to note that the  $\psi_B(\rho)$  solution is effectively zero; this component of the Dirac spinor seems to contribute almost nothing to the solution.

The difference between the theoretical and computed eigenvalues has decreased. This makes sense; we should expect that with greater energies, the electron's wavefunction will grow larger, and thus it will spend more time farther away from the nucleus.

Finally, the second excited state:



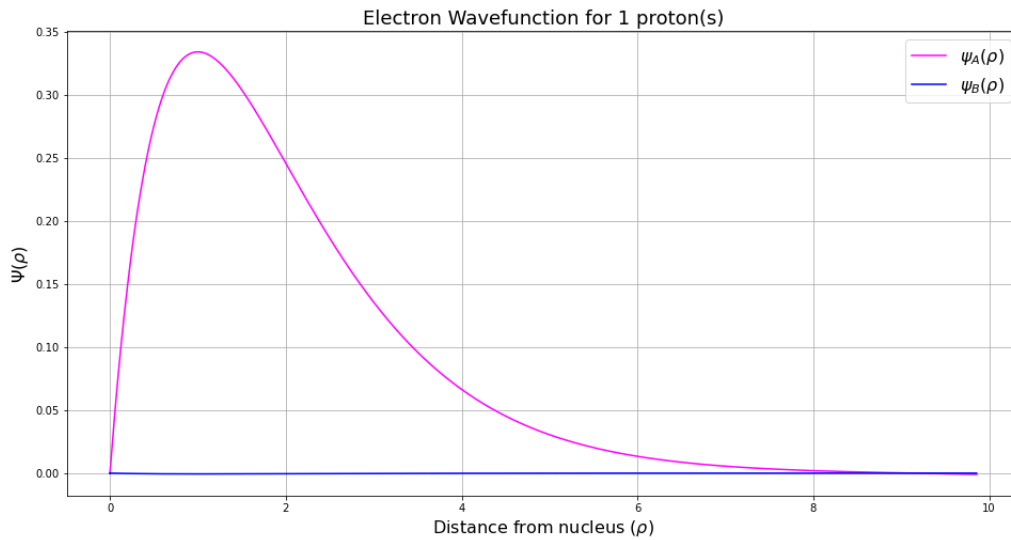
```

gamma = 0.0012162799493749968
Z = 1
n = 3
l = 0
n' = 3
Computed E': -1.511995900541615 eV
Theoretical E' (6th order): -1.5118424602866973 eV
Difference (6th order): 0.00015344025491770275 eV
Radius: 0.8783 fm

```

We can see the difference has shrunk even more so and the solution maintains accuracy to four significant figures. This shows that our method works well for the case of the relativistic hydrogen atom.

### Eigenstates for $k = 2$ and $k = 3$

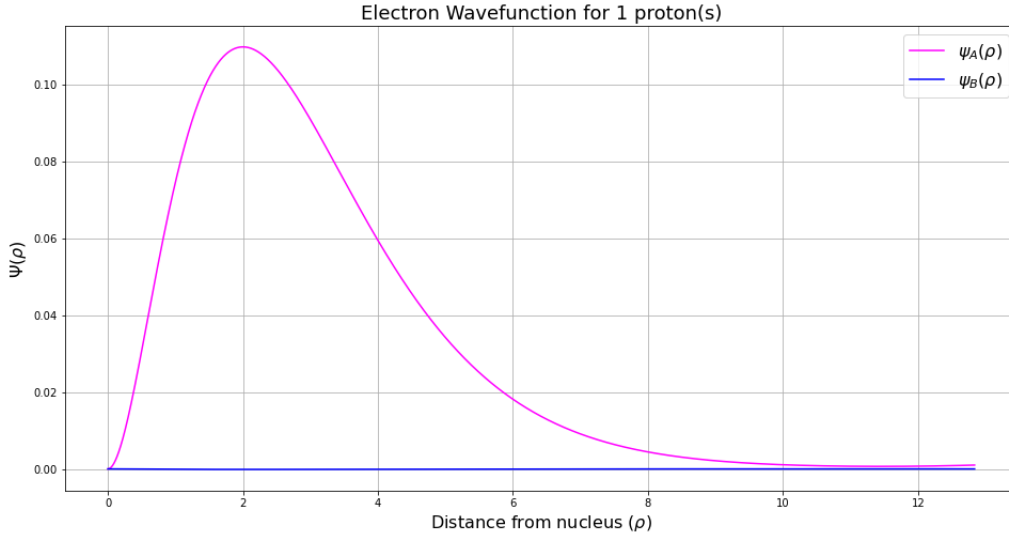


```

gamma = 0.0018241901056249973
Z = 1
n = 1
l = 1
n' = 2
Computed E': -3.4011274601886434 eV
Theoretical E' (6th order): -3.401679547484522 eV
Difference (6th order): 0.0005520872958784118 eV
Radius: 0.8783 fm

```





```

gamma = 0.0012162799493749968
Z = 1
n = 1
l = 2
n' = 3
Computed E': -1.511995900541615 eV
Theoretical E' (6th order): -1.5118603913942172 eV
Difference (6th order): 0.0001355091473977943 eV
Radius: 0.8783 fm

```

The eigenvalues of greater angular momentum clearly display the degeneracy of the hydrogen atom system; the ground state of  $k = 2$  has the same energy eigenvalue as the first excited state of  $k = 1$ , and  $k = 3$  has the same eigenvalue as the second.

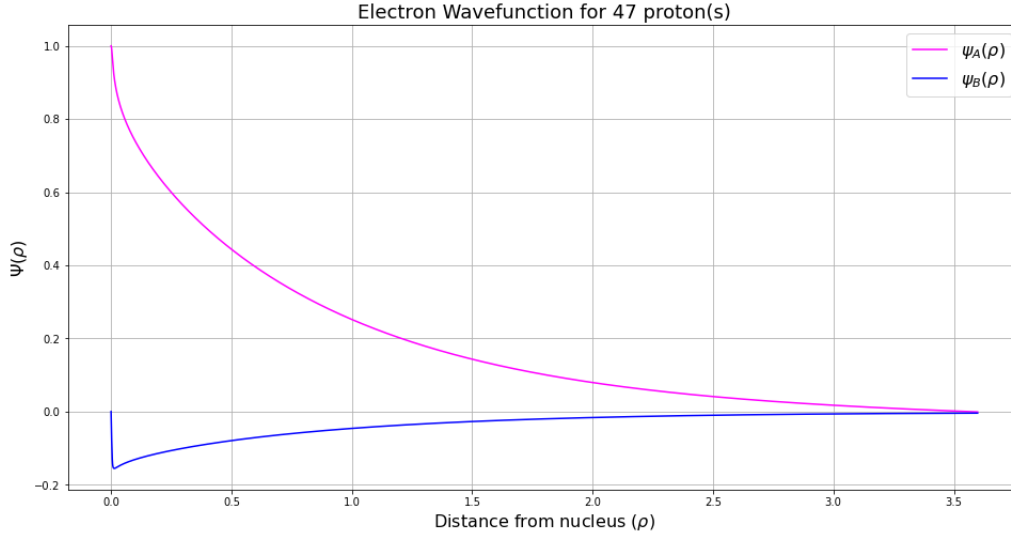
With higher angular momentum, the wavefunctions appear to spread out a little as well, which is perhaps the reason there is an even smaller difference between the theoretical and found eigenvalues.

## IV.2 Silver ( $Z = 47$ )

Silver, with 47 protons in its nucleus, is a good example of a larger element to compare against hydrogen. Whereas hydrogen's nucleus is less than a femtometer in radius, silver's is roughly seven times larger.

### Eigenstates for $k = 1$

The ground state of silver shows a significantly larger  $\psi_B$  component in its wavefunction, as well as a greater difference between the theoretical and found eigenvalues:



```
gamma = 0.172438106839375
Z = 47
n = 1
l = 0
n' = 1
Computed E': -29513.806206014906 eV
Theoretical E' (6th order): -30057.228758518355 eV
Difference (6th order): 543.422552503449 eV
Radius: 6.339263892371632 fm
```

It seems, then, that with larger  $Z$ ,  $\psi_B$  contributes more to the solution, and it might be tantalizing to consider one of the most interesting features of the Dirac Equation for an explanation: the prediction of antimatter. However, in a bound state, it is not as simple to separate “particleness” or “anti-particleness” between the two spinors of the Dirac spinor; we can be sure there is *no* antimatter hiding here.

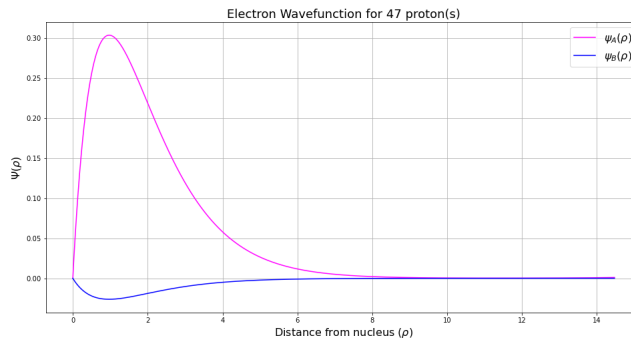
For brevity, I will only show the wavefunction of the ground state, and compare the eigenvalues of the first and second excited states; the wavefunctions follow a very predictable pattern.

```
gamma = 0.08774377090187493
Z = 47
n = 2
l = 0
n' = 2
Computed E': -7808.829432956883 eV
Theoretical E' (6th order): -7281.1610699397515 eV
Difference (6th order): 527.668363017131 eV
Radius: 6.339263892371632 fm
```

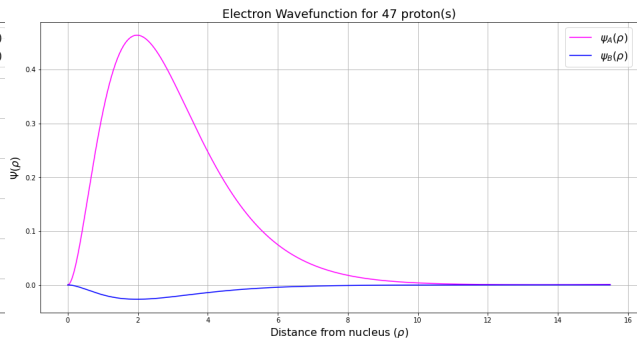
As expected, we see that the difference decreases (albeit not drastically) as the energy level increases.

```
gamma = 0.058144649808124914
Z = 47
n = 3
l = 0
n' = 3
Computed E': -3443.7997746093656 eV
Theoretical E' (6th order): -3252.1162775171115 eV
Difference (6th order): 191.68349709225413 eV
Radius: 6.339263892371632 fm
```

### Eigenstates for $k = 2$ and $k = 3$



(a) Ground state for  $k = 2$ .



(b) Ground state for  $k = 3$ .

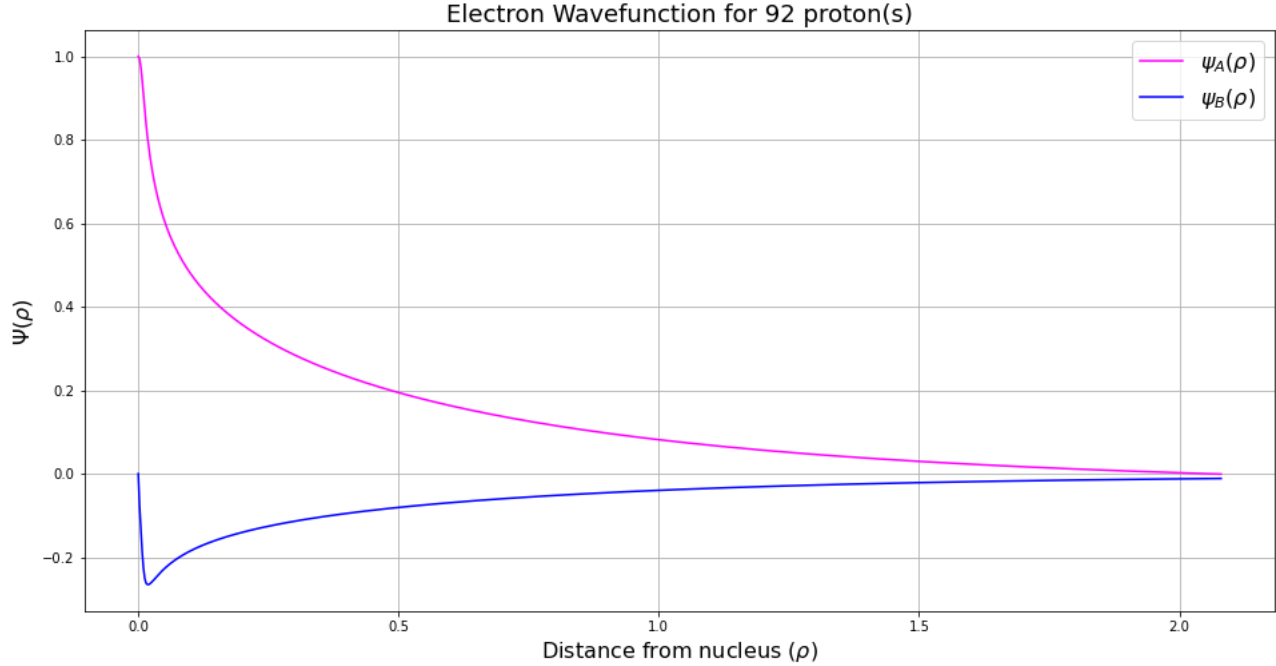
```
gamma = 0.08638390762062495
Z = 47
n = 1
l = 1
n' = 2
Computed E': -7570.439642044716 eV
Theoretical E' (6th order): -7991.979028767132 eV
Difference (6th order): 421.53938672241657 eV
Radius: 6.339263892371632 fm
```

```
gamma = 0.05735070449562491
Z = 47
n = 1
l = 2
n' = 3
Computed E': -3350.700267039955 eV
Theoretical E' (6th order): -3773.5884279942657 eV
Difference (6th order): 422.8881609543105 eV
Radius: 6.339263892371632 fm
```

### IV.3 Uranium ( $Z = 92$ )

Finally, we examine Uranium, with a very large nucleus in terms of its proton content; in terms of size, it is only about one femtometer larger in radius than silver.

Eigenstates for  $k = 1$



```
gamma = 0.336341847139375
Z = 92
n = 1
l = 0
n' = 1
Computed E': -103872.7686234106 eV
Theoretical E' (6th order): -151907.24123807362 eV
Difference (6th order): 48034.47261466303 eV
Radius: 7.929920271153631 fm
```

We see now a drastic deviation from the theoretical value by about  $48\text{keV}$ , confirming the idea that larger and larger nuclei will cause significant change in the energy eigenvalue as compared to the assumption of a point-like nucleus.

```
gamma = 0.18600151510814156
Z = 92
n = 2
l = 0
n' = 2
Computed E': -34177.95656574773 eV
Theoretical E' (6th order): -27158.435157006013 eV
Difference (6th order): 7019.521408741715 eV
Radius: 7.929920271153631 fm
```

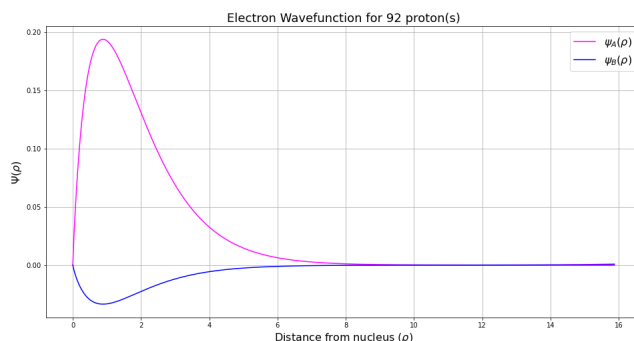
```

gamma = 0.12062602682689874
Z = 92
n = 3
l = 0
n' = 3
Computed E': -14658.599508438852 eV
Theoretical E' (6th order): -11952.247111204508 eV
Difference (6th order): 2706.3523972343446 eV
Radius: 7.929920271153631 fm

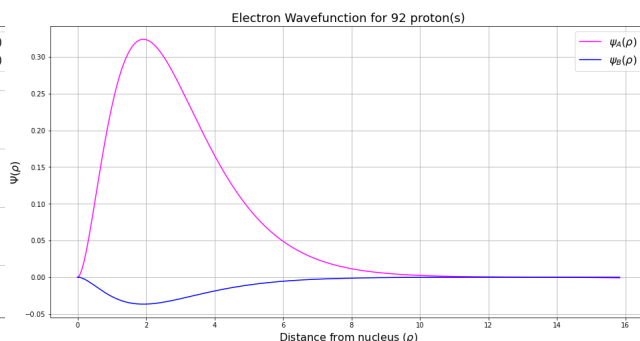
```

We see with the first two excited states that the difference continues to decrease, and we can be certain that for even larger atoms, the effects of the finite nucleus would continue to have an effect on the energy eigenvalues.

### Eigenstates for $k = 2$ and $k = 3$



(a) Ground state for  $k = 2$ .



(b) Ground state for  $k = 3$ .

```

gamma = 0.17285405417064298
Z = 92
n = 1
l = 1
n' = 2
Computed E': -29652.225869176433 eV
Theoretical E' (6th order): -57957.07239461392 eV
Difference (6th order): 28304.846525437486 eV
Radius: 7.929920271153631 fm

```

```

gamma = 0.11332964010814955
Z = 92
n = 1
l = 2
n' = 3
Computed E': -12960.709881769551 eV
Theoretical E' (6th order): -37657.002719967386 eV
Difference (6th order): 24696.292838197834 eV
Radius: 7.929920271153631 fm

```

# Appendices

## A Binomial Expansion of Relativistic Energy

Starting with the expression<sup>10</sup> for total energy as a function of the principle quantum number and  $s = \sqrt{k^2 + \alpha^2}$ :

$$E = mc^2 \left[ 1 + \frac{\alpha^2}{(s + n')^2} \right]^{1/2} \quad (\text{A.1})$$

We consider the expansion up to order  $x^3$ :

$$(1 + x)^n \approx 1 + nx + \frac{n(n-1)}{2!}x^2 + \frac{n(n-1)(n-2)}{3!}x^3 \quad (\text{A.2})$$

This is valid for sufficiently small  $x$ ; that is, if  $x < 1$ , and recall that  $\alpha \approx 1/137$ . The goal is to expand Equation A.1 as:

$$E \approx mc^2 \left[ 1 - \frac{1}{2} \left( \frac{\alpha^2}{(s + n')^2} \right) + \frac{3}{8} \left( \frac{\alpha^4}{(s + n')^4} \right) - \frac{5}{16} \left( \frac{\alpha^6}{(s + n')^6} \right) \right] \quad (\text{A.3})$$

to the order  $\alpha^6$ .  $s$  contains  $\alpha$  dependence, so it must be expanded as well:

$$s = \sqrt{k^2 + \alpha^2} \quad (\text{A.4})$$

$$s = k \left( 1 + \frac{\alpha^2}{k^2} \right)^{1/2} \quad (\text{A.5})$$

$$s \approx k \left( 1 - \frac{\alpha^2}{2k^2} + \frac{3\alpha^4}{8k^4} \right) \quad (\text{A.6})$$

Then, inside Equation A.3:

$$\frac{1}{(s + n')^2} \approx \frac{1}{[k(1 - \frac{\alpha^2}{2k^2} + \frac{3\alpha^4}{8k^4}) + n']^2} \quad (\text{A.7})$$

$n = n' + k$ , so distributing  $k$  yields:

$$\frac{1}{(s + n')^2} \approx \frac{1}{[n - \frac{\alpha^2}{2k} + \frac{3\alpha^4}{8k^3}]^2} \quad (\text{A.8})$$

$$\frac{1}{(s + n')^2} \approx \frac{1}{n^2} \left[ 1 - \frac{\alpha^2}{2kn} + \frac{3\alpha^4}{8k^3n} \right]^{-2} \quad (\text{A.9})$$

Performing another binomial expansion:

$$\frac{1}{n^2} \left[ 1 - \frac{\alpha^2}{2kn} + \frac{3\alpha^4}{8k^3n} \right]^{-2} \approx \frac{1}{n^2} \left[ 1 + \frac{\alpha^2}{kn} - \frac{3\alpha^4}{4k^3n} + \frac{3\alpha^4}{4k^2n^2} \right] \quad (\text{A.10})$$

$$\frac{1}{n^2} \left[ 1 - \frac{\alpha^2}{2kn} + \frac{3\alpha^4}{8k^3n} \right]^{-2} \approx \frac{1}{n^2} \left[ 1 + \frac{\alpha^2}{kn} - \frac{3\alpha^4}{4k^3n} \left( 1 - \frac{k}{n} \right) \right] \quad (\text{A.11})$$

---

<sup>10</sup>Tarun Biswas, *Quantum Mechanics: Concepts and Applications* (New York: 1999): 176.

Then, Equation A.3 is:

$$E \approx mc^2 \left[ 1 - \frac{\alpha^2}{2n^2} \left[ 1 + \frac{\alpha^2}{kn} - \frac{3\alpha^4}{4k^3n} \left( 1 - \frac{k}{n} \right) \right] + \frac{3}{8} \left( \frac{\alpha^4}{(s+n')^4} \right) - \frac{5}{16} \left( \frac{\alpha^6}{(s+n')^6} \right) \right] \quad (\text{A.12})$$

Notice first that in the final term, since we are only keeping up to  $\alpha^6$ , we need only keep the  $5\alpha^6/16n^6$  term:

$$E \approx mc^2 \left[ 1 - \frac{\alpha^2}{2n^2} \left[ 1 + \frac{\alpha^2}{kn} - \frac{3\alpha^4}{4k^3n} \left( 1 - \frac{k}{n} \right) \right] + \frac{3}{8} \left( \frac{\alpha^4}{(s+n')^4} \right) - \frac{5\alpha^6}{16n^6} \right] \quad (\text{A.13})$$

Finally then, we expand the third ( $\alpha^4$ ) term. We can cut off the expansion of  $s$  at the second order of  $\alpha$  here, since  $\alpha^4\alpha^2 = \alpha^6$ :

$$\frac{1}{(s+n')^4} \approx \frac{1}{\left[ n - \frac{\alpha^2}{2k} \right]^4} \quad (\text{A.14})$$

$$\frac{1}{(s+n')^4} \approx \frac{1}{n^4} \left[ 1 - \frac{\alpha^2}{2kn} \right]^{-4} \quad (\text{A.15})$$

This can, of course, be approximated as:

$$\frac{1}{n^4} \left[ 1 - \frac{\alpha^2}{2kn} \right]^{-4} \approx \frac{1}{n^4} \left[ 1 + \frac{2\alpha^2}{kn} \right] \quad (\text{A.16})$$

Collecting  $\alpha^2$ ,  $\alpha^4$  and  $\alpha^6$  terms yields our final approximation:

$$E = mc^2 \left[ 1 - \alpha^2 \left( \frac{1}{2n^2} \right) + \alpha^4 \left( \frac{3}{8n^4} - \frac{1}{2kn^3} \right) + \alpha^6 \left( \frac{3}{8k^3n^3} \left( 1 - \frac{k}{n} \right) + \frac{3}{4kn^5} + \frac{5}{16n^6} \right) \right] \quad (\text{A.17})$$

which can be rearranged to form Equation III.6:

$$E_n(Z) = mc^2 - mc^2 \frac{Z^2\alpha^2}{2n^2} - mc^2 \frac{Z^4\alpha^4}{2n^4} \left( \frac{n}{k} - \frac{3}{4} \right) - mc^2 \frac{Z^6\alpha^6}{4n^6} \left[ \frac{3n^3}{2k^3} \left( 1 - \frac{k}{n} + \frac{2k^2}{n^2} \right) + \frac{5}{4} \right]$$

## References

- [1] Biswas, Tarun. *Quantum Mechanics: Concepts and Applications*. New York: 1999. <http://www.engr.newpaltz.edu/~biswast/qmbook/qmbook.shtml>.
- [2] Blomquist, Emil and Trotte Boman. “The Dirac Equation for a Particle in a Spherical Box Potential with Application in Bag Modeling.” *Royal Institute of Technology (KTH)* (2015). <http://www.diva-portal.org/smash/get/diva2:815669/FULLTEXT01.pdf>.
- [3] Griffiths, David J., and Darrel F. Schroeter. *Introduction to Quantum Mechanics*. 3rd ed. Cambridge: Cambridge University Press 2018.
- [4] Marinova, Krassimira, Istvan Angeli. “Nuclear Charge Radii.” International Atomic Energy Agency: Nuclear Data Services. Accessed February 22, 2024. <https://www-nds.iaea.org/radii/>.