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Effect of Compactified Dimensions on the Ground State Energy of the Hydrogen Atom

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The University of Southern Mississippi

Effect of Compactified Dimensions on the Ground State Energy of the
Hydrogen Atom

by

Floyd Maseda

A Thesis

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Abstract

The three-dimensional Hydrogen atom has been explored extensively, and a wavefunction and energy expression can be found in closed form. Little work, however, has been done with higher-dimensional atoms. This discussion focuses on the effects of adding first one then two compactified dimensions to a Hydrogen atom. The metric of the 4-D Hydrogen atom is taken to be $\mathbb{R}^3 \times \mathbb{S}^1$ while the 5-D metric is taken to be $\mathbb{R}^3 \times \mathbb{S}^2$. We first determine the form of the Laplacian operator in each space and use it to find the respective atomic potentials. The variational method is used to determine an upper bound on the ground state energy as a function of the size of the extra dimension(s). Equating the 4- and 5-D variational energy functions with the experimentally confirmed 3-D Hydrogen atom ground state, an upper bound on the size the compacted dimension(s) must be in order to have not yet been detected is calculated.

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Introduction

The Schrödinger equation is used in quantum mechanics to determine permissible energy levels for a particle in a given electric, nuclear, or other potential. Not only do the outputs of the equation depend on the potential in the vicinity of the particle, but the very nature of the space in which the particle exists can tremendously change the permissible energy levels. As such, the energy levels of a particle in a three-dimensional space may differ greatly from those in a four-, five-, or higher-dimensional space. Though most calculations with the Schrödinger equation are performed in “normal” three-dimensional space, advances in physics beginning in the late 20th century have necessitated the addition of more dimensions in order to successfully combine many of the laws of nature into a single equation—a theory of everything. Many physicists theorize that if these extra dimensions do exist in reality, they must be small enough to be undetectable at low energy levels; therefore, the dimensions must be compactified, or wrapped up upon themselves, in a manner that makes them detectable only at sufficiently high energy levels which scientists have thus far not been able to reach.

This discussion will focus on the effects of adding first one then two compactified dimensions to a Hydrogen atom. We first determine the form of the atomic potential in each space using a modified Laplacian operator corresponding to our chosen metric. We determine an estimate of the ground state energy of a four- and a five-dimensional Hydrogen atom using a common mathematical method in quantum mechanics, the variational method. We hypothesize that the higher-dimensional ground state energies will take a form that forces the extra dimensions to be extremely small, consistent with the idea that they have not yet been detected at current energies. Using the ground state energy expressions, the researcher will determine the maximum size the compactified dimension(s) could be without having yet been detected.

Background

String Theory

The last century of physics has been largely about an idea called “unification.” In the late nineteenth century, Maxwell was able to describe electricity and magnetism in a single set of equations, thus unifying the two previously independent forces into a single force—electromagnetism. Later on in the twentieth century, there was a unification of electromagnetism with quantum mechanics, and in the 1960s and 1970s, the weak nuclear force was unified with the electromagnetic force, giving rise to electroweak theory. By the latter half of the twentieth century, all fundamental forces and particles—with the painful exception of gravity—were unified into a single model, called the Standard Model.[1]

As Kiritsis explains in [1], there have been many attempts since the formation of the Standard Model to remedy its downfalls. Ideas like supersymmetry, higher-dimensional spaces, and even new fundamental forces were introduced to try to forge the elusive “Theory of Everything” (TOE). The leading candidate for this TOE over the past two decades has been String Theory, which postulates that particles are not zero-dimensional, point-like objects (as is assumed in the Standard Model) but rather extremely small, one-dimensional, extended “strings.”

There are many different versions of String Theory, but one of the common denominators in all of them is that they all require the dimensionality of space to be higher than seems intuitive.[2] All theories require at least a ten-dimensional spacetime—as opposed to the “normal” 4-dimensional space (three spatial + time) to which we are accustomed—and some require as many as twenty-six dimensions. For a detailed explanation of the reasoning behind the different number of dimensions, the reader is referred to [3].

As Becker explains in [2], the usual explanation for String Theory’s requirement of higher dimensions is that all other dimensions except the four to which we are accustomed must be “compactified” or wrapped up upon themselves in such a way as to have avoided detection thus far. A common example for how these dimensions can be undetectable is that of a telephone cable, shown in Figure 1. If the telephone cable has a sufficiently small radius or likewise if the wire is viewed from a sufficiently large distance, it appears to be simply a one-dimensional line with

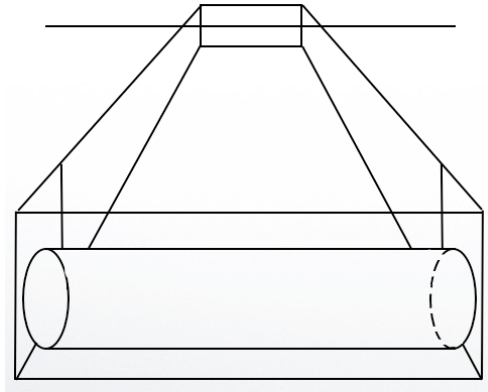


Figure 1: From far away, a telephone cable appears as if it is a one-dimensional object. Upon closer inspection, though, the cable’s surface is actually a two-dimensional plane wrapped upon itself.

no thickness. Upon closer inspection, though, the surface of the wire is actually a two-dimensional plane wrapped upon itself. In much the same way, physicists theorize that the “radius” of these higher dimensions is extremely small and thus undetectable at current energies. As experiments are fine-tuned and the ability to produce more and more energy at once is enhanced, these compactified dimensions may become detectable. This discussion hypothesizes the detection of these dimensions by assuming that at least one exists and observing the effect of adding it to the Schrödinger equation, which is discussed in the next section.

Schrödinger Equation

The Schrödinger Equation was developed by Erwin Schrödinger in 1926. It describes the quantum state of a particle and how it evolves over time. For the purposes of this research, only the non-relativistic, time-independent Schrödinger Equation will be considered. The fact that the equation does not depend on time means that a particle is in a well-defined energy state, i.e. that there is no energy being added to the system or being taken away. The equation makes use of a “wavefunction,” ψ , which is the probability amplitude of a particle’s position. The magnitude of the square of the wavefunction, $|\psi^2|$, is called the probability density. When integrated over an interval, the function returns the probability that a particle will be at some location in that interval. The general form

of the equation used in this research is as follows:

$$\left[-\frac{\hbar^2}{2m} \vec{\nabla}_k^2 + V(\vec{r}) \right] \psi(\vec{r}) = E\psi(\vec{r}) \quad (\text{i.1})$$

where \hbar (read “h-bar”) = $1.05457148 \times 10^{-34} m^2 \cdot kg \cdot s^{-1}$ is called Planck’s constant, m is the mass of a particle, k is the number of dimensions in a system, $\vec{\nabla}_k^2$ is the Laplacian operator in k dimensions, \vec{r} is the set of coordinates (x_1, x_2, \dots, x_k) , $V(\vec{r})$ is the potential energy of the particle as a function of the coordinates, and E is the energy of the particle.

The expression in brackets is known as the Hamiltonian operator, H , and it consists of two parts which correspond to kinetic and potential energy. In classical mechanics, the kinetic energy of a particle is represented as $p^2/2m$, where p is the momentum of the particle. In quantum mechanics, all observables such as momentum correspond to a mathematical operator which acts on a state and produces a number. The momentum operator is $\hat{p} = i\hbar\vec{\nabla}_k$, and $\hat{p}^2/2m = -\frac{\hbar^2}{2m}\vec{\nabla}_k^2$, the first term in the Hamiltonian shown in Equation (i.1).

Thus, the only two things one needs to form the Schrödinger Equation in some space is the Laplacian operator and the potential energy in that space, both of which are explained in more detail in the next two sections.

Laplacian operator

The Laplacian operator, $\vec{\nabla}_k^2$, is dependent on the number and structure of the dimensions in a space, so changing that space (by, perhaps, adding compactified dimensions) will also change the output of the Schrödinger Equation. It is the Laplacian’s spatial dependence that this research shall rely upon.

In a regular Euclidian, rectilinear space with coordinates (x, y, z) , the Laplacian takes on a rather simple form,

$$\vec{\nabla}_3^2(x, y, z) = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

If instead of (x, y, z) rectilinear coordinates, spherical coordinates (r, θ, ϕ) are used [See Figure 2], the Laplacian takes the more complicated form,

$$\vec{\nabla}_3^2(r, \theta, \phi) = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$$

This more complicated expression is due to the fact that in spherical coordinates, a change in the θ -direction also varies with r , the distance from the origin. A small change in θ results in a longer arclength traced out at large r than at small r . A change in the ϕ -direction varies with both r and θ . This interdependence causes each term of the Laplacian to include more than one variable.

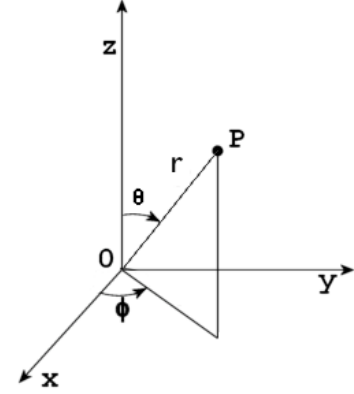


Figure 2: Spherical coordinates shown in relation to regular Cartesian coordinates.

For every different coordinate system, there is a different Laplacian. A general expression for any Laplacian (known as the Laplace-Beltrami operator) is given in terms of the metric of a space as follows:

$$\vec{\nabla}_k^2 = \frac{1}{\sqrt{|\det(g)|}} \sum_{i=1}^k \sum_{j=1}^i \frac{\partial}{\partial x^i} \left(g^{ij} \sqrt{|\det(g)|} \frac{\partial}{\partial x^j} \right) \quad (\text{i.2})$$

where g represents the metric of the space in matrix form, $\det(g)$ is the determinant of that matrix, and g^{ij} is the entry in the i th row and j th column of the *inverse* of the metric, g .

Potential energy, $V(\vec{r})$

Any electrostatic potential, $\Phi(\vec{r})$, where \vec{r} is a set of k coordinates, must satisfy Poisson's Equation in k dimensions,

$$\vec{\nabla}_k^2 \Phi(\vec{r}) = -\frac{\rho(\vec{r})}{\epsilon_0} \quad (\text{i.3})$$

where $\rho(\vec{r})$ is a given charge distribution of a source, and $\epsilon_0 = 8.8541878 \times 10^{-12} \text{ m}^{-3} \cdot \text{kg}^{-1} \cdot \text{s}^4 \cdot \text{A}^2$ is the electric constant (often called the vacuum permittivity) and is included as a standardized constant factor because of accepted units conventions. For the purposes of this research, the source will be a point charge of magnitude $e = 1.60217646 \times 10^{-19} \text{ C}$ at the origin of the coordinate system,

i.e. $\rho(\vec{r}) = e \delta(\vec{r})$, where $\delta(\vec{r})$ is the Dirac delta function in k dimensions.

In three dimensions, using spherical coordinates (r, θ, ϕ) ,

$$\Phi(\vec{r}) = \frac{e}{4\pi\epsilon_0 r}$$

Since the potential in question is an electrostatic one, the transformation from the potential, $\Phi(\vec{r})$, caused by the source to the potential energy of the particle, $V(\vec{r})$, is simple;

$$V(\vec{r}) = q \Phi(\vec{r})$$

where q is the electric charge of the particle.

Because a Hydrogen atom is simply an electron with charge $-e$ captured in the electrostatic field of a proton, the potential energy, $V(\vec{r})$, of the electron in three dimensions is given by

$$V(\vec{r}) = -\frac{e^2}{4\pi\epsilon_0 r}$$

Adding more dimensions changes the Laplacian operator and thus modifies the solution to Poisson's Equation. We therefore need to develop an expression for the potential due to a point charge in a four-dimensional space with a single compactified dimension and a five-dimensional space with two compactified dimensions.

Hydrogen atom

Using the Laplacian operator and potential energy derived in the previous section, the form of the Schrödinger Equation in a three-dimensional Hydrogen atom is

$$\left[-\frac{\hbar^2}{2\mu} \vec{\nabla}_3^2 - \frac{e^2}{4\pi\epsilon_0 r} \right] \psi(\vec{r}) = E\psi(\vec{r})$$

where \vec{r} is the set of spherical coordinates (r, θ, ϕ) , $\vec{\nabla}_3^2$ is the three-dimensional Laplacian operator in spherical coordinates, $\mu = \frac{m_e m_p}{m_e + m_p}$ is the “reduced mass” of the electron, m_e is the actual mass

of the electron, and m_p is the mass of a proton. Reduced mass is used to cancel out any effects of gravitation.

As shown in [4], the solution to the above equation is

$$\psi(r, \theta, \phi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}} \cdot e^{-\frac{r}{na_0}} \left(\frac{r}{na_0}\right)^\ell L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0}\right) Y_\ell^m(\theta, \phi)$$

where $a_0 = \frac{4\pi\epsilon_0\hbar^2}{\mu e^2} = 0.529177 \times 10^{-10}$ m is the Bohr radius, $n = 1, 2, 3, \dots$ is the principal quantum number, $\ell = 0, 1, \dots, n-1$ is the angular quantum number, and $m = -\ell, \dots, \ell$ is the magnetic quantum number. $L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0}\right)$ are generalized Laguerre polynomials of degree $n-\ell-1$ and are defined as

$$L_{a-p}^p(x) = (-1)^p \frac{d^p}{dx^p} \left[e^x \frac{d^a}{dx^a} (e^{-x} x^a) \right]$$

$Y_\ell^m(\theta, \phi)$ are spherical harmonics of order m and degree ℓ , defined by

$$Y_\ell^m(\theta, \phi) = \sqrt{\frac{(2\ell+1)(\ell-|m|)!}{4\pi(\ell+|m|)!}} \cdot e^{im\phi} P_\ell^m(\cos\theta)$$

where $P_\ell^m(\cos\theta)$ are associated Legendre polynomials of degree ℓ and order m ,

$$P_\ell^m(x) = (1-x^2)^{|m|/2} \frac{d^{|m|}}{dx^{|m|}} \left[\frac{1}{2^\ell \ell!} \frac{d^\ell}{dx^\ell} \left((x^2-1)^\ell \right) \right]$$

These quantum numbers and special functions arise from the nature of solving the partial differential equation and asserting that the solution be normalizable.

The allowable energy levels for the Hydrogen atom, E_n , are

$$E_n = - \left[\frac{\mu e^4}{32\hbar^2 \pi^2 \epsilon_0^2} \right] \frac{1}{n^2} = - \left[\frac{\hbar^2}{2\mu a_0^2} \right] \frac{1}{n^2} = \frac{E_1}{n^2}$$

where $E_1 = -13.6$ eV = -2.179×10^{-18} J is the ground state energy of the Hydrogen atom. This result is only valid for a three dimensional space. Adding extra dimensions changes the Laplacian operator and thus alters the final solution. We do not attempt to solve the differential equations

directly but take a simple approach using the variational method, discussed later.

Previous compactification in a Hydrogen atom

In 2007, Martin Bureš published a paper, [5], in which he compactified a dimension inside of a Hydrogen atom. He first tried adding a fourth *extended* dimension to the atom (making it a 3-sphere), which changed the potential from being proportional to $1/r$ (as in three dimensions) to being proportional to $1/r^2$. This potential is found by solving Poisson’s equation with a 4-dimensional hyperspherical Laplacian,

$$\vec{\nabla}_4^2(r, \eta, \theta, \phi) = \frac{1}{r^3} \frac{\partial}{\partial r} \left(r^3 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \eta} \left[\frac{\partial}{\partial \eta} \left(\sin^2 \eta \frac{\partial}{\partial \eta} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]$$

derived in Appendix A of [5] using the Laplace-Beltrami operator, (i.2). After inserting the new potential and Laplacian into the Schrödinger Equation, Bureš examined three different cases corresponding to three types of modified Bessel functions and showed that an extra extended dimension makes the atom unstable (i.e. all energies are positive). Bureš noted, however, that there are several solutions to the Schrödinger equation that are stable with higher numbers of extended dimensions, although these solutions restrict the potential to only three dimensions. For more information about these solutions, the reader is directed to the references in [5].

Bureš also attempted to add a fourth *compactified* dimension into the Hydrogen atom. Still using the non-compactified potential, proportional to $1/r^2$, he employed what he called the “method of images” to sum up the force the electron would feel from multiple “images” of the nucleus. Bureš in effect “unwrapped” the compactified dimension and simulated compactification by treating an electron in that dimension as a collection of repeated point charges, each $2\pi R$ away from each other, where R is the radius of compactification. He then summed up the force felt by each of these images by simply changing the denominator of the potential to reflect a 2-dimensional distance. The “attractive” potential energy was thus modified to

$$V_{attract} = - \sum_{n=0}^{\infty} \frac{e^2}{r^2 + (w - 2\pi nR)^2}$$

where r is the radial distance in three dimensions, and w is the location in the compactified dimension. Because of the repeating behavior of the electron, Bureš was also forced to include a repulsive term to account for the electron interacting with its own images. This term turned out to simply be a constant factor,

$$V_{anti} = +\frac{e^2}{12R^2}$$

It is necessary to point out that the method of images only *simulates* a compactified dimension. The potential energy expression that Bureš used is merely a modification of the non-compactified 4-D potential. Using this potential, Bureš explored the effects of the compactified dimension using perturbation theory to find an estimate for the ground state energy of a four-dimensional Hydrogen atom.

We attempt to derive a possibly more accurate estimate of the ground state energy using a different Laplacian, configured to implicitly include the compactified dimension. The variational method, detailed in the next section, is used with the compactified potential to estimate the ground state energy. This method is then extended into five dimensions, a system which Bureš's method cannot address.

Variational Method

The variational method is used to determine an upper bound of the ground state energy of any system.[6] Choosing any normalized function, ϕ , whatsoever and calculating $\tilde{E} = \langle \phi | H | \phi \rangle = \int \phi^* H \phi dV$, where H is the Hamiltonian operator and dV is the volume element in the space, the result is guaranteed to be greater than or (in the case of finding the wavefunction exactly) equal to E_G , the actual ground state energy of the system, i.e.

$$\tilde{E} = \langle \phi | H | \phi \rangle \geq E_G \tag{i.4}$$

This can be shown by taking advantage of the *completeness* of the set of orthonormalized eigenfunctions of H . Because the set of orthonormalized eigenfunctions is complete, any normalized function can be represented as a linear combination of the individual eigenfunctions, ψ_n . One can

thus express (assuming $n = 1$ is the ground state as in the Hydrogen atom)

$$\phi = \sum_{n=1}^{\infty} c_n \psi_n$$

Because ϕ is normalized, $\langle \phi | \phi \rangle = 1$. Inserting the above for ϕ ,

$$\langle \phi | \phi \rangle = \left\langle \sum_{m=1}^{\infty} c_m \psi_m \left| \sum_{n=1}^{\infty} c_n \psi_n \right. \right\rangle = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} c_m^* c_n \langle \psi_m | \psi_n \rangle$$

Since the individual eigenfunctions are orthonormalized, $\langle \psi_m | \psi_n \rangle = \delta_{mn}$, which only has value when $m = n$; therefore,

$$\langle \phi | \phi \rangle = \sum_{n=1}^{\infty} |c_n|^2 = 1$$

Using the same method to calculate $\tilde{E} = \langle \phi | H | \phi \rangle$, where $H | \psi_n \rangle = E_n | \psi_n \rangle$, one finds

$$\tilde{E} = \langle \phi | H | \phi \rangle = \sum_{n=1}^{\infty} E_n |c_n|^2$$

From the above two expressions, it is clear that

$$E_G = E_G \sum_{n=1}^{\infty} |c_n|^2 = \sum_{n=1}^{\infty} E_G |c_n|^2 \leq \sum_{n=1}^{\infty} E_n |c_n|^2 = \tilde{E}$$

because for any $n \geq 1$, $E_n \geq E_G$. Thus, we have proven (i.4).

Methodology

Instead of simply modifying the 4-dimensional potential found by solving Poisson's equation with a hyperspherical Laplacian as Bureš did in [5], we use the Laplace-Beltrami operator, (i.2), to determine a compactified Laplacian. The metric of our space is taken to be $\mathbb{R}^3 \times \mathbb{S}^1$. This leads to the Laplacian,

$$\vec{\nabla}_4^2(r, \theta, \phi, w) = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial w^2} \quad (\text{ii.1})$$

where w corresponds to location in the compactified dimension, which is periodic with period a . In other words a is the circumference of the compactified dimension. This Laplacian is used in Poisson's equation, (i.3), and the differential equation is solved. As in three dimensions, the potential will not depend on the θ - and ϕ -directions, so our Poisson equation in four dimensions simply reads

$$\left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{\partial^2}{\partial w^2} \right] \Phi(r, w) = -\frac{e}{\epsilon_0 J} \delta(r) \delta(w/a) \quad (\text{ii.2})$$

where $J = 4\pi a r^2$, and the right side of the equation comes from expressing the multi-dimensional delta function in (i.3) as a product of the one-dimensional delta functions and asserting they integrate out to equal unity.

In five dimensions, the process is the same, with the metric now taken to be $\mathbb{R}^3 \times \mathbb{S}^2$. This leads to a five-dimensional Poisson equation of the form

$$\left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{a^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{a^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \Phi(r, w) = -\frac{e}{\epsilon_0 J} \delta(r) \delta(\theta) \delta(\phi) \quad (\text{ii.3})$$

where $J = 4\pi a^2 r^2 \sin \theta$, a is the radius of the compactified 2-sphere, and θ and ϕ correspond to angles in the *compactified* dimensions, not the regular angles.

After determining the form of the potential, the variational method is used in both cases to estimate the ground state energy of the Hydrogen atom with compactified dimensions. A trial function with one or more parameters is developed for each case, and the trial function is minimized with respect

to the parameters using a FORTRAN program and the "fit" tool in gnuplot. After determining estimates of the ground state energies in each space, the results are equated to the three-dimensional ground state energy, and a maximum size that the compactified dimension(s) could be without having yet been detected is determined.

Determination of the potential energy

In four dimensions

The right side of Poisson's equation in four dimensions, (ii.2), equals zero for all points in space except the origin of the coordinate system. We can thus solve the easier expression

$$\left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{\partial^2}{\partial w^2} \right] \Phi(r, w) = 0 \quad (1.1)$$

called Laplace's equation, and equate the solution to the right side of (ii.2) to determine any arbitrary constants found in solving Equation (1.1). This equation can be solved using the separation of variables technique. The potential, $\Phi(r, w)$ is assumed to be separable, i.e.

$$\Phi(r, w) = R(r)Q(w) \quad (1.2)$$

Inserting (1.2) into (1.1) and dividing the entire equation by $\Phi(r, w)$ yields

$$\frac{1}{r^2 R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) = -\frac{1}{Q} \frac{d^2 Q}{dw^2} \quad (1.3)$$

Because the right and left sides of (1.3) are functions of different variables, they must both equal the same constant, which we will call α^2 . The original PDE is thus split into two ODE's,

$$\frac{1}{r^2 R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) = \alpha^2 \quad (1.4a)$$

$$\frac{1}{Q} \frac{d^2 Q}{dw^2} = -\alpha^2 \quad (1.4b)$$

The general solution to (1.4b) is

$$Q(w) = A \sin(\alpha w) + B \cos(\alpha w)$$

where A and B are constants. Using the boundary condition $Q(w) = Q(w + a)$ (where a is the period of the compactified dimension), one finds

$$\alpha = \frac{2n\pi}{a} \quad (1.5)$$

$$Q_n(w) = A_n \sin\left(\frac{2n\pi w}{a}\right) + B_n \cos\left(\frac{2n\pi w}{a}\right) \quad (1.6)$$

where $n \in \mathbb{Z}$. Inserting the value of α , (1.5), into the R equation, (1.4a), yields

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) - \frac{4n^2\pi^2}{a^2} R = 0 \quad (1.7)$$

Using the substitution $u(r) = rR(r)$ such that $\frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) = r \frac{d^2u}{dr^2}$, the equation is transformed to

$$\frac{d^2u}{dr^2} - \frac{4n^2\pi^2}{a^2} u = 0 \quad (1.8)$$

which has a general solution

$$u(r) = C_1 e^{2n\pi r/a} + C_2 e^{-2n\pi r/a}$$

Because the final form of the potential must satisfy $\lim_{r \rightarrow \infty} \Phi = 0$, C_1 must equal 0. The other constant, C_2 , can be absorbed into the constants in the Q equation. The final solution to (1.7) is thus

$$R_n(r) = \frac{u(r)}{r} = \frac{e^{-2n\pi r/a}}{r} \quad (1.9)$$

and now n must be restricted to non-negative integers. Combining (1.6) and (1.9), a particular solution to the PDE, (1.1), is thus

$$\Phi_n(r, w) = R_n(r)Q_n(w) = \frac{e^{-2n\pi r/a}}{r} \left[A_n \sin\left(\frac{2n\pi w}{a}\right) + B_n \cos\left(\frac{2n\pi w}{a}\right) \right]$$

The general solution is the linear combination of all the particular solutions, i.e.

$$\Phi(r, w) = \sum_{n=0}^{\infty} \frac{e^{-2n\pi r/a}}{r} \left[A_n \sin\left(\frac{2n\pi w}{a}\right) + B_n \cos\left(\frac{2n\pi w}{a}\right) \right] \quad (1.10)$$

This solution is valid for all points in space except the origin. To find the unique solution to Poisson's equation, (ii.2), we set our solution, (1.10), equal to the right side of (ii.2) to yield

$$\sum_{n=0}^{\infty} \frac{e^{-2n\pi r/a}}{r} \left[A_n \sin\left(\frac{2n\pi w}{a}\right) + B_n \cos\left(\frac{2n\pi w}{a}\right) \right] = -\frac{e}{4\pi a r^2 \epsilon_0} \delta(r) \delta(w/a) \quad (1.11)$$

To find the value of these constants, we use the orthogonality of sines and cosines. We multiply both sides of (1.11) by $\cos\left(\frac{2n'\pi w}{a}\right)$ and integrate over all space, i.e. limits $r \in [0, \infty)$, $\theta \in [0, \pi)$, $\phi \in [0, 2\pi)$, and $w \in [-a/2, a/2)$. The volume element in this space is $r^2 \sin(\theta) dr d\theta d\phi dw$. Performing the integration, all terms except when $n = n'$ cancel out, and we find

$$B_n = \frac{2\pi n^2 e}{a^3 \epsilon_0}$$

Performing the same operation on (1.11), using a sine instead of a cosine, we find

$$A_n = 0$$

and thus

$$\Phi(r, w) = \sum_{n=1}^{\infty} \frac{2\pi n^2 e}{a^3 \epsilon_0} \cos\left(\frac{2n\pi w}{a}\right) \frac{e^{-2n\pi r/a}}{r} \quad (1.12)$$

where the $n = 0$ term can be dropped. To transform this potential into the potential energy, V , of a particle in the vicinity of this point charge, we multiply by the charge of that particle, which in our case is an electron with charge $-e$. We thus find for the potential energy of the electron,

$$V(r, w) = -\sum_{n=1}^{\infty} \frac{2\pi n^2 e^2}{a^3 \epsilon_0} \cos\left(\frac{2n\pi w}{a}\right) \frac{e^{-2n\pi r/a}}{r} \quad (1.13)$$

It can be shown [See Appendix A] that this infinite sum can be written in closed form as

$$V(r, w) = -\frac{\pi e^2}{4a^3 \epsilon_0 r} \left[\coth\left(\frac{\pi}{a}(r - iw)\right) \operatorname{csch}^2\left(\frac{\pi}{a}(r - iw)\right) + \coth\left(\frac{\pi}{a}(r + iw)\right) \operatorname{csch}^2\left(\frac{\pi}{a}(r + iw)\right) \right] \quad (1.14)$$

The expression is periodic in the w -direction with period a , and the radial part of the potential

resembles the three-dimensional $-1/r$ potential in form. These characteristics will be utilized in forming a variational function; for performing the actual calculations, however, we revert back to the series form of the potential.

In five dimensions

In five dimensions, the process of determining the potential energy is nearly identical to the four-dimensional case. Poisson's equation in five dimensions, (ii.3) is reduced to Laplace's equation in five dimensions,

$$\left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{a^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{a^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \Phi(r, w) = 0 \quad (1.15)$$

The solution of this equation is found using the same method used in four dimensions—separation of variables. When the equation is separated, we find

$$\frac{a^2}{r^2 R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) = \ell(\ell + 1) \quad (1.16a)$$

$$\frac{1}{Y \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} = -\ell(\ell + 1) \quad (1.16b)$$

The angular equation, (1.16b), is recognized to be the differential equation corresponding to spherical harmonics,

$$Y_\ell^m(\theta, \phi) = \sqrt{\frac{(2\ell + 1)(\ell - |m|)!}{4\pi(\ell + |m|)!}} \cdot e^{im\phi} P_\ell^m(\cos \theta)$$

The solution to (1.16a) is found using the same u -substitution:

$$R(r) = A_{\ell m} \frac{e^{-\sqrt{\ell(\ell+1)}r/a}}{r}$$

where $A_{\ell m}$ is a normalization constant. The general solution to Laplace's equation in five dimensions is thus

$$\Phi(r, \theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} A_{\ell m} Y_\ell^m(\theta, \phi) \frac{e^{-\sqrt{\ell(\ell+1)}r/a}}{r} \quad (1.17)$$

Using the orthogonality of the spherical harmonics,

$$A_{\ell m} = \frac{\ell(\ell + 1)e}{a^4\epsilon_0}$$

and multiplying (1.17) by $-e$, the charge of the electron, we find

$$V(r, \theta, \phi) = - \sum_{\ell=1}^{\infty} \sum_{m=-\ell}^{\ell} \frac{\ell(\ell + 1)e^2}{a^4\epsilon_0} Y_{\ell}^m(\theta, \phi) \frac{e^{-\sqrt{\ell(\ell+1)}r/a}}{r} \quad (1.18)$$

Unlike the four-dimensional potential, this sum cannot be written in closed form. It still adheres to the requirements of periodicity in the compactified dimensions due to the spherical harmonic, and the radial part of the function resembles both the four-dimensional and three-dimensional radial potentials.

Four-dimensional ground state energy

Now that we have an expression for the potential energy of an electron in a Hydrogen atom with one compactified dimension (Equation 1.14), we can express the entire Hamiltonian in four dimensions:

$$H = T + V = -\frac{\hbar^2}{2\mu} \vec{\nabla}_4^2 - \sum_{n=1}^{\infty} \frac{2\pi n^2 e^2}{a^3 \epsilon_0} \cos\left(\frac{2n\pi w}{a}\right) \frac{e^{-2n\pi r/a}}{r} \quad (2.1)$$

We are now faced with the task of using this Hamiltonian to find an upper bound on the ground state energy of the atom. To do this, we must develop a reasonable guess for the form of the ground state wavefunction based on the shape of the potential.

First we assume that the trial wavefunction, ϕ , is separable, i.e. $\phi(r, w) = R(r)Q(w)$. The r portion of the potential closely resembles a 3-dimensional $-1/r$ potential. This is a strong indicator that the radial part of the 4-dimensional ground state wavefunction will take approximately the same form as the 3-dimensional ground state wavefunction,

$$\psi_{100}(r, \theta, \phi) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

where a_0 is the Bohr radius. Any change in the wavefunction can likely be accounted for by a multiplicative constant or by modifying the scaling factor in the exponential term. We therefore assume that the radial part of the wavefunction takes the form

$$R(r) = A e^{-\beta r}$$

where A is a normalization constant and β is a parameter that will later be minimized.

Periodic trial function

Since the potential is periodic in the w direction, we first try a wavefunction that is also periodic. Absorbing normalization constants into the radial part of the equation, we assume the w part of

the wavefunction takes the form

$$Q(w) = e^{i\alpha w}$$

where α is another parameter.

Combining Q and R ,

$$\phi(r, w) = Ae^{i\alpha w}e^{-\beta r}$$

Asserting that $\langle \phi | \phi \rangle = 1$ (i.e. ϕ is normalized) forces $A = \sqrt{\frac{\beta^3}{\pi a}}$, and thus

$$\phi(r, w) = \sqrt{\frac{\beta^3}{\pi a}} e^{i\alpha w} r e^{-\beta r} \quad (2.2)$$

Using the normalized trial function, (2.2), we now compute $\tilde{E} = \langle \phi | H | \phi \rangle$, where H is defined in (2.1). The integral can be split up into two separate integrals,

$$\langle \phi | H | \phi \rangle = \langle \phi | T + V | \phi \rangle = \langle \phi | T | \phi \rangle + \langle \phi | V | \phi \rangle$$

The first integral represents the expectation value of the kinetic energy of the particle, and the second integral represents the expectation value of the potential energy. The kinetic energy integral is rather straightforward to compute:

$$\begin{aligned} \langle \phi | T | \phi \rangle &= -\frac{\hbar^2 \beta^3}{2\pi a \mu} \int_{-a/2}^{a/2} \int_0^\infty \int_0^{2\pi} \int_0^\pi e^{-i\alpha w} e^{-\beta r} \vec{\nabla}_4^2 \left[e^{i\alpha w} e^{-\beta r} \right] r^2 \sin(\theta) d\theta d\phi dr dw \\ &= -\frac{2\beta^3 \hbar^2}{\mu} \int_0^\infty e^{-2\beta r} [\beta^2 r^2 - 2\beta r - r^2 \alpha^2] dr \\ &= -\frac{2\beta^3 \hbar^2}{\mu} \left[\frac{1}{8\beta} \Gamma(3) - \frac{1}{2\beta} \Gamma(2) - \frac{\alpha^2}{8\beta^3} \Gamma(3) \right] \\ &= \frac{\hbar^2}{2\mu} (\beta^2 + \alpha^2) \end{aligned} \quad (2.3)$$

where $\Gamma(x)$ is the Gamma function.

The potential energy integral, though, reveals a problem with the trial function, (2.2). Because the w part of the function is a complex exponential, it cancels with its complex conjugate and leaves

only the potential to be integrated in the w dimension:

$$\begin{aligned}\langle\phi|V|\phi\rangle &= -\frac{8\beta^3\pi e^2}{a^4\epsilon_0}\int_{-a/2}^{a/2}\int_0^\infty r e^{-2\beta r}\sum_{n=1}^\infty n^2\cos\left(\frac{2n\pi w}{a}\right)e^{-2n\pi r/a}dr dw \\ &= -\frac{8\beta^3\pi e^2}{a^4\epsilon_0}\sum_{n=1}^\infty n^2\int_{-a/2}^{a/2}\cos\left(\frac{2n\pi w}{a}\right)dw\int_0^\infty r e^{-2\beta r}e^{-2n\pi r/a}dr\end{aligned}$$

The w integral, for any $n \in \mathbb{Z}$, results in zero. The trial function then is forced to take some other form in order to contribute to the integral and avoid the zero. It can be checked that trying both sine and cosine as a trial function lead to the same result. Because of this, the possibility of a periodic trial function is eliminated (all periodic functions can be written as a linear combination of sines and cosines, called a Fourier expansion).

Non-periodic trial function

While a non-periodic function would seem to be less accurate than one that is periodic, the variational method does not require the most accurate function to yield relevant results. *Any* trial function can be used to provide an upper bound on the ground state energy, so long as the function is normalizable.

Many times the term “normalizable” is interpreted to mean that a function must approach the same finite value at positive infinity as it does at negative infinity, i.e.

$$\lim_{x \rightarrow \infty} f(x) = \lim_{x \rightarrow -\infty} f(x) = C$$

where C is some finite value. In actuality, though, all that is required for the function to be normalizable is that the function satisfies the boundary condition that its value at both extremes of the domain equals the same finite number. Usually the extremes of a function’s domain are $x = \pm\infty$. In the case of our compactified dimension, however, the extremes of the domain are just $w = \pm a/2$; the behavior of the function at the infinities is irrelevant. Any function, $Q(w)$, that satisfies the condition $Q(-a/2) = Q(a/2)$ can thus be used as a trial function. One such function is an inverted parabola of the form $Q = -C_1 w^2 + C_2$, or (if we so choose) $Q = C_2(1 - C_1' w^2)$, where C_2 functions as a normalization constant and C_1' is the variational parameter. The revised trial

function is thus (after normalization):

$$\phi(r, w) = \sqrt{\frac{240\beta^3}{\pi(240a - 40\alpha a^3 + 3\alpha^2 a^5)}} \cdot (1 - \alpha w^2)e^{-\beta r} \quad (2.4)$$

We attempt to compute $\tilde{E} = \langle \phi | H | \phi \rangle$, again calculating the kinetic and potential integrals separately.

The kinetic energy integral, though a little more complicated this time, is again straightforward to compute:

$$\begin{aligned} \langle \phi | T | \phi \rangle &= -\frac{A^2 \hbar^2}{2\mu} \cdot 4\pi \int_{-a/2}^{a/2} \int_0^\infty (1 - \alpha w^2) e^{-\beta r} \vec{\nabla}_4^2 \left[(1 - \alpha w^2) e^{-\beta r} \right] r^2 dr dw \\ &= -\frac{2A^2 \hbar^2 \pi}{\mu} \left[\int_{-a/2}^{a/2} (1 - \alpha w^2)^2 dw \int_0^\infty e^{-2\beta r} (\beta^2 r^2 - 2\beta r) dr \right. \\ &\quad \left. - 2\alpha \int_{-a/2}^{a/2} (1 - \alpha w^2) dw \int_0^\infty r^2 e^{-2\beta r} dr \right] \\ &= -\frac{2A^2 \hbar^2 \pi}{\mu} \left[\frac{240a - 40\alpha a^3 + 3\alpha^2 a^5}{240} \left(\frac{1}{8\beta} \Gamma(3) - \frac{1}{2\beta} \Gamma(2) \right) \right. \\ &\quad \left. - 2\alpha \cdot \frac{12a - \alpha a^3}{12} \cdot \frac{1}{8\beta^3} \Gamma(3) \right] \\ &= -\frac{2A^2 \hbar^2 \pi}{\mu} \left[\frac{240a - 40\alpha a^3 + 3\alpha^2 a^5}{240} \left(-\frac{1}{4\beta} \right) - \frac{12\alpha a - \alpha^2 a^3}{24\beta^3} \right] \\ &= \frac{\hbar^2}{2\mu} \left[\beta^2 + \frac{40\alpha(12 - \alpha a^2)}{240 - 40\alpha a^2 + 3\alpha^2 a^4} \right] \quad (2.5) \end{aligned}$$

Comparing the results, (2.3) and (2.5), altering the trial function has only changed the term dependent on α , the constant associated with the w direction.

The potential energy integral itself, $\langle \phi | V | \phi \rangle$, is straightforward to compute as well, but integrating does not yield a summable expression. Because of this, some approximating will be necessary. The

integral is as follows:

$$\begin{aligned}
\langle \phi | V | \phi \rangle &= -\frac{8A^2\pi^2e^2}{a^3\epsilon_0} \int_0^\infty \int_{-a/2}^{a/2} (1-\alpha w^2)^2 r e^{-2\beta r} \sum_{n=1}^\infty n^2 \cos\left(\frac{2n\pi w}{a}\right) e^{-2n\pi r/a} dw dr \\
&= -\frac{8A^2\pi^2e^2}{a^3\epsilon_0} \sum_{n=1}^\infty n^2 \int_0^\infty r e^{-2(\beta-n\pi/a)r} dr \int_{-a/2}^{a/2} (1-\alpha w^2)^2 \cos\left(\frac{2n\pi w}{a}\right) dw \\
&= -\frac{8A^2\pi^2e^2}{a^3\epsilon_0} \sum_{n=1}^\infty n^2 \left[\frac{a^2}{4(a\beta+n\pi)^2} \right] \left[\frac{(-1)^n}{4n^4\pi^4} (n^2\pi^2\alpha^2a^5 - 4n^2\pi^2\alpha a^3 - 6\alpha^2a^5) \right] \\
&= -\frac{A^2e^2a^2\alpha}{2\pi^2\epsilon_0} \sum_{n=1}^\infty \frac{n^2(-1)^n}{(a\beta+n\pi)^2} \left[\frac{\pi^2\alpha a^2}{n^2} - \frac{4\pi^2}{n^2} - \frac{6\alpha a^2}{n^4} \right] \\
&= -\frac{A^2e^2a^2\alpha}{2\pi^2\epsilon_0} \left[\pi^2(\alpha a^2 - 4) \sum_{n=1}^\infty \frac{(-1)^n}{(a\beta+n\pi)^2} - 6\alpha a^2 \sum_{n=1}^\infty \frac{(-1)^n}{n^2(a\beta+n\pi)^2} \right] \tag{2.6}
\end{aligned}$$

We call the first infinite series S_1 and the second one S_2 . To approximate the two infinite series, we refer to the three-dimensional Hydrogen atom. In the 3-D case, $\beta = 1/a_0$, where a_0 is the Bohr radius, comparable to 10^{-10} m. Because a_0 is in the denominator, β is an extremely large number. On the other hand a , defined as the ‘‘circumference’’ of the compactified dimension, will more than likely be a very small number—even smaller than the Bohr radius. In fact, the hypothesis that the dimension is extremely small is one of the driving forces of this research. Assuming that $a < a_0$ means the value $a\beta$ is restrained to the interval $(0, 1)$, as long as β is not changed much from the 3-D case.

To approximate the series, we plot the first 100 terms of each series for values of $a\beta$ ranging from 0 to 1. We then use a curve fitting procedure to express the series as functions of $a\beta$, i.e. S_1 and S_2 are approximated to become $S_1(a\beta)$ and $S_2(a\beta)$. A FORTRAN program [See Appendix B] is used to approximate the series and return data points. Running the program and plotting the results in gnuplot [See Figure 3] shows $S_1(a\beta)$ and $S_2(a\beta)$ appear nearly linear for very small values of $a\beta$ and curve away from the line for larger values. Though a linear approximation breaks down for larger values, we make the reasonable assumption that a will not be as large as a_0 , the Bohr radius, but rather many times smaller than a_0 , so the linear approximation will be reasonable for those values, as shown in the insets of the graphs below.

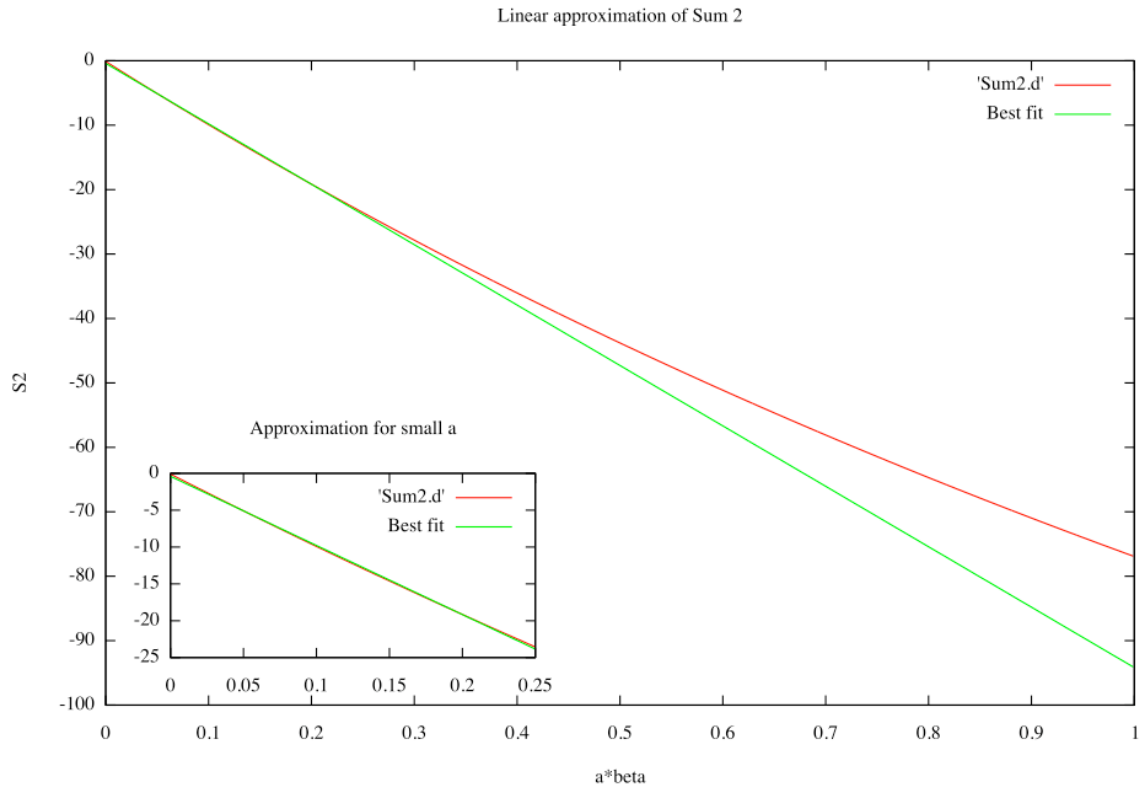
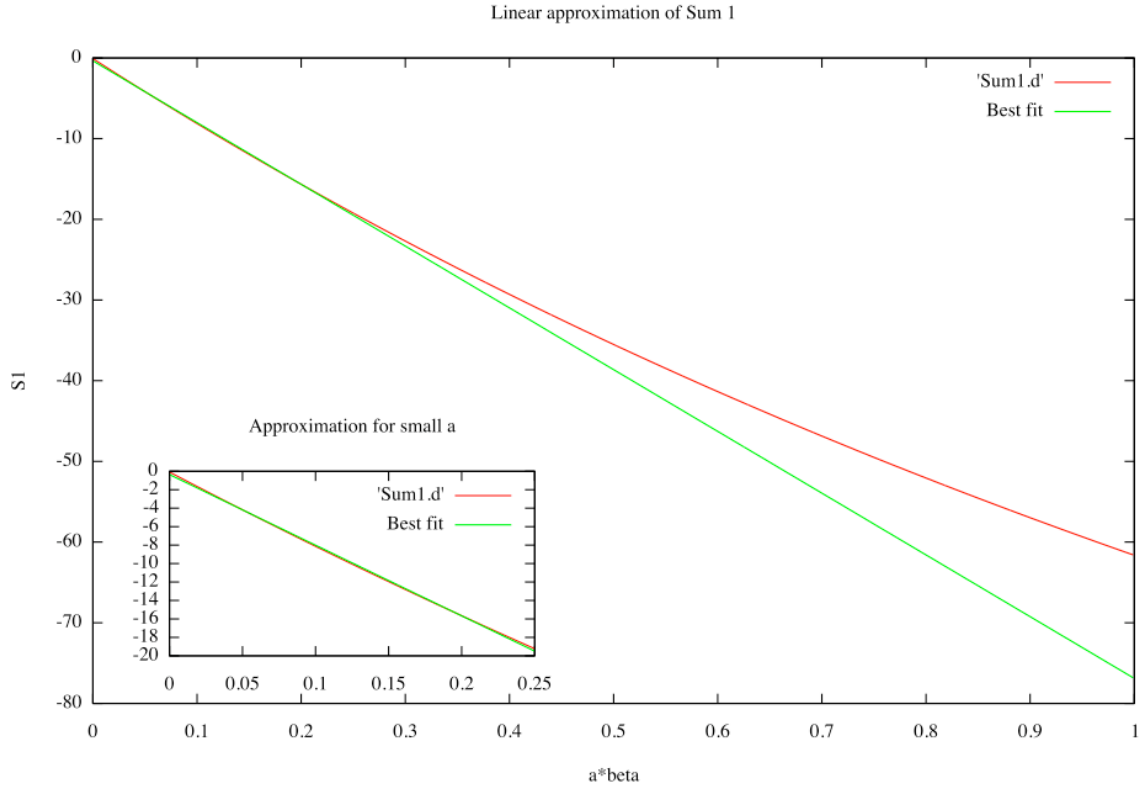


Figure 3: Graph of the first 100 terms of S_1 and S_2 as functions of $a\beta$

The lines of best fit (for small a) of S_1 and S_2 are [See Appendix B]

$$S_1(a\beta) = -76.5427a\beta - 0.356926 \quad (2.7)$$

$$S_2(a\beta) = -93.7695a\beta - 0.406147 \quad (2.8)$$

Plugging (2.7) and (2.8) into (2.6) yields

$$\begin{aligned} \langle \phi | V | \phi \rangle &\approx -\frac{120e^2\beta^3 a\alpha}{\pi^3\epsilon_0(240 - 40\alpha a^2 + 3\alpha^2 a^5)} \left[\pi^2(\alpha a^2 - 4)(-76.5427a\beta - 0.356926) \right. \\ &\quad \left. - 6\alpha a^2(-93.7695a\beta - 0.406147) \right] \\ &= -\frac{\hbar^2}{\mu} \underbrace{\left[\frac{480\alpha a}{\pi^2 a_0(240\dots)} \right]}_{=C} \left[\pi^2(\alpha a^2 - 4)(-76.5427a\beta^4 - 0.356926\beta^3) \right. \\ &\quad \left. - 6\alpha a^2(-93.7695a\beta^4 - 0.406147\beta^3) \right] \\ &= \frac{\hbar^2\beta^4}{\mu} [76.5427aC\pi^2(\alpha a^2 - 4) - 562.617C\alpha a^3] \\ &\quad + \frac{\hbar^2\beta^3}{\mu} [.356926C\pi^2(\alpha a^2 - 4) - 2.436882C\alpha a^2] \quad (2.9) \end{aligned}$$

Combining the kinetic expectation, (2.5), and the potential expectation, (2.9), we now have a full expression for an upper bound on the ground state energy of a Hydrogen atom in four dimensions,

$$\begin{aligned} \tilde{E} &= \frac{\hbar^2}{\mu} \left[\beta^4 [76.5427aC\pi^2(\alpha a^2 - 4) - 562.617C\alpha a^3] \right. \\ &\quad \left. + \beta^3 [.356926C\pi^2(\alpha a^2 - 4) - 2.436882C\alpha a^2] \right. \\ &\quad \left. + \frac{\beta^2}{2} + \frac{20\alpha(12 - \alpha a^2)}{(240 - 40\alpha a^2 + 3\alpha^2 a^5)} \right] \quad (2.10) \end{aligned}$$

Minimizing the variational energy

Now that an expression for an upper bound on the ground state energy, we minimize it with respect to the parameters α and β to get as close to the actual ground state energy as possible. The equation can be minimized in β by hand. After factoring and cancelling a factor of \hbar^2/μ , the β -minimization expression is

$$\begin{aligned} \frac{\partial \tilde{E}}{\partial \beta} = & \beta^3 [306.1708aC\pi^2(\alpha a^2 - 4) - 2250.468C\alpha a^3] \\ & + \beta^2 [1.070778C\pi^2(\alpha a^2 - 4) - 7.310976C\alpha a^2] + \beta = 0 \end{aligned}$$

which is a simple quadratic that can be solved using the quadratic formula.

Minimizing in α , however is not as easy. To minimize the equation, we again make use of FORTRAN and gnuplot. We numerically calculate \tilde{E} , using 1000 points of α from 0 to 10 and 1000 points of a from 0 to a_0 , giving a total of 1 million points. We take the minimum of the curve at each step in a [See Appendix B] and find a line of best fit for the resulting data. This line of best fit is denoted $\tilde{E}_{min}(a)$ and has the form $\tilde{E}_{min}(a) = -A/a^n$, where A and n are constants. We use the sequence in Appendix C to fit the constants and find

$$A = 4.03532 \times 10^{-16}$$

$$n = 2$$

The final, minimized expression for an upper bound on the ground state energy of a Hydrogen atom in four dimensions is

$$\tilde{E}_{min}(a) = -4.03532 \times 10^4 \frac{\hbar^2}{\mu a^2} = -4.92922 \times 10^{-34} \cdot \frac{1}{a^2} \quad (2.11)$$

Five-dimensional ground state energy

With the four-dimensional case complete, we now focus on the five-dimensional ground state before comparing and contrasting the results. Combining the kinetic energy, $\hat{p}^2/2m$, with the potential energy function found in Equation 1.18, we can write the entire 5-D Hamiltonian:

$$H = -\frac{\hbar^2}{2\mu} \vec{\nabla}_5^2 - \sum_{\ell=1}^{\infty} \sum_{m=-\ell}^{\ell} \frac{\ell(\ell+1)e^2}{a^4\epsilon_0} Y_{\ell}^m(\theta, \phi) \frac{e^{-\sqrt{\ell(\ell+1)}r/a}}{r} \quad (3.1)$$

We again assume that the trial function is separable and that the radial part will closely resemble the 3-D ground state. Because the potential itself includes spherical harmonics (and because the integral will work out nicely), we choose the angular part of our trial function to be another spherical harmonic. Because we do not want a factor of a^2 floating around from the volume element, we also choose to divide the trial function by a factor of a so that when it is squared, it cancels with the volume element. Our trial function is thus taken to be

$$\phi(r, \theta, \phi) = \sqrt{\frac{\beta^3}{\pi}} e^{-\beta r} \frac{Y_{\ell}^m(\theta, \phi)}{a} \quad (3.2)$$

where the function has been normalized.

Kinetic energy

The expectation value of the kinetic energy can then be found by integrating

$$\begin{aligned} \langle \phi | T | \phi \rangle &= \underbrace{-\frac{\beta^3 \hbar^2}{2\pi a^2 \mu} \cdot 4\pi}_{=A} \int_0^{\infty} \int_0^{\pi} \int_0^{2\pi} e^{-\beta r} (Y_{\ell}^m)^* \vec{\nabla}_5^2 [e^{-\beta r} Y_{\ell}^m] r^2 \sin \theta \, dr \, d\theta \, d\phi \\ &= A \left[\int e^{-2\beta r} |Y|^2 dV - \int e^{-2\beta r} \cdot \frac{2\beta}{r} |Y|^2 dV + \int \frac{e^{-2\beta r}}{a^2} Y \frac{\partial^2 Y}{\partial \theta^2} dV \right. \\ &\quad \left. + \int \frac{e^{-2\beta r}}{a^2} Y \frac{\partial Y}{\partial \theta} \cot \theta dV + \int \frac{e^{-2\beta r}}{a^2} Y \frac{\partial^2 Y}{\partial \phi^2} \csc^2 \theta dV \right] \end{aligned}$$

The first and second integrals are relatively easy, producing a combined result of

$$I_1 + I_2 = -\frac{1}{4\beta} \quad (3.3)$$

For the third integral, we make use of the identity

$$\begin{aligned} \frac{\partial^2 Y_\ell^m}{\partial \theta^2} &= m(m \cot^2 \theta - \csc^2 \theta) Y_\ell^m + \sqrt{(\ell - m)(\ell + m + 1)(2m + 1)} e^{-i\phi} \cot \theta Y_\ell^{m+1} \\ &\quad + \sqrt{(\ell - m)(\ell - m - 1)(\ell + m + 1)(\ell + m + 2)} e^{-2i\phi} Y_\ell^{m+2} \end{aligned}$$

and realize that when the last two terms are integrated against another Y_ℓ^m , they vanish. Thus the third integral becomes

$$I_3 = \frac{m^2}{4\beta^3 a^2} \int_0^{2\pi} \int_0^\pi |Y|^2 \frac{\cos^2 \theta}{\sin \theta} d\theta d\phi - \frac{m}{4\beta^3 a^2} \int_0^{2\pi} \int_0^\pi |Y|^2 \csc \theta d\theta d\phi \quad (3.4)$$

The fourth integral makes use of the identity

$$\frac{\partial Y_\ell^m}{\partial \theta} = m \cot \theta Y_\ell^m + \sqrt{(\ell - m)(\ell + m + 1)} e^{-i\phi} Y_\ell^{m+1}$$

where again the second term vanishes when integrated. Thus the fourth integral becomes

$$I_4 = \frac{m}{4\beta^3 a^2} \int_0^{2\pi} \int_0^\pi |Y|^2 \frac{\cos^2 \theta}{\sin \theta} d\theta d\phi \quad (3.5)$$

Finally, the fifth integral uses the identity

$$\frac{\partial^2 Y_\ell^m}{\partial \phi^2} = -m^2 Y_\ell^m$$

so it becomes

$$I_5 = -\frac{m^2}{4\beta^3 a^2} \int_0^{2\pi} \int_0^\pi |Y|^2 \csc \theta d\theta d\phi \quad (3.6)$$

Adding up all the integrals, (3.3) + (3.4) + (3.5) + (3.6), we find

$$\begin{aligned}
\langle T \rangle &= \frac{A}{4\beta^3} \left[-\beta^2 + \frac{m(m+1)}{a^2} \left(\int |Y|^2 \frac{\cos^2 \theta}{\sin \theta} - \int |Y|^2 \csc \theta \right) \right] \\
&= \frac{\hbar^2}{2\mu} \left[\beta^2 - \frac{m(m+1)}{a^2} \left(\int |Y|^2 \csc \theta - \int |Y|^2 \sin \theta - \int |Y|^2 \csc \theta \right) \right] \\
&= \frac{\hbar^2}{2\mu} \left[\beta^2 + \frac{m(m+1)}{a^2} \right]
\end{aligned} \tag{3.7}$$

Potential energy

Now, we examine the expectation value of the potential energy function, (1.18). We find

$$\begin{aligned}
\langle \phi | V | \phi \rangle &= -\frac{\beta^3}{\pi} \frac{4\pi a^2}{a^2} \sum_{\ell', m'} \frac{\ell'(\ell'+1)e^2}{a^4 \epsilon_0} \iiint e^{-\beta r} (Y_{\ell'}^m)^* \left[\frac{e^{\sqrt{\ell'(\ell'+1)}r/a}}{r} Y_{\ell'}^{m'} \right] e^{-\beta r} Y_{\ell'}^m r^2 \sin \theta \, dr \, d\theta \, d\phi \\
&= -\frac{(-1)^m 4\beta^3 e^2}{a^2 \epsilon_0} \sum_{\ell', m'} \frac{\ell'(\ell'+1)}{(2\beta a + \sqrt{\ell'(\ell'+1)})^2} \iint Y_{\ell'}^{-m} Y_{\ell'}^{m'} Y_{\ell'}^m d\Omega \\
&= \frac{(-1)^{m+1} 2\beta^3 e^2}{a^2 \epsilon_0 \sqrt{\pi}} (2\ell+1) \sum_{\ell', m'} \frac{\ell'(\ell'+1)}{(2\beta a + \sqrt{\ell'(\ell'+1)})^2} \sqrt{2\ell'+1} \begin{pmatrix} \ell & \ell' & \ell \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell & \ell' & \ell \\ -m & m' & m \end{pmatrix}
\end{aligned}$$

where the integral of three spherical harmonics gives rise to the symbols at the end of the last step, known as Wigner 3-j symbols or just 3-j symbols. The 3-j symbols are related to Klebsch-Gordon coefficients and follow the same selection rules, i.e. for a generic 3-j symbol $\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix}$, the result is zero unless

1. $d + e + f = 0$
2. $|a - b| \leq c \leq a + b$
3. $a + b + c$ is even

Applying these conditions forces $m' = 0$ and $\ell' \in (0, 2\ell] \cap 2\mathbb{Z}$. The 3-j symbols are also invariant among even permutations, so the final expression for $\langle V \rangle$ is

$$\frac{(-1)^{m+1} 2\beta^3 e^2}{a^2 \epsilon_0 \sqrt{\pi}} (2\ell+1) \sum_{\substack{\ell'=2 \\ \ell' \text{ even}}}^{2\ell} \frac{\ell'(\ell'+1)}{(2\beta a + \sqrt{\ell'(\ell'+1)})^2} \sqrt{2\ell'+1} \begin{pmatrix} \ell & \ell' & \ell' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell & \ell' & \ell' \\ m & -m & 0 \end{pmatrix} \tag{3.8}$$

Unlike in four dimensions, we cannot approximate this sum because there are no reasonable general

formulas for both 3-j symbols. We thus choose several special cases ($\ell = 1, 2, 3$) and examine each case individually.

Equation (3.8) when $\ell = 1$ only includes a single term from the sum. Looking up the values of the 3-j symbols, the expectation value of the potential energy when $\ell = 1$ is found to be

$$\langle V \rangle = \frac{(-1)^{m+1}}{(1-m)!(1+m)!} \frac{24e^2}{\sqrt{5\pi}a^2\epsilon_0} \frac{\beta^3}{(2\beta a + \sqrt{6})^2} \quad (3.9)$$

and using the identity $\frac{e^2}{\epsilon_0} = \frac{4\pi\hbar^2}{\mu a_0}$, we can write the entire variational energy with a leading factor of $\frac{\hbar^2}{2\mu}$. We use the notation \tilde{E}_ℓ^m to mean the variational energy at a specific ℓ and m .

$$\tilde{E}_1^m = \frac{\hbar^2}{2\mu} \left[\beta^2 + \frac{m(m+1)}{a^2} + \frac{(-1)^{m+1}}{(1-m)!(1+m)!} \frac{192\pi}{\sqrt{5\pi}a^2a_0} \frac{\beta^3}{(2\beta a + \sqrt{6})^2} \right] \quad (3.10)$$

When $\ell = 1$, m can be $-1, 0$, or 1 . We use the program in Appendix C to minimize each case with respect to the parameter β and observe that only $m = 0$ gives negative (i.e. bound) energies. The $\ell = 1, m = 0$ energy graph is shown in Figure 4, and the $\ell = 0, m = \pm 1$ energy graph is shown in Figure 5.

The $\ell = 2$ case contains two terms from the sum, and the variational energy can be written

$$\begin{aligned} \tilde{E}_2^m = \frac{\hbar^2}{2\mu} \left[\beta^2 + \frac{m(m+1)}{a^2} + \frac{480\pi(m^2-2)}{7\sqrt{5\pi}a^2a_0} \frac{\beta^3}{(2\beta a + \sqrt{6})^2} \right. \\ \left. + \frac{(-1)^{m+1}}{(2-m)!(2+m)!} \frac{7680\pi}{7\sqrt{\pi}a^2a_0} \frac{\beta^3}{(2\beta a + \sqrt{20})^2} \right] \quad (3.11) \end{aligned}$$

The choices for m range from -2 to 2 in integer steps, all of which are minimized using FORTRAN. We observe that again only $m = 0$ gives negative energies while $m = \pm 1, \pm 2$ gives positive, unbounded energies. The graph of the bounded energy ($m = 0$) is shown in Figure 4, and the graphs of the unbounded energies are shown in Figure 5.

We finally find the energy corresponding to $\ell = 3$ and minimize all possibilities of m from -3 to 3 .

The energy expression is

$$\begin{aligned} \tilde{E}_3^m = \frac{\hbar^2}{2\mu} & \left[\beta^2 + \frac{m(m+1)}{a^2} + \frac{32\pi(m^2-4)}{\sqrt{5\pi a^2 a_0}} \frac{\beta^3}{(2\beta a + \sqrt{6})^2} \right. \\ & + \frac{(-1)^m}{(3-m)!(3+m)!} \frac{7680\pi(11m^2-9)}{11\sqrt{13\pi a^2 a_0}} \frac{\beta^3}{(2\beta a + \sqrt{20})^2} \\ & \left. + \frac{(-1)^{m+1}}{(3-m)!(3+m)!} \frac{806400\pi}{11\sqrt{13\pi a^2 a_0}} \frac{\beta^3}{(2\beta a + \sqrt{42})^2} \right] \end{aligned} \quad (3.12)$$

We observe a difference between the $\ell = 3$ case and the previous two. Not only does $m = 0$ produce negative energies but also $m = \pm 2$. Positive energies are still produced when $m = \pm 1, \pm 3$. Again, the bounded energies are displayed in Figure 4, and the unbounded energies in Figure 5.

We use gnuplot to find a line of best fit for the bounded energies. Using the procedure in Appendix C, we find that the energy curves corresponding to each bounded energy state are

$$(\tilde{E}_1^0)_{min} = -19661.4 \cdot \frac{1}{a^2} \quad (3.13a)$$

$$(\tilde{E}_2^0)_{min} = -32901.1 \cdot \frac{1}{a^2} \quad (3.13b)$$

$$(\tilde{E}_3^0)_{min} = -34931.7 \cdot \frac{1}{a^2} \quad (3.13c)$$

$$(\tilde{E}_3^{\pm 2})_{min} = -1665.82 \cdot \frac{1}{a^2} \quad (3.13d)$$

These numbers are *much* larger than the line of best fit found for the four-dimensional case, found in Equation (2.11), though the energies are still inversely proportional to the square of the size of the compactified dimension(s).

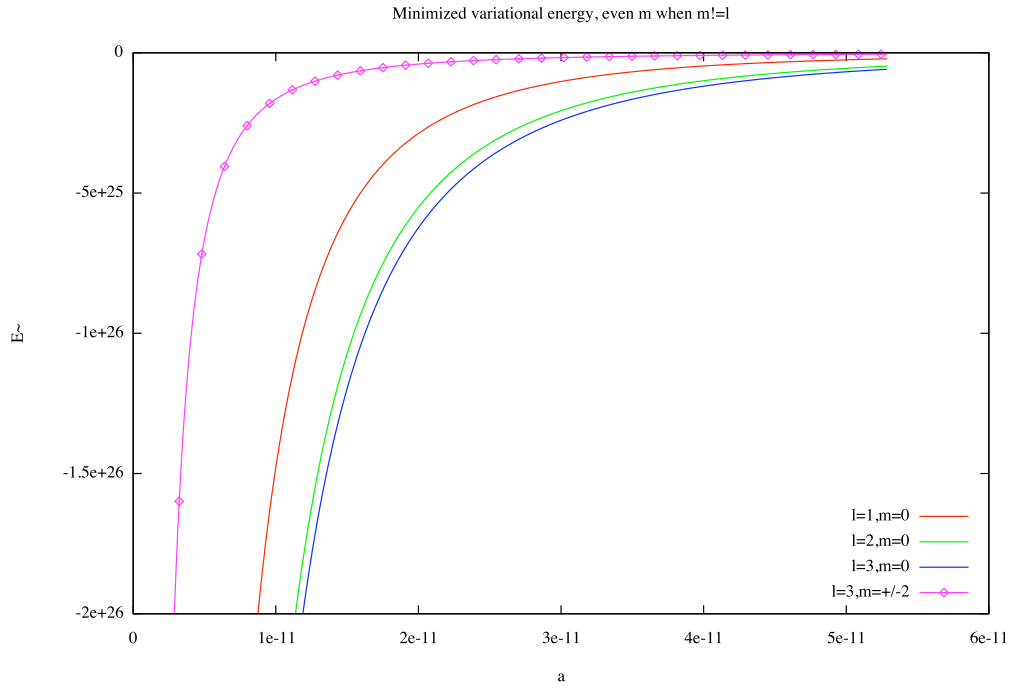


Figure 4: Only even m and $m \neq \ell$ yield negative, bounded energies. As ℓ increases, the energies become more negative, and as m increases (only one $m \neq 0$ is visible here), energies become less negative.

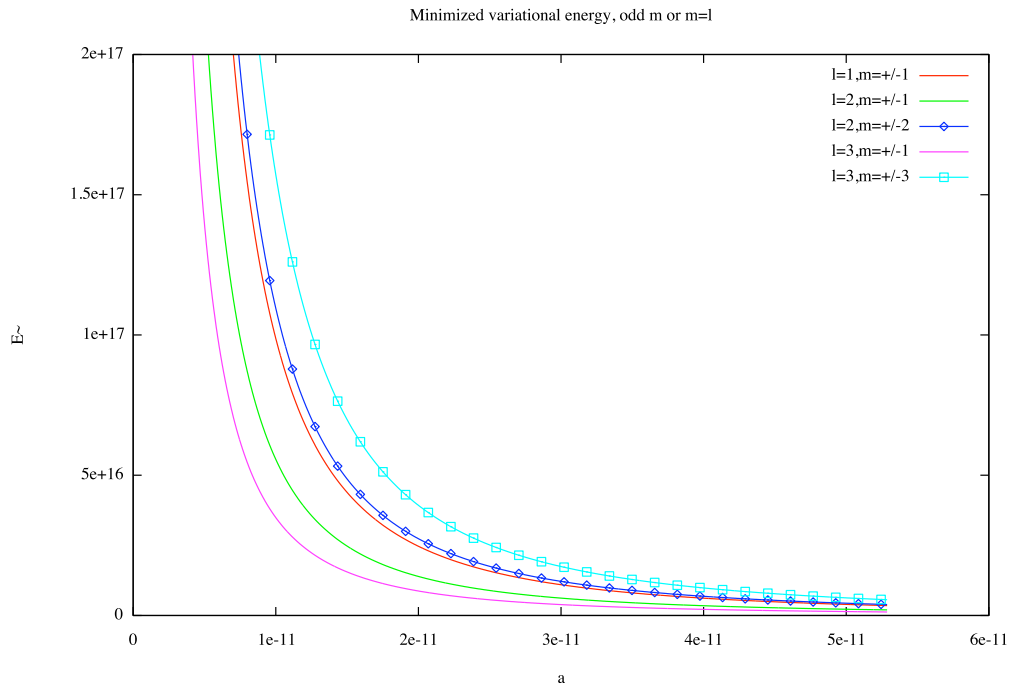


Figure 5: If m is odd or $m = \ell$, the variation produces positive, unbounded energies. As ℓ increases, the energies become less positive, and as m increases, it appears that energies become more positive.

Conclusions

From the variational method, the minimized ground state energy found in each case above is known to be an *upper bound* on the actual ground state energy of a four- or five-dimensional Hydrogen atom, E_G . That is,

$$\tilde{E}_{min} \geq E_G$$

E_G , however, is a quantity which can be directly measured in a lab, independent of the number of dimensions that exist in space; it is simply a scalar quantity with no dependence whatsoever. From numerous experiments in the lab, the ground state energy of a Hydrogen atom is known to be $E_G = -2.179 \times 10^{-18}$ J. It is worth noting that the three-dimensional solution to the Hydrogen atom problem predicts this number almost exactly. Because the four- and five-dimensional energies determined here are continuous functions of the size of the extra dimension(s), there is some value of a for which the energies found here will exactly match the measured ground state. Because our variational energy is just an upper bound, the relation will be an inequality that can be solved for a , thus yielding an expression for an upper bound on the size of the extra dimension(s).

Single compactified dimension

Setting the upper bound on the ground state energy of a Hydrogen atom with a single compactified dimension, found in Equation (2.11), equal to the experimentally verified ground state energy of an actual Hydrogen atom, we find

$$\tilde{E}_{min}(a) = -4.92922 \times 10^{-34} \cdot \frac{1}{a^2} \geq -2.179 \times 10^{-18} = E_G$$

$$a \leq 2.262 \times 10^{-16} \text{ m}$$

Recall that a corresponds to the circumference of the compactified dimension, so the radius of the dimension,

$$r_a \leq 3.600 \times 10^{-17} \text{ m} \tag{4.1}$$

which is about 1/24 the size of a proton's charge radius—*extremely* small.

To determine this number, all calculations were analytical until the determination of the expectation value of the potential energy, $\langle\phi|V|\phi\rangle$, when assumptions and approximations were necessary. The expectation value included an infinite sum that could not be written in closed form. Using FORTRAN and gnuplot, the sum was approximated as a linear function of a parameter $a\beta \in [0, 1]$. In order for the linear approximation to be reasonable, the assumption that the size of the compactified dimension, a , must be less than the Bohr radius, $a_0 = 0.529177 \times 10^{-10}$ m, was necessary. This assumption was reasonable since the driving force behind this research is that any compactified dimensions must be sufficiently small as to have not yet been detected.

When minimizing the energy produced by the variational method, more approximation was necessary. The energy expression could be minimized analytically in β , but it was not minimizable analytically in α , so FORTRAN and gnuplot were used again to determine the minimum. The result of the FORTRAN program was a function $\tilde{E}_{min}(a)$, which was approximated by a line of best fit in gnuplot. This line of best fit was then equated to the experimentally verified ground state energy of a Hydrogen atom and manipulated to yield an expression for the maximum size of the compactified dimension. The result of that manipulation is consistent with the assumption that the size of the dimension is smaller than the Bohr radius.

Though the result is valid, there is still room for improvement. A better trial function—perhaps one with more parameters or one that is not separated into radial and compactified parts—could be developed. It is also possible to determine a better approximation of the infinite series in the expectation value of the potential energy. One might use a quadratic or higher-order function rather than a linear function to produce more accurate results, or one might also fit the function specifically in the range of $a = 10^{-16}$ m to provide a better estimate. It is also possible to minimize the function more accurately in α , possibly using smaller steps in the FORTRAN program or by developing an entirely different method of minimization.

Two compactified dimensions

Unlike the four-dimensional case, the trial function used in five dimensions contained parameters ℓ and m itself which vary independent of the variational parameters. We thus took several special cases with small ℓ —specifically $\ell = 1, 2$, and 3 ($\ell = 0$ produces an energy of zero).

In the case of $\ell = 1$, we found that only the $m = 0$ state produced a negative energy for the atom. When $\ell = 2$, we found $m = 0$ gave a negative energy while $m = \pm 1, \pm 2$ produced positive energies. When $\ell = 3$, we found $m = 0, \pm 2$ gave negative energies while $m = \pm 1, \pm 3$ gave positive energies. As in four dimensions, we equate these minimized energy expressions with the experimentally verified ground state of Hydrogen to find an estimate of the upper bound on the size of the compactified 2-sphere. For each of the cases with negative energies, we find

$$\ell = 1, m = 0 \longrightarrow a \leq 9.499 \times 10^{10} \text{ m} \quad (4.2)$$

$$\ell = 2, m = 0 \longrightarrow a \leq 1.229 \times 10^{11} \text{ m} \quad (4.3)$$

$$\ell = 3, m = 0 \longrightarrow a \leq 1.266 \times 10^{11} \text{ m} \quad (4.4)$$

$$\ell = 3, m = \pm 2 \longrightarrow a \leq 2.765 \times 10^{10} \text{ m} \quad (4.5)$$

not *nearly* as small as the four-dimensional case, despite using nearly exactly the same method. In fact, more of this calculation was done analytically than in the four-dimensional case. The only margin for error in this calculation is the FORTRAN minimization and the gnuplot line of best fit. Perhaps a better method of minimization can be found, in which the function is analytically minimized in β (the resulting equation is a cubic polynomial) or in which a better step-method is developed. It may be beneficial to use a different trial function, possibly with more parameters. It is possible that the use of only one parameter in this case (as opposed to two in the four-dimensional case) greatly hindered accuracy, so including more parameters may lower these numbers to more reasonable levels. It may also be necessary to choose some other angular function than a spherical harmonic, although this could force a numerical approximation of the integrals involved.

Despite these possible sources of error, the method by which both the four- and five-dimensional energies were calculated is strikingly similar, so that leads to the conclusion that if a compactified

space takes on the metric of a 2-sphere as opposed to a circle, the size the compactified space could be without having yet been detected increases (though not likely by as much as these results suggest).

Other two-dimensional compactified spaces (e.g. a torus, two disjoint circles, or a multitude of other metrics) could produce different results, so that could possibly be explored in future research. Higher dimensional spaces such as a 3-sphere or a plethora of other metrics may be explored. The driving theory behind this exploratory research is that a six-dimensional compactified space should exist (according to string theory), but the problem is no one knows the structure of that space. Even in two dimensions, there are many different possible metrics, and the number of possibilities only grows with the addition of still more dimensions.

As we have given rough evidence for here, the presence of more compactified dimensions could even increase the maximum size of the compact space. It is also possible that other metrics may decrease the upper bound on dimensional size. There are many different setups that can be tested in the manner set forth here, providing for many more research opportunities in the area of compactified dimensions in a Hydrogen atom or other systems.

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Appendix A: Writing the 4-D potential in closed form

We now check to see if the series, (1.13), converges to a specific value and can be written in closed form. Combining all factors without an n into a multiplicative constant, $A = -\frac{2\pi e^2}{a^3 \epsilon_0 r}$, we find

$$V(r, w) = A \sum_{n=1}^{\infty} n^2 \cos\left(\frac{2n\pi w}{a}\right) e^{-2n\pi r/a}$$

The cosine function is only defined over the range $[-1, 1]$, so

$$S_1 = \sum_{n=1}^{\infty} \left| n^2 \cos\left(\frac{2n\pi w}{a}\right) e^{-2n\pi r/a} \right| \leq S_2 = \sum_{n=1}^{\infty} n^2 e^{-2n\pi r/a}$$

By the comparison test, if it can be shown that S_2 converges, S_1 must also converge. Using the ratio test on S_2 ,

$$\lim_{n \rightarrow \infty} \frac{(n+1)^2 e^{-2(n+1)\pi r/a}}{n^2 e^{-2n\pi r/a}} = \lim_{n \rightarrow \infty} \left(1 + \frac{1}{n}\right)^2 e^{-2\pi r/a} = e^{-2\pi r/a} < 1$$

so S_2 converges; therefore, S_1 must also converge.

To find the value to which S_1 converges, we write the cosine in terms of complex exponentials, i.e.,

$$V(r, w) = A \sum_{n=1}^{\infty} n^2 \left(\frac{e^{i2n\pi w/a} + e^{-i2n\pi w/a}}{2} \right) e^{-2n\pi r/a}$$

Combining the factor of $1/2$ into the constant A , such that A now equals $-\frac{\pi e^2}{a^3 \epsilon_0 r}$, we split the sum into two parts,

$$V(r, w) = A \left[\underbrace{\sum_{n=1}^{\infty} n^2 e^{\frac{2n\pi}{a}(iw-r)}}_{S_A} + \underbrace{\sum_{n=1}^{\infty} n^2 e^{-\frac{2n\pi}{a}(iw+r)}}_{S_B} \right] \quad (\text{A.1})$$

S_A and S_B can both be manipulated to resemble a geometric series, a series with a known sum.

$$\begin{aligned}
S_A &= \sum_{n=1}^{\infty} n^2 \left[\underbrace{e^{\frac{2\pi}{a}(iw-r)}}_x \right]^n = \sum_{n=1}^{\infty} (n^2 - n)x^n + \sum_{n=1}^{\infty} nx^n \\
&= x^2 \sum_{n=1}^{\infty} n(n-1)x^{n-2} + x \sum_{n=1}^{\infty} nx^{n-1} = x^2 \left(\frac{1}{1-x} \right)'' + x \left(\frac{1}{1-x} \right)' \\
&= -\frac{x(x+1)}{(x-1)^3}
\end{aligned} \tag{A.2}$$

The same method can be used to find

$$S_B = -\frac{y(y+1)}{(y-1)^3} \tag{A.3}$$

where $y = e^{-\frac{2\pi}{a}(iw+r)}$. Plugging (A.2) and (A.3) back into (A.1),

$$\begin{aligned}
V(r, w) &= A \left[-\frac{x(x+1)}{(x-1)^3} - \frac{y(y+1)}{(y-1)^3} \right] \\
&= -\frac{\pi e^2}{a^3 \epsilon_0 r} \left[-\frac{e^{\frac{2\pi}{a}(iw-r)} \left(e^{\frac{2\pi}{a}(iw-r)} + 1 \right)}{\left(e^{\frac{2\pi}{a}(iw-r)} - 1 \right)^3} - \frac{e^{-\frac{2\pi}{a}(iw+r)} \left(e^{-\frac{2\pi}{a}(iw+r)} + 1 \right)}{\left(e^{-\frac{2\pi}{a}(iw+r)} - 1 \right)^3} \right]
\end{aligned}$$

which can alternatively be written in the form

$$\begin{aligned}
V(r, w) &= -\frac{\pi e^2}{4a^3 \epsilon_0 r} \left[\coth\left(\frac{\pi}{a}(r-iw)\right) \operatorname{csch}^2\left(\frac{\pi}{a}(r-iw)\right) \right. \\
&\quad \left. + \coth\left(\frac{\pi}{a}(r+iw)\right) \operatorname{csch}^2\left(\frac{\pi}{a}(r+iw)\right) \right]
\end{aligned} \tag{A.4}$$

where $\coth(x)$ is the hyperbolic cotangent function, and $\operatorname{csch}(x)$ is the hyperbolic cosecant function.

Appendix B: Approximating infinite series in FORTRAN

When determining the upper bound on the ground state energy of a four dimensional atom, we use a Fortran program to calculate the first 100 terms of each series for 1000 values between $a\beta = 0$ and $a\beta = 1$. The program write the points to data files, 'Sum1.d' and 'Sum2.d', to be interpreted by gnuplot later. The program is written as follows:

```
PROGRAM Summation
  REAL::abeta,part1,part2,sum1,sum2
  INTEGER::i,j

  pi = 3.14159265358979
  sum1 = 0
  sum2 = 0

  OPEN(7,file='Sum1.d', status='unknown')
  OPEN(8,file='Sum2.d', status='unknown')
  DO i=1,1000
    abeta = .001*(i-1)
    DO j=1,100
      part1 = (-1)**j*(abeta+j*pi)**(-2)
      sum1 = sum1 + part1
      part2 = part1*j**(-2)
      sum2 = sum2 + part2
    END DO
    WRITE(7,*) abeta, sum1
    WRITE(8,*) abeta, sum2
  END DO
END PROGRAM Summation
```

A plot of the results can be seen in Figure 3.

To plot the results in gnuplot and determine a line of best fit for small a , the following sequence is used:

```
gnuplot> FIT_LIMIT = 1e-18
gnuplot> S1(abeta) = m*abeta+b
gnuplot> fit [0:0.25] S1(x) 'Sum1.d' via m,b
...
Final set of parameters          Asymptotic Standard Error
=====
m              = -76.5427        +/- 0.1057      (0.1381%)
b              = -0.356926       +/- 0.01528     (4.28%)
...
gnuplot> S2(abeta) = m*abeta+b
gnuplot> fit [0:0.25] S2(x) 'Sum2.d' via m,b
...
Final set of parameters          Asymptotic Standard Error
=====
m              = -93.7695        +/- 0.1179     (0.1258%)
b              = -0.406147       +/- 0.01704    (4.196%)
...
gnuplot> plot 'Sum1.d' w l, S1(x) title 'Best fit'
gnuplot> plot 'Sum2.d' w l, S2(x) title 'Best fit'
```

These values are then used to approximate the series in the expression, (2.6).

Appendix C: Minimizing variational energy using FORTRAN and gnuplot

To minimize the variational energy in four dimensions, (2.10), we represent the function numerically (without the prefactor \hbar^2/μ) and find a minimum at each of 1000 steps in a . The program writes the points to a file, 'Emin.d', and gnuplot is used to plot the points and find a line of best fit. The points are scaled by a factor of 10^{-20} to make them easier for gnuplot to handle. After determining a line of best fit, that prefactor is divided out. The program is as follows:

```
PROGRAM Minimization
  REAL*8,DIMENSION(2,1000)::E
  INTEGER::i,k
  REAL*8 min,tempmin,deltaa,deltaalpha,a,alpha
  REAL*8 g,c,Abeta,Bbeta,Cbeta,beta,Epart1,Epart2,Epart3,Epart4

  pi = 3.14159265358979D+0
  a_0 = 5.29177D-11
  h = 1.22085D-38
  E(1:2,1:1000) = 0.
  deltaa = 5.29177E-14
  deltaalpha = .01

  OPEN(7,file='Emin.d', status='unknown')

  DO i=2,1000
    a = deltaa*(real(i)-1)
    DO k=2,1000
      alpha = deltaalpha*(real(k)-1)
      g = 240. - 40.*alpha*a**2. + 3.*alpha**2.*a**4.
      c = 480.*a*alpha/(pi**2.*a_0*g)
      Abeta = 306.1708*a*c*pi**2.*(alpha*a**2.-4.)
      Abeta = Abeta-2250.468*c*alpha*a**3.
      Bbeta = 1.070778*c*pi**2.*(alpha*a**2.-4.)
      Bbeta = Bbeta-7.310967*c*alpha*a**2.
      Cbeta = 1.
      beta = abs((-Bbeta+sqrt(Bbeta**2.-4.*Abeta*Cbeta))/(2.*Abeta))

      Epart1 = 76.5427*a*c*pi**2.*(alpha*a**2.-4.)
      Epart1 = Epart1 - 562.617*c*alpha*a**3.
      Epart1 = Epart1*beta**4.
    
```



```

Epart2 = .356926*c*pi**2.*(alpha*a**2.-4.)
Epart2 = Epart2 - 2.436882*c*alpha*a**2.
Epart2 = Epart2*beta**3.
Epart3 = beta**2./2.
Epart4 = -20.*alpha*(12.-alpha*a**2)/g

tempmin = 1e-20*(Epart1+Epart2+Epart3+Epart4)

IF (k == 2) THEN
    min = tempmin
END IF
IF (tempmin <= min) THEN
    min = tempmin
    E(1,i) = a
    E(2,i) = min
END IF
END DO
WRITE(7,*) E(1:2,i)
END DO
END PROGRAM Minimization

```

The resulting points are then plotted using gnuplot and the following sequence is used to determine a line of best fit:

```

gnuplot> FIT_LIMIT = 1e-18
gnuplot> E(a) = -A/(a**n)
gnuplot> fit E(x) 'Emin.d' via A,n

```

...

| Final set of parameters | Asymptotic Standard Error |
|-------------------------|----------------------------|
| ===== | ===== |
| A = 4.03532e-16 | +/- 2.066e-29 (5.121e-12%) |
| n = 2 | +/- 1.628e-15 (8.14e-14%) |

These values are then used to compare the four-dimensional energy with the three-dimensional energy and determine the maximum size of the compactified dimension.

A similar program is used to minimize the five-dimensional variational energy. Three different programs are used for $\ell = 1, 2$, and 3 , and each steps forward in β from 0 to $1/a_0$ (where a_0 is the Bohr radius) for 1000 steps. The local minimum of \tilde{E} is taken at each of 1000 steps in a from 0 to the Bohr radius. The points are sent to data files specified for each (ℓ, m) pair, and the points are fitted using the same procedure as above in gnuplot. An example program used when $\ell = 1$ is shown below.

```

PROGRAM Energy_l=1
  DOUBLE PRECISION::size,a_step,b_step,const,beta
  DOUBLE PRECISION::h,mu,e,e0,a0,E1,E2,E3,tempmin,min
  INTEGER::i,j,m

  h = 1.05457148D-34
  mu = 9.104423456D-31
  pi = 3.14159265
  a0 = 5.2917721092D-11

  OPEN(7,file='Energy_l=1,m=-1.d', status='unknown')
  OPEN(8,file='Energy_l=1,m=0.d', status='unknown')
  OPEN(9,file='Energy_l=1,m=1.d', status='unknown')

  a_step = 5.29177210D-14
  b_step = 1.88972612D7

  DO m=-1,1
    DO i=2,1000
      size = a_step*(real(i)-1)

      const = (-1)**(m+1)*192.*pi/(sqrt(5.*pi)*size**2.*a0)
      const = const/(fact(1-m)*fact(1+m))

      DO j=2,1000
        beta = b_step*(real(j)-1)

        E1 = beta**2.
        E2 = m*(m+1)/(size**2.)
        E3 = const*beta**3./((2*beta*size+sqrt(6.))**2.)
        tempmin = h**2./(2.*mu)*(E1+E2+E3)

        IF (j == 2) THEN
          min = tempmin
        END IF
      END DO
    END DO
  END DO

```

```

        IF (tempmin <= min) THEN
            min = tempmin
        END IF
    END DO

    WRITE(m+8,*) size,min
END DO
END DO
END PROGRAM Energy_l=1

```

```

FUNCTION fact(N)
    fact=1
    IF (N>1) THEN
        DO k=2,N
            fact=fact*k
        END DO
    END IF
    RETURN
END

```

The output is plotted using gnuplot and a line of best fit is found using the same method as above.

The example below is fitting the data for $\ell = 3, m = \pm 2$.

```

gnuplot> FIT_LIMIT = 1e-18
gnuplot> E(a) = -A/(a**2)
gnuplot> fit E(x) 'Energy_l=3,m=2.d' via A
...
Final set of parameters          Asymptotic Standard Error
=====                          =====
A                = 1665.82      +/- 0.0007737    (4.644e-05%)

```