Bound State

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The ground state energy of the hydrogen atom is computed from a relativistic wave equation based on finite structure for elementary particles and the results fall within the experimental measurement error unlike the results from the Schrödinger and Dirac equations. The solution exposes the origin of both the Pauli Principle and the attraction for forming Bose-Einstein condensations. More importantly, it shows that the γ of special relativity for the bound states takes on values less than one. [a]

CONTENTS

I. HYDROGEN ATOM

In 1947 Polykarp Kusch and Henry Foley reported their experiment of the gyromagnetic ratio of the electron (Foley and Kusch, 1948). This finding was eventually titled by others as the anomalous magnetic moment, being a correction to the magnetic moment derived from the Dirac equation. There was an intense effort both experimental and theoretical to establish the spectroscopic structure of the hydrogen atom through out the 1930s and 1940s (Schweber, 1994). This work on the magnetic moment in part gave rise to a theory called quantum electrodynamics that was used to compute the corrections to the Dirac electron theory. Until the early 1960s P. Kusch had no public problem with quantum electrodynamics but by 1967 he had come to the conclusion it was not valid physics. The troubling experimental question was the discrepancy in the ground state energy of hydrogen $^2\mathbf{S}_{\frac{1}{2}}$. The experimental discrepancy to both the Schrödinger and Dirac equations computed values were large, $> .003$ eV. To a spectroscopist this is a large discrepancy. Kusch was a stickler for semantics and the adjective anomalous applied to his earlier experimental work might be considered a slur. In the academic year 1966-67 when he took over the Columbia Radiation Laboratory on I.I. Rabi's retirement and initiated an investigation using a post doctoral student and an undergraduate to perform a more accurate measurement of the $^2\mathbf{S}_{\frac{1}{2}}$ state using electron scattering to ionize hydrogen. That work was never completed as the 1968 riots moved Kusch to become university vice president.

Neither the Schrödinger nor the Dirac equations are directly derived from the relativistic conservation of energy relation. In addition is their failure to recognize that the γ of special relativity can take on values less than one for the bound state. It did not help that they treated particles as mathematical points with no structure.

[a] submitted to Reviews of Modern Physics, https://vixra.org/pdf/2103.0026v2.pdf, https://www.castinganalysis.com/files/boundstate.pdf

II. SOLVING THE RELATIVISTIC WAVE EQUATION

There are a pair of laboratory frame wave equation derived from the relativistic conservation of energy that replace the Schrödinger and Dirac equations (Wallace and Wallace, 2020).

$$\nabla^2\Phi - \frac{1}{c^2}\frac{\partial^2\Phi}{\partial t^2} = \frac{2m_o}{\hbar^2}\{-i\hbar\frac{\partial\Phi}{\partial t} + V(1+\frac{V}{2m_oc^2})\Phi\}$$
$$i\hbar\frac{\partial\Phi}{\partial t} = -\frac{\hbar^2}{m_o(1+\gamma)}\nabla^2\Phi + \frac{2V}{1+\gamma}(1+\frac{V}{2m_oc^2})\Phi \quad (1)$$

The upper equation describes the behavior of a free field that can be massless or massive and the lower equation describes the relative dynamics of a particle, free or bound in a potential such as the hydrogen atom. The upper equation naturally integrates electromagnetic theory into quantum mechanics and is useful for problems dealing with refraction of both photons and neutrinos (Wallace and Wallace, 2018) (Wallace and Wallace, 2023). By dropping the quadratic potential term and setting γ to one results in the Schrödinger equation that has now been properly derived as an approximation. Both equations 1 are derived from $E^2 = p^2c^2 + (m_oc^2)^2$ where m_o is the rest mass of the particle.

A. Solution for the Coulomb Potential

Applying the lower equation 1 to hydrogen atom with the Coulomb potential was first not even considered because the point charge of the Coulomb potential is not valid because the electron has a finite structure (Wallace and Wallace, 2015). However, Peter Hagelstein in looking for a problem to give his quantum mechanics class found a simple solution to the upper equation 1 using the Coulomb potential. His three dimensional spherically symmetric trial solution is $\phi(r) \sim r^s e^{-\beta r}$ happens also to solve the lower equation for a bound $^2\mathbf{S}_{\frac{1}{2}}$ ground state.

The trial solution for the time dependent portion of the wave function:

$$\Phi(r,t) = \phi(r)e^{-\frac{iE_{rel}t}{\hbar}} \quad (2)$$

producing.

$$E_{rel}\ \phi(r) = -\frac{\hbar^2}{m_o(1+\gamma)}\nabla^2\phi + \frac{2V}{1+\gamma}(1+\frac{V}{2m_oc^2})\phi \quad (3)$$

Taking $\phi(r) = r^s e^{-\beta r}$ yields in 3D spherical coordinates:

$$E_{rel}\ \phi(r) = -\frac{\hbar^2}{m_o(1+\gamma)}\{\beta^2 - \frac{2\beta(s+1)}{r} + \frac{s(s+1)}{r^2}\}\phi(r) + \frac{2V}{1+\gamma}(1+\frac{V}{2m_oc^2})\phi(r) \quad (4)$$

B. Relativistic Wave Equation Trial Solution

Applying the Coulomb potential to the two potential terms the relativistic wave equation becomes:

$$V + \frac{V^2}{2m_oc^2} = -\frac{Ze^2}{2(1+\gamma)\pi\epsilon_o r} + \frac{1}{(1+\gamma)m_oc^2}\frac{Z^2e^4}{(4\pi\epsilon_o)^2r^2} \quad (5)$$

Separating the terms in powers of r allows E_{rel}, s and β to be computed as all factors of r^m must equal zero.

$$E_{rel} + \frac{\hbar^2\beta^2}{m_o(1+\gamma)} = \frac{1}{r}\{-\frac{2\hbar^2\beta(s+1)}{m_o(1+\gamma)} - \frac{Ze^2}{2(1+\gamma)\pi\epsilon_o}\} + \frac{1}{r^2}\{-\frac{\hbar^2 s(s+1)}{m_o(1+\gamma)} + \frac{1}{(1+\gamma)m_oc^2}\frac{Z^2e^4}{(4\pi\epsilon_o)^2}\} \quad (6)$$

Solving for s and then substituting for the fine structure constant α:

$$s^2 + s = \frac{Z^2e^4}{(4\pi c\hbar\epsilon_o)^2} = \alpha^2Z^2 \quad (7)$$

$$s = \sqrt{1+4Z^2\alpha^2} - 1 \quad (8)$$

For β the equation is simplified by using the Bohr radius a_o:

$$\beta = \frac{1}{s+1}\frac{m_o}{\hbar^2}\frac{Ze^2}{4\pi\epsilon_o} = \frac{Z\alpha}{\sqrt{1+4Z^2\alpha^2}}\frac{m_oc}{\hbar} = \frac{Z}{a_o\sqrt{1+4Z^2\alpha^2}} \quad (9)$$

Then the expression for the ground state energy of the $^2\mathbf{S}_{\frac{1}{2}}$ state when the factor representing the reduce mass effect is applied where m_N is the nucleon mass. (Bethe and Salpeter, 1957).

$$E_{rel} = -\frac{m_oc^2}{(1+\gamma)}\ \frac{Z^2\alpha^2}{1+4Z^2\alpha^2}\frac{m_N}{m_o+m_N} \quad (10)$$

The γ dependence can be factored out by using the expression for total energy $E_t = \gamma m_oc^2$.

$$E_{rel} = E_t - m_o c^2 = m_o c^2(\gamma - 1) \tag{11}$$

Substituting into equation 10 to remove γ yields:

$$E_{rel}^2 + 2m_o c^2 E_{rel} - 4(m_o c^2)^2 \frac{Z^2\alpha^2}{1+4Z^2\alpha^2}\frac{m_N}{m_o+m_N} = 0 \tag{12}$$

$$E_{rel} = -m_o c^2\{-1 + \sqrt{1 + \frac{Z^2\alpha^2}{1+4Z^2\alpha^2}\frac{m_N}{m_o+m_N}}\} \tag{13}$$

The wave function then becomes:

$$\Phi(r,t) = Ar^{\sqrt{1+4Z^2\alpha^2}-1} \quad e^{-\frac{Zr}{a_o\sqrt{1+4Z^2\alpha^2}} - i\frac{Et}{\hbar}} \tag{14}$$

The ground state energies for the three different wave equations are computed in Table I. γ in the bound state now takes on values less than one as the self-energy is reduced to supplying the field that binds the state. The change in γ can be computed using equation 11.

C. Increasing Z

There is a strong divergence between the behavior of the ground state energy from the relativistic wave equation verse the Schrödinger and Dirac equations as shown in Figure 1. There is no single electron ionization data at high **Z** and the best data is that of **K**-shell x-ray data from electron scattering. Care has to be taken since NIST tables report ionization data for high **Z** that are only calculations and not experimental.

The reason the **K**-shell x-ray data is interesting is that Moseley's law breaks down (Condon and Shortley, 1951) in the same area where the ground state energies diverge for the three relations. This indicates the source of the binding energy is altered.

In the limit of infinite charge γ does not go to zero. The bound state energy is limited to a finite value independent of Z limiting the electrostatic potential strength.

$$E_{rel} \quad \geq \quad -m_o c^2 \, \{\sqrt{\frac{5}{4}} - 1\} \quad = \quad \textbf{- .11803} \; m_o c^2 \tag{15}$$

The ground state energies when computed from both the Schrödinger and Dirac equation do not remain finite, but continue to decrease with increasing **Z**. This finite binding occurs for potentials generated from the self-energy of the particles themselves. That is not the case for the gravitational potential, which enters the field equation in a different way (Wallace and Wallace, 2024). In the opposite limit when **Z**$\rightarrow$ 0 then E goes to zero but not in the case of the Dirac equation solution. The Dirac equation still produces a bound state with no potential. At high **Z** the **K**-shell electron contribution to binding is exhausted and they are crushed between the nuclear charge and the outer electrons.

Table I **H**ydrogen ground state energy from Bohr (Bohr, 1913) the Schrödinger Equation (Bethe and Salpeter, 1957) , modified Dirac equation (Gordon, 1928), and the relativistic wave ground state energy (eq. 13). The experimentally measured ground state energy is **-13.595** eV (Moore, 1971).

Bohr	**1913**
-13 eV	planetary atomic quantized model $E_{Bohr} = \frac{R}{2}$
Schrödinger equation	**1926**
solution relativity	regular at origin not considered
ground state energy **-13.5984** eV deviation **-.0034** eV $\gamma \;=\; 1$	$E_{Schro.} =$ $-\frac{Z^2 m_o e^4}{2(4\pi\epsilon_o)^2\hbar^2}\frac{m_N}{m_o+m_N}$
mod. Dirac Equation	**1928**
solution relativity	singular at origin incorrectly applied
ground state energy **-13.5986** deviation **-.0036** eV $\gamma \;=\; 1$	$E_{Dirac} =$ $-\frac{m_o c^2\sqrt{1-Z^2\alpha^2}m_N}{m_o+m_N}$
Relativistic Wave Equation	**2023**
solution relativity	regular at origin correctly applied
ground state energy **-13.5953** eV deviation **-.0003** eV $\gamma \;=\; .9997339$	$E_{rel} = m_o c^2\{1-$ $\sqrt{1+\frac{Z^2\alpha^2}{(1+Z^2\alpha^2)}\frac{m_N}{m_o+m_N}}\}$

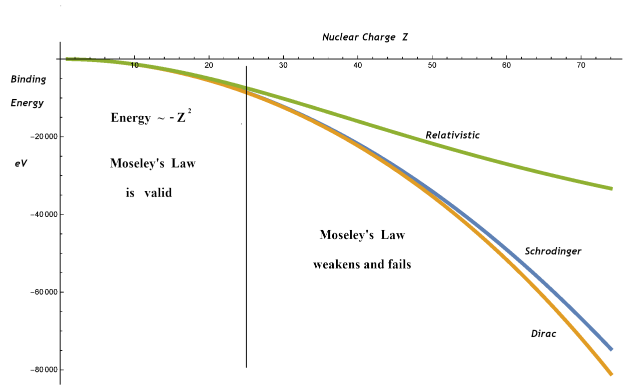

Figure 1 **Binding energy of hydrogen like ions taking Z from 1 to 74 in eV for three models.**

Table II **Ground state binding limits for the three wave equations as a function of Z.**

Analysis	**Z** $\rightarrow 0$	**Z** $\rightarrow \infty$
Schrödinger fails at upper limit	0	**-**∞
Dirac fails at both limits	Bound State?	**Complex** ∞
Relativistic predicts limit to Moseley's Law	0	$> \ .12\ m_o c^2$ Limit to Binding

III. PARTICLES WITH STRUCTURE

The question remains of why the computed energy from the relativistic wave equation for the hydrogen ground state is within the error bounds of the experimental value when a singular Coulomb potential, $\frac{1}{r}$ is being used? Neither the electron nor proton are point charges (Wallace and Wallace, 2015) (Wallace and Wallace, 2019). The proton's charge density is more compact than that of the electron, however, it plays the dominant role in defining the central force potential field due to its greater mass. The proton's potential is well approximated by the singular Coulomb potential. The size effect of the electron's charge distribution will be reduced by the ratio of its much smaller mass. All calculations are done in center of mass coordinates and similar to the use of the reduced mass, the same constraints operate on the contribution of the individual charge distributions.

The necessary correction to the electrostatic potential of the electron due to its structure can be computed from the electrons state function in its self-reference frame, $u^*(r)u(r)$ and is shown in Figure 2.

$$V_{Coul.}(r) = -\frac{Ze^2}{4\pi\epsilon_o r} \tag{16}$$

$$\Delta V(r) = V_{Coul}(r) - \int_{\infty}^{r} u^{f*}(x)u^f(x)dx \tag{17}$$

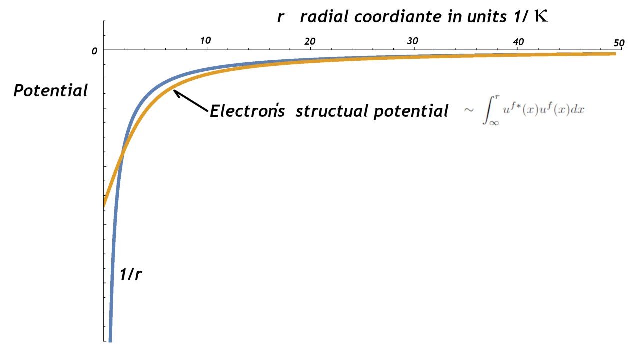

Figure 2 **The difference between the** $1/r$ **potential of a point charge and the electron's structural potential is significant in the electrons core region. In the plot** $r = 1$ **represent the electron's Compton scale of** $\hbar/mc = 3.86 \times 10^{-13} m$ **(Wallace and Wallace, 2015).**

The classical potential that is singular at the origin can be corrected for the fact the electron has a distributed charge. The Coulomb potential does not take into account the electron's finite size that rolls off close to the origin. This correction is small for the hydrogen atom's ground state and the nuclear charge distribution effect is even smaller (Wallace and Wallace, 2015), however, the energy correction will grow for higher Z single electron ions. The first order perturbation contribution due to the electrons charge distribution is calculated as $< 1S|\delta V(r)|1S >= .007098 eV$ (Wallace and Wallace, 2015). With the center of mass correction this is reduced to $3.863 \times 10^{-6} eV$ or an insignificant contribution to the ground state energy.

A weak point in the argument for the Dirac relativistic wave equation is being solely for the electron. The second point of failure is that the electron is represented as a mathematical point. Its possible to produce a general derivation for the particle structure in its own frame of reference using a second order equation to generate a pair of solutions, for both a fermion and boson in three spatial dimensions. The restriction to a single spatial spherically symmetric variable, r, ensures $U(1)$ group symmetry. Where $u^f(r;\kappa,n,\gamma)$ one for fermion and one $u^b(r;\kappa,n,\gamma)$ for a boson dependent on three parameter: n the dimension (1, 2, or 3), κ inverse particle scale. Dynamics is not expressed in this space, except indirectly through the relativistic parameter γ (Wallace and Wallace, 2014).

The electron's architectural description defines its static electric field, $u^*(r)u(r)\widehat{\mathbf{r}}$, that is dependent on two parameter: inverse scale κ and γ (Wallace and Wallace, 2014). In the self-reference frame where there are no internal dynamics γ is a function of the particle's relative environment and that includes not only relative motion to another free particle that defines kinetic energy, but also what occurs in a bound state under the restraints of an external potential.

The spatial expression $u^f(r)$ and $u^b(r)$ for 3D elementary massive fermion and boson in their own frame of reference, which for the fermion solution will be taken as an electron is one of the two solutions of equation 19. The lower solution being for the boson where ${}_1F_1$ and U are confluent hypergeometric functions (Wallace and Wallace, 2014).

$$
\begin{aligned}
u^f(r) &= Ae^{-\kappa r}{}_1F_1[\frac{2}{1+i\gamma},2,(1+i\gamma)\kappa r] \\
u^b(r) &= Ae^{-\kappa r}U[\frac{2}{1+i\gamma},2,(1+i\gamma)\kappa r]
\end{aligned}
\quad (18)
$$

The field equation that produced these solution is derived from the behavior of a longitudinal field when coupled to the laboratory frame relativistic wave equation that can generate pair-production of the same particle. This annihilation renewal process isolates the two spaces because of the statistical independence generated by the loss of a history as to which particles annihilate (Wallace and Wallace, 2014).

$$
\frac{\partial^2 u(r)}{\partial r^2}+(\frac{n-1}{r}+\kappa\{1-i\gamma\})\frac{\partial u(r)}{\partial r}-i\kappa^2\gamma u(r)=0 \quad (19)
$$

A. Origin of Fermion and Boson Statistics

The role of γ for the bound state and its effect on structure of the particle is of interest for both bosons and fermions. The simplest way to display the effect is to plot the particle's density function comparing values of γ, when both greater and less than one.

The effect of an external binding potential in altering γ acts differently on fermions and bosons. This can be seen in their density function, $u^*(r)u(r)r^{n-1}$ for the three dimensional solutions.

In the electron's own frame of reference, its self-reference frame, γ modifies the electron's structure. In free space for $\gamma<1$ the electron expands, its wave function is divergent and grows, inhibiting additional occupation of the same state.

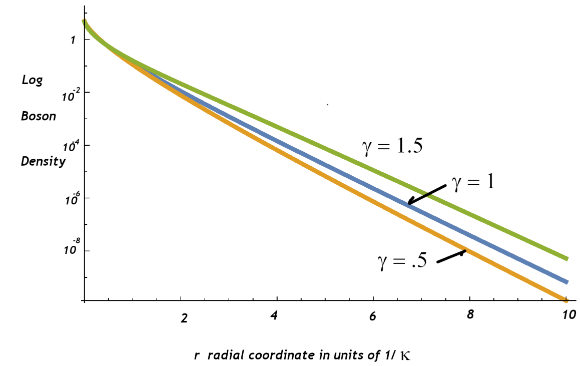

Figure 3 **Origin of the Bose-Einstein condensate is seen in the shrinkage of the boson density function in the self-reference frame with an external binding potential.**

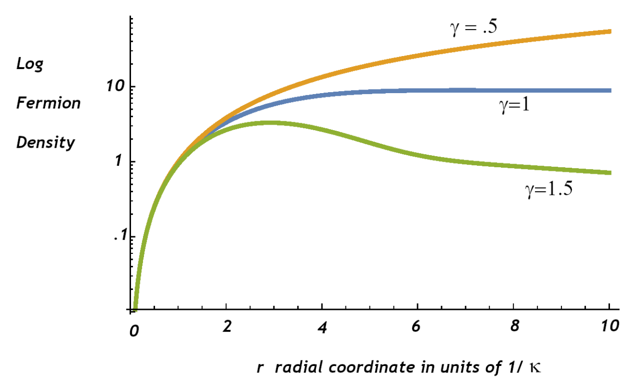

Figure 4 **Origin of fermion repulsion is seen in the density function diverging in an external binding potential.**

IV. DISCUSSION

The bound quantum particle's equivalent response to a tidal force has been ignored. The effect of tidal force can now be computed. The severe restrictions on a quantum particle's structure found in their individual self-reference frame does not allow a tidal like shape change as these quantum particles have only one free variable that can be affected, their radial scale (Wallace and Wallace, 2014). Any response would have to change the particle's density profile while preserving spherical symmetry.

In addition to the origin of quantum statistics, the defect in special relativity has been partially solved. The surprise result was that the additional corrections to the ground state energy of hydrogen due to the finite size of the electron are small.

V. ACKNOWLEDGMENT

To Polykarp Kusch and Patrick Cahill for introducing us to hydrogen ground state problem and Jack Steinberger for insisting that longitudinal fields in physics must be better understood. Also to John David Jackson who helped in getting our original experimental data that peered into the self-reference frame of a Bose-Einstein condensate published. Finally to Peter Hagelstein for a useful method to solve the bound state relativistic wave equation in the laboratory frame.

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