Quantum Mechanical Bound States of the Yukawa Potential (or some better title)

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Ellen M. McManis

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Nelia Mann

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Abstract

Math and computers and stuff gave me results!

Introduction

The Yukawa potential governs the force between protons and neutrons in the nucleus of the atom. It is

$$V(r) = -\frac{C}{r}e^{-r/l}, \tag{1}$$

where C and l are constants. C sets the strength of the force; l acts as a length scale. The exponential term provides an effective cutoff once r gets much larger than l, as the exponential term drops off quite rapidly. The simplest system in which the potential can be studied is the deuterium nucleus. The system of a single neutron and proton can be expressed as a reduced mass orbiting the center of mass.

The force comes from the exchange of virtual pions between the two nucleons. The limited range is due to the fact that pions have mass. The mass of the pion then generates the length scale:

$$l = \frac{\hbar}{m_\pi c} \approx 1.41 \times 10^{-15} \text{ m} \tag{2}$$

The strength of the force C is only known experimentally; it has been found to be about 2.96×10^{-6} eV*m[1][1].

In general, the time-independent Schrödinger wave equation for a particle under the influence of some $V(r)$ is

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(r,\phi,\theta) + V(r)\psi(r,\phi,\theta) = E\psi(r,\phi,\theta) \tag{3}$$

where μ is the reduced mass of the system. Because we are working with nuclei in atoms, it makes the most sense to express this in spherical coordinates, as above. With the Yukawa potential, this equation cannot be solved analytically, as the exponential term messes things up. However, we *can* solve the more simple system described by the potential without the exponential term, that is,

$$V(r) = -\frac{C}{r}. \tag{4}$$

This problem is equivalent to solving the wave equation for the Coulomb potential in hydrogen; in that case, $C = \frac{e^2}{4\pi\epsilon_0}$. Plugging the above potential into the wave equation, we have

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(r,\phi,\theta) - \frac{C}{r}\psi(r,\phi,\theta) = E\psi(r,\phi,\theta). \tag{5}$$

[1] Get a better citation for this than Eisberg and Resnick

This equation can be solved analytically by separation of variables. The wave function can be expressed as the product of three functions

$$\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi) \tag{6}$$

with the values

$$\begin{aligned}
\Phi_{m_l}(\phi) &= e^{im_l\phi} \\
\Theta_{lm_l}(\theta) &= \sin^{|m_l|}\theta F_{lm_l}(\cos\theta) \\
R_{nl}(r) &= e^{-C\mu r/n\hbar^2}\left(\frac{C\mu r}{\hbar^2}\right)^l G_{nl}\left(\frac{C\mu r}{\hbar^2}\right)
\end{aligned}$$

Here, l, m_l, and n are quantum numbers, and F_{lm_l} and G_{nl} are polynomials in $\cos\theta$ and $\left(\frac{C\mu r}{\hbar^2}\right)$, respectively. The energy for the particle described by this wave function is just a function of n (the radial quantum number), and is equal to

$$E_n = -\frac{\mu C^2}{2\hbar^2 n^2}. \tag{7}$$

All of these functions can be simplified further by introducing a length scale,

$$\alpha = \frac{\hbar^2}{C\mu}. \tag{8}$$

α is a constant with units of length, defined in terms of the other constants of the problem. In hydrogen, this is the Bohr radius, and reduces to the familiar $a_o = \frac{4\pi\epsilon_0\hbar^2}{\mu e^2}$. Physically, it represents the radius of the smallest orbit in a Bohr hydrogen atom (the ground state), making it a natural length scale for the problem.

The ground state for the wave function $(n = 1, l = 0, m_l = 0)$ is

$$\frac{1}{\sqrt{\pi}}\left(\frac{1}{\alpha}\right)^{3/2} e^{-r/\alpha}. \tag{9}$$

The ground state wave function is spherically symmetric, meaning that ψ there is only a function of r. In general, the spherically symmetric wave functions have the form

$$\psi(r) = e^{-r/\alpha} G_n\left(\frac{1}{\alpha}\right) \tag{10}$$

where G_n is the same polynomial as earlier. As n increases, so do the possible values of r, and the particle can be found further and further from the center of mass of the system. This can be seen in figure 1, in which $\psi(r)$ is plotted for several values of n. As this happens, E_n gets closer and closer to zero, but never quite reaches it – there are an infinite number of bound states possible. This is shown in figure 2.

Going back to the more-complicated Yukawa potential, the exponential term in the potential means that its range is limited in a way the Coulomb potential's isn't, because e^{-x} drops off much faster than $1/x$. We expect that this will limit the number of bound states as well, to some number whose rs are less than l.

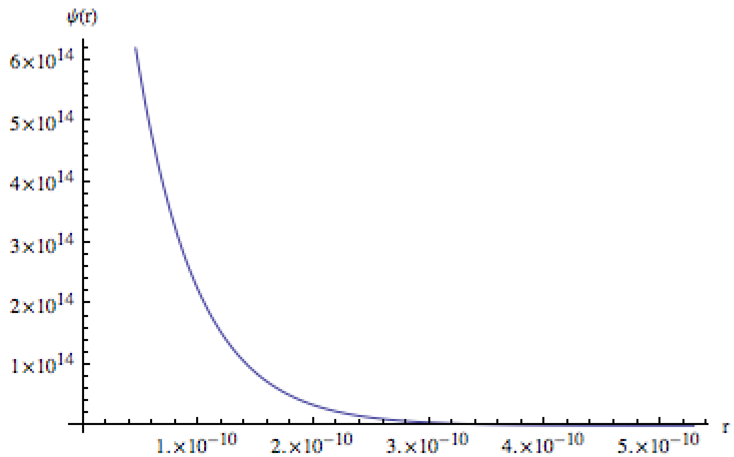

Figure 1: The ground state ($n = 1$, $l = 0$, $m_l = 0$) wave function for hydrogen

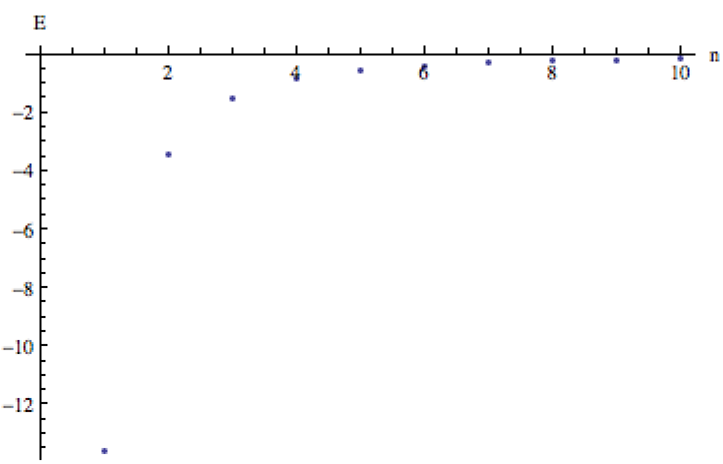

Figure 2: The energies of the first 10 bound states of the electron in the hydrogen atom

Chapter 1

Semi-Classical Approximation and Numerical Setup

1.1 The Bohr Model

The similarity between the Yukawa potential in deuterium and the Coulomb potential in hydrogen suggests treating them similarly. The Bohr model is a semi-classical view of the electron orbiting the nucleus in hydrogen. The postulates of the model are as follows:

1. Electrons move in circular orbits around the nucleus under the influence of the Coulomb force. They obey all the laws of classical mechanics.

2. Angular momentum is quantized; $L = n\hbar$ where n is a positive integer.

3. The energy of the electron in an orbit remains constant.

4. If an electron changes orbits, electromagnetic radiation is emitted with frequency $\nu = \frac{E_i - E_f}{h}$

We can easily use this model with the Yukawa potential instead of the Coulomb to get a qualitative idea of where we expect bound states to be found.

First, we look at the classical energy of a particle (here, the reduced mass of the neutron-proton system) moving under the influence of the Yukawa potential:

$$E = \frac{1}{2}\mu\dot{r}^2 + \frac{1}{2}\frac{L^2}{\mu r^2} - \frac{C}{r}e^{-r/l}. \tag{1.1}$$

To make this easier to work with, we use the length scale from (8), the "Bohr radius" for this problem. We then use this to nondimensionalize r, defining

$$\rho \equiv \frac{r}{\alpha}. \tag{1.2}$$

Finally, we define a time scale:

$$\beta \equiv \frac{c^2 m}{\hbar^3}. \tag{1.3}$$

We can now substitute in ρ, α, and $\tau = \beta t$:

$$E = \frac{1}{2}m\left(\frac{d\rho}{d\tau}\alpha\beta\right)^2 + \frac{1}{2}\frac{c}{\rho^2\alpha}(n^2 - \rho e^{-(\rho\alpha)/l}) \tag{1.4}$$

$$= \frac{1}{2}\frac{c}{\alpha}\rho'^2 + \frac{1}{2}\frac{c}{\alpha}\frac{1}{\rho^2}(n^2 - \rho e^{-(\rho\alpha)/l}) \tag{1.5}$$

$$\frac{2\alpha}{c}E = \tilde{E} = \rho'^2 + \frac{1}{\rho^2}(n^2 - 2\rho e^{-\rho/\lambda}) \tag{1.6}$$

In the last line, we have used $\lambda = \frac{l}{\alpha}$, relating the strength of the force and the length scale of the problem. We now have a dimensionless effective potential,

$$V_{eff} = \frac{1}{\rho^2}(n^2 - 2\rho e^{-\rho/\lambda}) \tag{1.7}$$

to use for further analysis.

We now turn our attention to the number of bound states allowed by this potential. We expect that the exponential term will act as a cutoff, limiting the number of bound states to some finite quantity. As a really naive approximation of this behavior, we can use the Bohr model to look at a system where $V(r) = -\frac{C}{r}$ for r <l, and $V(r) = 0$ everywhere else.

This system is equivalent to hydrogen for $r < l$, so we solve it the same way. We know that

$$\frac{C}{r^2} = F = \mu a = \mu\frac{v^2}{r} \tag{1.8}$$

and

$$\mu v r = n\hbar \tag{1.9}$$

from the postulates. Solving for v and substituting, we find that

$$r = \frac{n^2\hbar^2}{\mu C} \tag{1.10}$$

Substituting in our length scale gets us

$$r = n^2\alpha. \tag{1.11}$$

The physical interpretation of α is clear here – in the ground state ($n = 1$), $r = \alpha$. Substituting our nondimensionalized ρ makes the expression even simpler: we get

$$\rho = n^2. \tag{1.12}$$

This can be rearranged to be $n = \sqrt{\rho}$. For some λ, then, there will be $\lfloor\sqrt{\lambda}\rfloor$ bound states, and a new bound state will appear when $\sqrt{\lambda} = n$.

To perform the analysis of the full potential, we look at the graph of the effective potential (figure [placeholder]). We can see that bound states exist for ρ where V_{eff} is less than 0, and these bound states have circular orbits at the minimum of V_{eff}

Keeping α and n constant, there will then be two critical values of λ – one where V_{eff} has no more true bound states, and one where V_{eff} doesn't produce any kind of dip.

The first of these critical values occurs when the minimum of V_{eff} is 0. To find it, we start by taking the derivative of (1.7) and setting it to 0, obtaining

$$\frac{dV}{d\rho_0} = -\frac{2n^2}{\rho_0^3} + \frac{2}{\rho_0^2}e^{-\rho_0/\lambda} + \frac{2}{\rho_0\lambda}e^{-\rho_0/\lambda} \tag{1.13}$$

$$0 = -2n^2 + 2\rho_0 e^{-\rho_0/\lambda} + 2\frac{\rho_0^2}{\lambda}e^{-\rho_0/\lambda} \tag{1.14}$$

where ρ_0 is the value of ρ when V_{eff} is minimized. This equation has no general solution, but we can find one for the specific case where $V_{eff}(\rho_0) = 0$ by solving the equation

$$V_{eff}(\rho_0) = 0 = n^2 - 2\rho_0 e^{-\rho_0/\lambda} \tag{1.15}$$

$$n^2 = 2\rho_0 e^{-\rho_0/\lambda} \tag{1.16}$$

and plugging it in to the previous, obtaining

$$0 = -2n^2 + n^2 + n^2\frac{\rho_0}{\lambda} \tag{1.17}$$

$$= -1 + \frac{\rho_0}{\lambda} \tag{1.18}$$

$$\rho_0 = \lambda. \tag{1.19}$$

Plugging this back into the equation for $V_{eff}(\rho_0)$ gives us

$$n = \sqrt{\tfrac{2}{e}}\sqrt{\lambda} \approx 0.857764\sqrt{\lambda} \tag{1.20}$$

which is pretty close to the naive $n = \sqrt{\lambda}$ from above.

For the second critical point, the one where V_{eff} has no minimum, we rewrite (1.14) to be

$$n^2 = \left(\rho + \frac{\rho^2}{\lambda}\right) e^{-\rho/\lambda} \tag{1.21}$$

The right side of this equation will have some maximum, which will be the last point for which the equation can be solved – after that, the value of n^2 will always be greater than the right side. To find this, we differentiate with respect to ρ and set to 0, obtaining

$$0 = (1 + 2\frac{\rho}{\lambda}) - \frac{1}{\lambda}(\rho + \frac{\rho^2}{\lambda}) \tag{1.22}$$

$$= 1 + \frac{\rho}{\lambda} + \frac{\rho^2}{\lambda^2}. \tag{1.23}$$

This is a quadratic in ρ and can be solved using the quadratic formula:

$$\rho = \frac{-\frac{1}{\lambda} \pm \sqrt{\left(\frac{1}{\lambda}\right)^2 + 4\frac{1}{\lambda^2}}}{-\frac{2}{\lambda^2}} \tag{1.24}$$

$$= \frac{\lambda}{2} \mp \frac{\lambda\sqrt{5}}{2} \tag{1.25}$$

As ρ is a real physical quantity that can't be negative, we can discard one solution, obtaining

$$\rho = \frac{\lambda}{2}(1+\sqrt{5}) \tag{1.26}$$

We can plug this in to (1.14) to find the relationship between λ and n:

$$n^2 = \lambda(1+\sqrt{5})\left(\frac{3+\sqrt{5}}{4}\right)e^{-(1+\sqrt{5})/2} \tag{1.27}$$

$$n = 0.916494\sqrt{\lambda} \tag{1.28}$$

From these equations, we expect the number of bound states to go up as the square root of λ.

1.2 Quantum Mechanics

Numerics and stuff goes here.

References

[1] Robert Eisberg and Robert Resnick. *Quantum Physics of Atoms, Molecules, Solids, Nuclei, and Particles*. Wiley, 1985.