Bound State

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Relativistic solutions of the bound state problem for the hydrogen atom and one electron ions using the uncorrected Coulomb potential and comparing those results with ones using the correct physical potential reveals that relativity's γ in the quantum bound state takes on values less than one. This also explains the physical origin of the Bose-Einstein and Fermi-Dirac statistics for bound state particles.

CONTENTS

I. HYDROGEN ATOM

With the new quantum mechanics of 1926 the picture of the orbiting electron was replaced by a density function. The solutions for the electron orbitals generated by the Schrödinger equation were a major advance on understanding the hydrogen atom. The Pauli's modified version of the relativistic Dirac equation took the solution further explaining the spectra in more detail from an expression for the electron's magnetic moment. Considering the matter for five years Dirac was dissatisfied and felt he might have gone wrong in generating a first order equation instead of a second order equation (Dirac, 1932). Pauli did not want to trash the hard won effort on modifying the Dirac equation and won the debate by default. It was a damaged prize because the equation was specific to only a structure-less electron, with both the electron and the nucleons treated as point masses and charges.

To patch things up following WWII with the energy levels of the hydrogen atom and the magnetic moment of the electron, perturbation corrections were attempted. These corrections were rightly challenged at the time for being non-physical (Schweber, 1994). Whether a correction is large or small should not enter the argument if a physical understanding is missing. The problems were the infinities, the main defect in the model that could not be overcome with the electron being a point mass and point charge. The perturbation corrections to solutions of Schrödinger/Dirac equations were a political winner because one could generate almost any desired solution, right or wrong (Consa, 2020).

By 2013 it was found that if relativistic energy conservation was strictly adhered to, particles like the electron gained a structure defined in their own self-reference frame as opposed to the laboratory frame where their dynamics were on display (Wallace and Wallace, 2014a). More importantly, the particle description in their own frame and a general dynamical equation in the laboratory

frame were not specific just to the electron (Wallace and Wallace, 2020). The free particle quantum solution now incorporated both time dilation and the Lorentz contraction as part of their normal solution, because the particles now had a physical structure. The Lorentz contraction of point is not a problem that can be dealt with.

The bound state problem is one of physic's oldest problem and as a classical problem it was never simply solved even for planetary motion as planets and moons are not points and tidal forces come into play. There should be no expectation that the quantum variant the hydrogen atom should be free of such complications. The planetary question was simple as long as it was assumed it could be treated with point masses located at the bodies center of mass as a first order approximation. With the particle structure defining its static fields opens up the question about the plasticity of these structures. Giving particle structure automatically generated the static fields for the electrostatic, weak, and the strong force (Wallace and Wallace, 2014b)(Wallace and Wallace, 2020). With structure this turns a very rigid model into one where the plasticity of the structure can be investigated.

The quantum particle's equivalent response to a tidal force has been ignored as the object that bind are assumed to be inert points of matter. Once the source of the electrostatic potential is tied to a particles structure and is no longer a mathematical point, the question of the affect of a tidal force can 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, 2014a). Any response would have to change the particle's density profile while preserving spherical symmetry and altering their energy. To expose this quantum problem of tides there is a solution to the ground state of a single bound electron where a dynamic equation is available, which does not assume the electron or the nucleons as being mathematical points that treats relativity properly (Wallace and Wallace, 2014a).

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

Relativity can now operate on the particle's scale in the bound state. The description in the particle's own self-reference frame that is statistically independent from the lab frame is derived from the free field equation $E = pc$. The solutions produce density structures in 1,2, and 3 dimension dependent on two parameter, κ an inverse scale parameter, and γ of relativity that is more broadly defined than it is dynamically defined in the laboratory frame. It is the behavior of both these parameters in the bound state that is of interest. The elementary fermion in three dimension, electron, that has long been treated

as a point now has been shown to have structure defining its static electric field(Wallace and Wallace, 2015) from which its charge density distribution and magnetic moment can be computed(Wallace and Wallace, 2020). How the electron's scale varies under the influence of an external potential in a bound state is equivalent to planetary tides that now can be explored.

II. HISTORY OF THE QUANTUM BOUND STATE

There is a detailed history of the Schrödinger and modified Dirac equation and how these equations were constructed along with their solutions found in Bethe and Salpeter *Quantum Mechanics of One and Two Electron Atoms* (Bethe and Salpeter, 1957). The Schrödinger equation is not derived and the modified Dirac equation also is only constructed by adding two terms to the base equation that are not derived.

Table I **The Z dependence of the Schrödinger Equation and modified Dirac equation ground state energy for one electron ions. (Bethe and Salpeter, 1957)**

Schrödinger equation	Comment
potential	singular at origin
solution	regular at origin
electron	point mass and charge
relativity	not considered
ground state	$E_{Schro.} = -\frac{Z^2 m_o e^4}{2(4\pi\epsilon_o)^2\hbar^2}\frac{m_N}{m_o+m_N}$
mod. Dirac Equation	**Comment**
potential	singular at origin
solution	singular at origin
electron	point mass and charge
relativity	application limited
ground state	$E_{Dirac} = -\frac{m_oc^2\sqrt{1-Z^2\alpha^2}m_N}{m_o+m_N}$

III. PARTICLES WITH STRUCTURE

The expression for the electron that generates its static electric field, $u^*(r)u(r)\hat{\mathbf{r}}$, is dependent on two parameter: inverse scale κ and γ. 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 to what occurs in a bound state with the restraints of a potential.

The 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 3. The lower solution being for the boson where $_1F_1$ and U are hypergeometric functions (Wallace and Wallace, 2014a).

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

The function $u(r)$ is dependent on three parameter κ the inverse scale, γ, and the dimension, n. In the derivation the γ was introduced from the ratio of E/mc^2 for the particle and no dynamical arguments were used in the derivation.

$$\frac{\partial^2 u(r)}{\partial r^2} + (\frac{n-1}{r} + \kappa\{1 - i\gamma\})\frac{\partial u(r)}{\partial r} - i\kappa^2\gamma u(r) = 0 \quad (3)$$

IV. SOLVING THE RELATIVISTIC WAVE EQUATION

There are actually 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).

$$\nabla^2\Phi - \frac{1}{c^2}\frac{\partial^2\Phi}{\partial t^2} = \frac{2m_o}{\hbar^2}\{-i\hbar\frac{\partial\Phi}{\partial t} + V(1 + \frac{V}{2m_oc^2})\Phi\}$$
$$(4)$$
$$i\hbar\frac{\partial\Phi}{\partial t} = -\frac{\hbar^2}{m_o(1+\gamma)}\nabla^2\Phi + \frac{2V}{1+\gamma}(1 + \frac{V}{2m_oc^2})\Phi$$

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. By dropping the quadratic potential term and setting γ to one the result is the relativistic origin of the Schrödinger equation that has now been properly derived as an approximation. Both equations 4 are derived from $E^2 = p^2c^2 + (m_oc^2)^2$ where m_o is the rest mass of the particle.

A. A Simple Solution for the Coulomb Potential

Applying equation 1 to hydrogen atom with the Coulomb potential was 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 problem to give his quantum mechanics class for a final

exam, found a simple ground state solution to the spatial part upper equation 4 using the Coulomb potential. His three dimensional spherically symmetric trial solution is $\phi(r) \sim r^s e^{-\beta r}$ also solves the lower equation for the bound ground state and thus allows the major corrections to this state to be computed for the error introduced by the Coulomb potential.

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

$$\Phi(r,t) = \phi(r)e^{-\frac{iEt}{\hbar}} \quad (5)$$

producing.

$$E\phi(r) = -\frac{\hbar^2}{m_o(1+\gamma)}\nabla^2\phi + \frac{2V}{1+\gamma}(1 + \frac{V}{2m_oc^2})\phi \quad (6)$$

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

$$E\phi(r) = -\frac{\hbar^2}{m_o(1+\gamma)}\{\beta^2 - \frac{2\beta(s+1)}{r} + \frac{s(s+1)}{r^2}\}\phi(r) +$$
$$\frac{2V}{1+\gamma}(1 + \frac{V}{2m_oc^2})\phi(r)$$
$$(7)$$

B. Approximate Trial Solution

The relativistic wave equation is completely general until one supplies a potential. In the case of the modified Dirac equation two parameters are added to account for the electrostatic field of a point charge and the electron's magnetic moment. However, necessary correction to the Coulomb potential because of the structure of the electron can easily be computed and shown in figure1.

$$V_{Coul.}(r) = -\frac{Ze^2}{4\pi\epsilon_o r} \quad (8)$$

$$\Delta V(r) = V_{Coul}(r) - \int_\infty^r u^{f*}(x)u^f(x)dx \quad (9)$$

The classical potential that is singular at the origin will be used and this can be partially corrected for the fact the electron has a distributed charge once an initial solution has been obtained. 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.

r radial coordiante in units $1/\Kappa$

Potential

Electron's structural potential
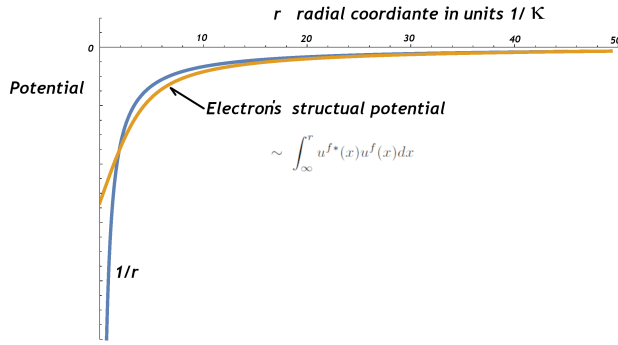
$\sim \int_{\infty}^{r} u^{f*}(x)u^f(x)dx$

1/r

Figure 1 **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 scale of $\hbar/mc = 3.86 \times 10^{-13}m$. (Wallace and Wallace, 2015)**

The two potential terms in the relativist wave equation become:

$$V + \frac{V^2}{2m_oc^2} = -\frac{Ze^2}{2(1+\gamma)\pi\epsilon_o r} + \frac{1}{(1+\gamma)m_oc^2}\frac{Z^2e^4}{(4\pi\epsilon_o)^2 r^2} \tag{10}$$

Substituting the classical potential and separating in terms of r allows E, s and β to be computed as all factors of r^m must be equal to zero.

$$E + \frac{\hbar^2\beta^2}{m_o(1+\gamma)} =$$
$$\frac{1}{r}\{-\frac{2\hbar^2\beta(s+1)}{m_o(1+\gamma)} - \frac{Ze^2}{2(1+\gamma)\pi\epsilon_o}\} + \tag{11}$$
$$\frac{1}{r^2}\{-\frac{\hbar^2 s(s+1)}{m_o(1+\gamma)} + \frac{1}{(1+\gamma)m_oc^2}\frac{Z^2e^4}{(4\pi\epsilon_o)^2}\}$$

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

$$s^2 + s = \frac{Z^2e^4}{(4\pi c\hbar\epsilon_o)^2} = \alpha^2 Z^2 \tag{12}$$

$$s = \sqrt{1 + 4Z^2\alpha^2} - 1 \tag{13}$$

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

$$\beta = \frac{1}{s+1}\frac{m_o}{\hbar^2}\frac{Ze^2}{4\pi\epsilon_o} = \frac{Z\alpha}{\sqrt{1+4Z^2\alpha^2}}\frac{m_oc}{\hbar} = \frac{Z}{a_o\sqrt{1+4Z^2\alpha^2}} \tag{14}$$

Then the expression for the ground state energy of the 1S state when the factor representing the reduce mass effect is applied where m_N is the nucleon mass. (Bethe and Salpeter, 1957).

$$E = -\frac{m_oc^2}{(1+\gamma)}\frac{Z^2\alpha^2}{1+4Z^2\alpha^2}\frac{m_N}{m_o+m_N} \tag{15}$$

The wave function then becomes:

$$\Phi(r,t) = Ar^{\sqrt{1+4Z^2\alpha^2}-1}\ e^{-\frac{Zr}{a_o\sqrt{1+4Z^2\alpha^2}}-i\frac{Et}{\hbar}} \tag{16}$$

where a_o is the Bohr radius. The interesting feature of the bound state wave function is that it does not contain γ as does the free particle relativistic wave function. Whereas, γ is firmly embedded in the ground state energy expression. It is also a principal parameter in the particle's own self-reference frame that can control the particle's convergence. In free space relativity functions to produce both spatial contraction and time dilation in all massive particle (Wallace and Wallace, 2014a). However, in a bound state we are not dealing with classical orbits rather the direct effect of a potential field on a particle's structure. The correction to the 1S ground state energy of hydrogen by the Schrödinger equation solution is small due to taking into account the difference between the static charge distribution and the point charge description of the electron (Wallace and Wallace, 2015).

The small wave function changes are found in table II in terms of the r^s factor that is practically a factor of 1 and the exponential factor is little changed from the Z scaling of the Schrödinger equation solution. So that the wave function is much the same as found in the ground state Schrodinger solution. The bound state wave function for the ground state in the laboratory frame is independent of γ, whereas the energy level is γ dependent. The modified Dirac ground state wave function is singular at the origin and will not be dealt with because its resulting energies for the ground state as a function of Z closely follow the Schrödinger energy values and will be similarly affected by the electron charge distribution correction (Bethe and Salpeter, 1957).

To expose the electron's structure in a bound structure, higher field levels are needed and are found in one electron ion's with higher nuclear charges, Z. There is no parameter γ in either the modified Dirac or Schrödinger ground state energy expressions. The energies of the ground state from the three different equations for hydrogen are shown in table III.

The shift in the ground state energy due to an elec-

Table II β **and** s **that yields** ~ 1 **for** $r \leq 1$ **with little affect on the the wave function in equation 16 close to the origin.**

Z	β	s
1	.998935	.000106497
2	1.99957	.000212983
4	3.99829	.000425920
8	7.99319	.000851659
16	15.9728	.001702594
32	31.8915	.003402299

Table III **All three ground state energies are close to the experimental value but that is not sufficient proof to find these numbers useful on their own. No corrections have been made for electron charge distribution that reduce the binding energy.**

Method	Energy eV	Difference eV
Experiment	-13.598433	-
Schrödinger Table I	-13.605693	+ 0.000146
Mod. Dirac Table I	-13.598468	- 0.000035
Rel. Wave eq. 1	-13.595391	+ 0.003042

Table IV **First order corrections to the Schrödinger ground state energies,** $< 1S|\Delta V|1S >$**, due to the finite scale of the electron that corrects the singular** $1/r$ **potential, (Wallace and Wallace, 2015). With increasing** Z **these are large corrections and close to the corrections for the modified Dirac equation ground state energies. The correction ruins the seemingly good** Z **dependence to both the Schrödinger and Dirac ground state energies in eV.**

Z	1S Table I	Correction	Exp.	Cor. col. # 2
1	-13.605693	+.0071189	**-13.598433**	**-13.598574**
2	-54.422772	+.1113908	**-54.41776**	**-54.308864**
4	-217.69109	+1.7035464	**-217.71858**	**-215.98754**
8	-870.76436	+24.88695	**-871.4101**	**-845.87741**
16	-3,483.0514	+332.8845	**-3,490.4189**	**-3,150.1729**
32	-13,932.23	+3,809.444	**-14,119.435**	**-10,122.79**

tron with structure take both the Schrodinger and Dirac ground state solutions far from the measured experimental values. Unlike the normal corrections to bound state energies eg. Lamb shift contribution these changes are large.

V. PARTICLES WITH STRUCTURE

A weak point in the Dirac and Pauli arguments for their relativistic wave equation is that it is specifically designed for the electron. With a general derivation for the particle structure in its own frame of reference the second order equations generate two solutions restricted to a single spatial spherically symmetric variable, r. 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, γ the ratio of the particle energy to its self-energy. Dynamics is not expressed in this space, except through the parameter γ for an unbound particle (Wallace and Wallace, 2014a).

A. Origin of Fermion and Boson Statistics

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

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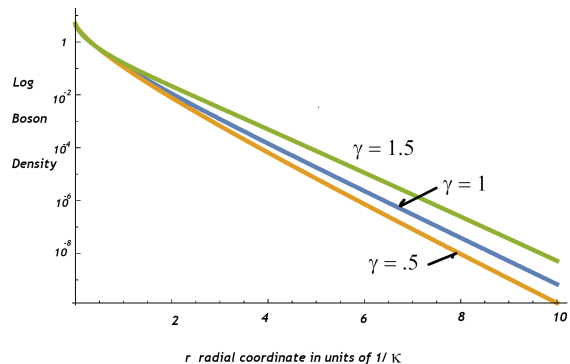

Figure 2 **Origin of the Bose-Einstein condensate is seen in the shrinkage of the boson density function in an external binding potential.**

As Z goes to higher values for the one electron ions the Dirac values for the ground state energy are quite good and close to the experimental values. However, the details are buried within the calculation of the ground state energy. In the development of the modified Dirac equation a set of corrections include the spin angular momentum of the electron and its associated field.
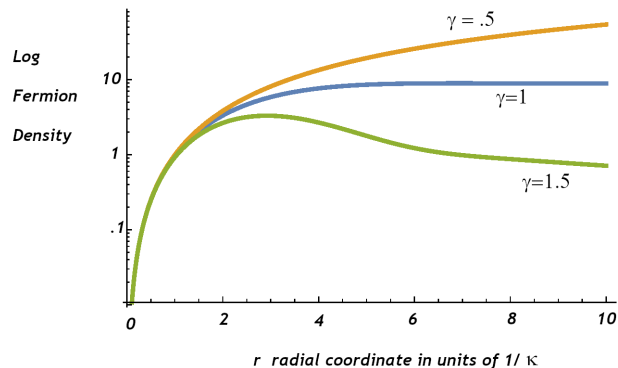
bound state   *rest*   *free*

Figure 3 **Origin of fermion repulsion is seen in the wave function diverging at large r in an external binding potential.**

$$0 < \gamma < 1 \quad \Longleftarrow \quad \gamma = 1 \quad \Longrightarrow \quad \gamma > 1$$

The two corrections in the modified Dirac equation deal with the electrostatic and magnetic fields, not the structure of the electron, which is still a point. There are no corrections in the Schrödinger equation that implies the corrections of the Dirac equation are canceling out each other. The finite core size of the electron only produces a small correction for the hydrogen atom. Conveniently the magnetostatic/angular moment contribution to the electron's ground state energy can be treated separately so that the relativistic wave equation potential only need contain the electrostatic field (Wallace and Wallace, 2020).

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 is not a stable particle, its wave function is divergent and grows. However, in a bound state this divergence is controlled by the binding potential and γ can take on values that are less than 1.

Table V **Computed values from equation 15 of γ an approximation to correct the bound state energies.**

z	γ estimate
1	.9995563
2	.998204
4	.9928343
8	.9715725
16	.8905061
32	.6200965

The main approximation that has been made in the examples thus far was that relativistic field equation was not solved with either a correct electron or nuclear electrostatic potentials as these become γ dependent and alter the entire problem. The solutions with classical Coulomb potential of equation 5 only can be used a guide. The reason is that γ decreases below 1 the bound state energy also drops to lower negative values making the binding stronger. Competing against that is the electron's distributed charge and the spreading of the electron wave function with increasing Z that will reduce the binding energy. The equations have to be solved numerical to minimize the energy because the potential is now coupled to the solution. Analogous to a return to Thomas-Fermi and the associated methods that followed.

At a $Z = 1$ the collection of corrections to the ground state energy are small. As Z increases the competition between greater binding and the electron's finite scale not helping brings in two large and competing contributions to the ground state energy that destroy the Schrödinger/Dirac approximations at increasing Z. The only way to recover the ground state energy is properly include the relativistic effect on energy with γ taking on values less than one. This single electron ion behavior at high Z is an extreme case, however, this changes the way normal nucleon binding with two competing fields, electrostatic and strong force, tied to boson and fermion structure respectively need to be treated.

VI. ACKNOWLEDGMENT

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