Hydrogen atom

Exotic state. Part two

Arayik Emilevich Danghyan E-mail <u>araik_d@hotmail.com</u>

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Introduction

In the study of the hydrogen atom, in order to reveal all the details of the behavior of an electron, one of the main conditions is the use of the correct, appropriate equations. Until recently, this applied Schrödinger equation, Klein-Gordon and Dirac. Schrödinger equation will not analyze because it is not relativistic, and therefore can not qualify for a full and accurate description of the range of high energies and velocities.

It will be shown as the Klein-Gordon equation is also unacceptable, because the assumption is deeply disguised errors in the derivation of this equation.

Since, in connection with the intended purpose, we will analyze the behavior of an electron in the states with energy below the ground state, it will be shown that the same should be treated with some suspicion in this regard to the results of the Dirac equation.

As a result, the only acceptable equation is the equation M2 [1].

An analysis of the equations of quantum mechanics

In the [1] work we can see a brief conclusion stationary Klein-Gordon equation (KGE). A key feature of the Klein-Gordon equation is the fact that it reflects, in the form of a differential equation, the ratio of the energy and momentum of the Special Theory of Relativity (SRT) $E^2 - p^2c^2 = m^2c^4$ (1.1)

Next in the work [1] are provided the analytical solutions of KGEfor the isoelectronic series of hydrogen in the ground state. As a result of the decision, a formula for the ground-state energy in the following form:

$$E_0(Z) = 27.2 * \left[\frac{\sqrt{c^4 + c^4 \sqrt{\frac{c^2 - 4Z^2}{c^2}}}}{\sqrt{2}} - c^2 \right] eV \quad (1.2)$$

Comparative analysis of the solutions obtained with the experimental data showed that with increasing deviation of the charge Z the nucleus greatly increase. Looking at the formula (1.2) can be seen that under the square root is the expression: $\frac{c^2 - 4Z^2}{c^2}$ Hence we can write $\frac{c^2 - 4Z^2}{c^2} \ge 0$ which

implies inequality $Z \le \frac{c}{2}$ (1.3) $r \exists e Z \in [1 \div 137]$ the charge of the nucleus of a hydrogen ion,

c = 137.03599971 speed of light in Hartree's atomic units. Hence from (1.3) we obtain $Z \le 68$. This means that the excess charge of the nucleus Z > 68 the solution of KGE frustrated and under the square root of a negative value is obtained.

The above calculation demonstrates the fallacy of Klein-Gordon equation, since this situation was due to happen at Z > 137 and not at Z > 68.

Now let's look at why there was this erroneous situation and what will eliminate this error.

When the derivation of the Klein-Gordon equation in the expression of the binding energy and momentum SRT (1.1) we substitute the expression of a square pulse of the wave function $p^{2} = -\frac{\hbar^{2}}{\Psi}\Delta\Psi$ we think that got relativistic pulse square. That is, we think that $-\frac{\hbar^{2}}{\Psi}\Delta\Psi = \frac{m^{2}v^{2}}{1-\frac{v^{2}}{c^{2}}}$

(Or rather thought so, Klein and Gordon in the derivation of the equation).

But in fact, the equation takes the expression $p^2 = -\frac{\hbar^2}{\Psi} \Delta \Psi$ (1.4) as a regular square of pulse

$$-\frac{\hbar^2}{\Psi}\Delta\Psi = m^2 v^2$$

Why it is like that? Let us leave this question to deep theorists. And we are interested in the practical side of the issue. That is, the elimination of errors in the Klein-Gordon equation.

In one word, the relativistic momentum of the square is not determined by the expression $p^2 = -\frac{\hbar^2}{W} \Delta \Psi$. And so we get the erroneous Klein-Gordon equation.

Now, if we rewrite the expression (1.1) in the unfolded state $E^2 - \frac{m^2 v^2}{1 - \frac{v^2}{c^2}}c^2 = m^2 c^4$ and make the

necessary changes: $E^2 - \frac{m^2 v^2}{1 - \frac{m^2 v^2}{m^2 c^2}} c^2 = m^2 c^4$ and substitute already normal square pulse $p^2 = m^2 v^2$ in

its place. We will get: $E^2 - \frac{p^2}{1 - \frac{p^2}{m^2 c^2}} c^2 = m^2 c^4$ (1.5). Rewriting the expression (1.5) in a suitable

form we get: $m^2c^2 - p^2 = \frac{m^4c^6}{E^2}$ (1.6), which is corresponding to expression (2.5) in the article <u>"The</u> new equation of relativistic quantum mechanics "[1].

Thus, for a proper understanding of the expression for the square pulse (1.4), instead of the erroneous Klein-Gordon equation, we get the correct equation M2.

$$\Delta \Psi - \frac{1}{\hbar^2} \left[\frac{m^4 c^6}{(E - U(\vec{r}))^2} - m^2 c^2 \right] \Psi = 0 \quad (1.7)$$

Comments on the Dirac equation we will give later, when comparing the solutions with solutions of the equation M2.

The radial equation M2 for the hydrogen atom

In work [2] was given enough the corner solution of the equation M2. So we go straight to the solution of the radial equation. It is important for us that the quantum number can take as whole and

half-integer values, including the value of $l = -\frac{1}{2}l = -\frac{1}{2}, 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}, \dots$ Justification is in the works [2] and [4]. A special case $l = -\frac{1}{2}$ we will be consider separately. Let us rewrite the radial equation M2 for hydrogen-like ions with nuclear charge Z:

$$\frac{d^{2}R}{dr^{2}} + \frac{2}{r}\frac{dR}{dr} - \frac{l(l+1)}{r^{2}}R - \frac{1}{\hbar^{2}}\left[\frac{m^{4}c^{6}}{\left(E + \frac{Ze^{2}}{4\pi\varepsilon_{0}r}\right)^{2}} - m^{2}c^{2}\right]R = 0 \quad (2.1)$$

Next we will apply the Hartree's atomic system of units. $a_0 = 1, m = 1, e = 1, \hbar = 1, c = 137.03599971, 4\pi\varepsilon_0 = 1.$

Let us rewrite the equation (1.1) in Hartree's atomic units:

$$\frac{d^{2}R}{dr^{2}} + \frac{2}{r}\frac{dR}{dr} - \frac{l(l+1)}{r^{2}}R - \left[\frac{c^{6}}{\left(E + \frac{Z}{r}\right)^{2}} - c^{2}\right]R = 0$$
(2.2)

To solve the resulting equation, we use mathematical Web Resources **WolframAlpha** <u>http://www.wolframalpha.com/</u>

The solution of equation (2.2) is the sum of two linearly independent parts. Generalized Laguerre polynomials and confluent hypergeometric function of the second kind.

Let us use a second linearly independent solutions. That is:

$$R(r) = \frac{1}{r}k_{1} \exp\left(-\frac{r\sqrt{c^{6}-E^{2}c^{2}}}{E}\right)(Er+Z)^{\frac{1}{2}\sqrt{4L+\frac{4Z^{2}c^{6}}{E^{4}}+1}+\frac{1}{2}} + \text{HypergeometricU}\left(\frac{\left(\sqrt{4L+\frac{4Z^{2}c^{6}}{E^{4}}+1}+1\right)E^{4}-c^{4}\left(\sqrt{4L+\frac{4Z^{2}c^{6}}{E^{4}}+1}+1\right)E^{2}+2Zc^{4}\sqrt{c^{6}-E^{2}c^{2}}}{2E^{2}(E^{2}-c^{4})}, \sqrt{4L+\frac{4Z^{2}c^{6}}{E^{4}}+1}+1, \frac{2\sqrt{c^{6}-E^{2}c^{2}}(Er+Z)}{E^{2}}\right)\right)$$

Where HypergeometricU is confluent hypergeometric function of the second kind, k_1 constant of integration. L = l(l+1) where l is orbital quantum number.

As it is known, the first parameter of the confluent hypergeometric function is the radial quantum number with a minus sign $-n_{rad}$.

From these considerations, we obtain the equation for determining the energy of the ground state and the excited states of hydrogen ions in the following form:

$$\left[\underbrace{\left(\sqrt{4L + \frac{4Z^2c^6}{E^4} + 1} + 1 \right) E^4 - c^4 \left(\sqrt{4L + \frac{4Z^2c^6}{E^4} + 1} + 1 \right) E^2 + 2Zc^4 \sqrt{c^6 - E^2c^2}}_{2E^2 \left(E^2 - c^4 \right)} \right] = -n_{rad} (2.3)$$

First, let us find the solution of equation M2 for ordinary hydrogen states. Solving the equation (2.3) with parameters $n_{rad} = 0$ and l = 0 we obtain the formula of energy of the ground state of hydrogenlike ions in Hartree's atomic units in the following form: $E_0(Z) = \sqrt{c^4 - c^2 Z^2}$ (2.4) Received energy includes energy electron rest. With this in mind, we write the final formula of the energy in electron-volts.

 $E_0(Z) = 27.2 * \left(\sqrt{c^4 - c^2 Z^2} - c^2\right) eV$ (2.5) The received formula for the ground state energy of a hydrogen number coincides exactly with the corresponding Dirac formula.

Let us define the energy of the hydrogen atom for the ground state l = 0, $n_{rad} = 0$ and the first excited state with orbital angular momentum l = 0, $n_{rad} = 1$.

Substituting values Z = 1, c = 137.03599971 in formula (2.5) we get the energy of the ground state:

$$E_0(1) = 27.2 * \left(\sqrt{137.03599971^4 - 137.03599971^21^2} - 137.03599971^2\right) = -13.6001810593938 \text{ eV}$$

Solving the equation (2.3) with parameters $l = 0, n_{rad} = 1, Z = 1, c = 137.03599971$ we obtain the energy of the first excited state: $E_1(1) = 27.2 * (-0.124997088038) = -3.3999207946 \text{ eV}.$

On the basis of energy, we build a graph of the normalized radial probability density for the ground state and the first excited state Pic.1.

From equation (2.3) we can get quite compact universal formula for calculating the number of hydrogen-energy, in the ground and excited states, for equation M2, under conditions of equality of radial and orbital quantum numbers: $n_{rad} = l = n$.

$$E = \pm \frac{c\sqrt{c^2 + 4c^2n + 4c^2n^2 - Z^2}}{\sqrt{1 + 4n + 4n^2}}$$
(2.6)

The quantum number *n* takes values from a number of $n = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}, \dots$ with the pitch $\frac{1}{2}$. There are some differences in the interpretation of quantum numbers of the Dirac equation and the equation M2. At that dwell in this paper we will not. If the value of the quantum number n = 0 formula (2.6) becomes the ground state energy of the formula (2.4) as it was expected.

We use only the positive values of energy, although the equation M2 provides symmetric solutions. Decisions by the formula (2.6) is in very good agreement with the experimental values.



Pic.1 Normalized radial probability density of the ground state and the first excited state in the Hartree's atomic units.

Exotic, highly localized, compact hydrogen status

Let us construct a graph of dependingenergy on the radial quantum number for a spherically symmetric states with orbital angular momentum l = 0 according to the equation (2.3) Pic.2. In the same figure we construct the corresponding graph l = 0 Dirac's equation for comparison. In the graph point 1 corresponds to the ground state l = 0, $n_{rad} = 0$. Point 2 corresponds to the first excited state l = 0, $n_{rad} = 1$.

As you can see, in the energy range above the ground state, that is above the point 1, the solution of the Dirac equation and M2 are exactly the same. This is the area of conventional excited states. However, at energies below the ground state, the behavior of the equations are fundamentally different. In this area the equation M2 has a characteristic bend. As a result of this behavior there is

formed point 3. This is the point of intersection of the graph energy with the line $n_{rad} = -\frac{1}{2}$. Point 3

is a potential solution to the high localization electronin the nucleus and a high binding energy. As you can see these solutions in the Dirac equation are missing. Therefore, as it was said, in the energy range below the ground state to the solutions of the Dirac equation given in various papers [5],[6],[7],[8], should be treated with caution.



Pic.2 The graph of the energy from the radial quantum number n_{rad} at l = 0 for the Dirac's equation and M2.

The assumption of the existence of compact localized states of the hydrogen atom, suggests the presence of high binding energy. The binding energy must be higher than the accepted ground state. And this in its turn requires displacement of the radial or orbital quantum number to negative values $n_{rad} < 0$ or l < 0. Looking at the graph of the energy of the quantum number n_{rad} Pic. 2. we can see

that this value is $n_{rad} = -\frac{1}{2}$. When l < 0 is special and will be considered separately. In this case the only possible negative value is $l = -\frac{1}{2}$.

Let us determine the energy of the localized state 3 by solving the equation (2.3) with parameters

 $l = 0, n_{rad} = -\frac{1}{2}$. The solution gives $E = \frac{\sqrt{c^4 - c^3 \sqrt{c^2 - 16Z^2}}}{\sqrt{2}}$ (3.1) Substituting in the formula we got the value of the speed of light c = 137.03599971 and the nuclear charge value Z = 1 we obtain

energy E = 274.10119971623305 in Hartree's atomic units. The energy includes energy electron rest mc^2 . With this in mind we define the binding energy and transform it into electron-volts $E = 27.2*(274.10119971623305 - 137.03599971^2) = -503329.5812570386 \text{eV}.$

Let us build the graph of the normalized radial wave function for the state 3. Pic. 3.





$E = -503329.5812570386 \,\mathrm{eV}$

As we can see the wave function tends to infinity $r \to 0$. But such behavior can not be considered natural because this is a consequence of an infinite increase in the negative direction of Coulomb potential when $r \to 0 - \frac{Z}{r} \to -\infty$. In reality, the potential is different from the Coulomb at $r \to 0$ is limited from below, since the core is not a point but has dimensions. Let us build a graph of normalized radial probability density for the state 3. Pic. 4.

Thus, we have shown the possibility of the existence of the hydrogen atom is strongly localized, compact states with high binding energy.



Manipulating the quantum numbers l and n_{rad} within the acceptable range, it is possible to obtain a family of solutions. We show this as a family of graphs Pic.5. Followed by a table of values corresponding to the energy and quantum numbers.



Pic.5 A family of graphs of energy from the radial quantum number n_{rad} for different values of the quantum number $l = 0, \frac{1}{2}, 1, \frac{3}{2}, 2$

l\n	-1/2	-1	-3/2	-2	-5/2	-3	-7/2	-4	-9/2	-5
0	-503330	-	-	-	-	-	-	-	-	-
1/2	-507058	-460092	-	-	-	-	-	-	-	-
1	-508300	-479790	-455327	-	-	-	-	-	-	-
3/2	-508921	-488160	-475050	-453404	-	-	-	-	-	-
2	-509294	-492901	-483786	-472899	-452362	-	-	-	-	-
5/2	-509543	-495977	-488919	-481637	-471665	-451708	-	-	-	-
3	-509720	-498141	-492348	-486844	-480348	-470863	-451259	-	-	-
7/2	-509853	-499749	-494819	-490371	-485555	-479486	-470300	-450933	-	-
4	-509957	-500992	-496692	-492945	-489107	-484673	-478869	-469883	-450684	-
9/2	-510040	-501982	-498164	-494917	-491718	-488225	-484030	-478405	-469561	-450488
5	-510107	-502789	-499353	-496483	-493732	-490847	-487573	-483541	-478043	-469305

The binding energies of a compact hydrogen atom, depending on the quantum numbers eV

Compact hydrogen atom and the annihilation peak

In various natural phenomena in the solar corona radiation, cosmic radiation, the study of storm clouds, is often observed gamma photons with energies $E = mc^2 \approx 511$ keV. Such radiation is usually explained by the annihilation of electron-positron pairs. But in many cases, to explain the existence of antimatter in the observed area, is simply impossible.

Researcher J.Va'vra [5] hypothesized that radiation 511 keV It may be due to electron trapping proton on a low orbit, during the formation of a compact hydrogen atom.

We currently test this hypothesis.

The radiation with energy mc^2 means that all the energy of the electron is emitted, and therefore should be substituted in the equation of energy value E = 0. Let us rewrite the equation M2 with

energy $E = 0 \Delta \Psi - \frac{1}{\hbar^2} \left[\frac{m^4 c^6}{(-U(\vec{r}))^2} - m^2 c^2 \right] \Psi = 0$ (4.1). In [2] it was enough given the corner solution

of the equation M2. So we go straight to the solution of the radial equation. We write the equation of the radial M2 Hartree's atomic units considering E = 0, Z = 1.

 $\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \frac{l(l+1)}{r^2}R - \left|\frac{c^6}{\left(\frac{1}{r}\right)^2} - c^2\right|R = 0 \quad (4.2) \text{ To solve the resulting equation, we use}$

mathematical Web Resources **WolframAlpha** <u>http://www.wolframalpha.com/</u> The solution has this form:

$$R(r) = \frac{k_{1}2^{\frac{1}{4}(1-2l)}(r^{2})^{\frac{1}{4}(1-2l)}e^{-\frac{1}{2}c^{3}r^{2}}}{r^{\frac{3}{2}}} \text{HypergeometricU}\left(\frac{-2lc+c-1}{4c},\frac{1}{2}-l,c^{3}r^{2}\right)}{k_{2}2^{\frac{1}{4}(1-2l)}(r^{2})^{\frac{1}{4}(1-2l)}e^{-\frac{1}{2}c^{3}r^{2}}}\text{LaguerreL}\left(-\frac{-2lc+c-1}{4c},-\frac{1}{2}-l,c^{3}r^{2}\right)}{r^{\frac{3}{2}}}$$

$$(4.3)$$

That is, the sum of two linearly independent parts. Confluent hypergeometric function of the second kind, and generalized Laguerre polynomials.

We use the first linearly independent solutions.

$$R(r) = \frac{k_1 2^{\frac{1}{4}(1-2l)} \left(r^2\right)^{\frac{1}{4}(1-2l)} e^{-\frac{1}{2}c^3 r^2} \text{HypergeometricU}\left(\frac{-2lc+c-1}{4c}, \frac{1}{2}-l, c^3 r^2\right)}{r^{\frac{3}{2}}}$$
(4.4)

Where HypergeometricU is confluent hypergeometric function of the second kind and k_1 integration constant.

As we consider the case when all of the energy of an electron emitted, it is natural to obtain state power $E_0 = -mc^2 = -(137.03599971)^2 = -18778.8652165$ in Hartree units. We transform into electron-volts $E_0 = 27.2 * (-18778.8652165) = -510785.13388932 \text{ eV}$. Now it's time to consider the special case when $l = -\frac{1}{2}$. We substitute this value in equation (4.4) and determine the constant of

integration k_1 from the normalization condition $\int_{0}^{\infty} k_1^2 R(r)^2 4\pi r^2 dr = 1 \quad (4.5). \quad k_1 = 361.23722848$





Let us plot the graph of normalized radial probability density at $l = -\frac{1}{2}$ Pic. 7.



We define the orbital radius, ie the distance from the origin to the point of maximum probability density. $r_0 = 0.00012715729$ in atomic units. Multiplying this value by the Bohr radius $a_0 = 52.9 \times 10^{-12}$ M we get $r_0 = 0.00012715729 \times 52.9 \times 10^{-12} = 0.006726620641 \times 10^{-12}$ M. Thus, by solving the equation M2, it was proved the possibility of existence, unknown to date state of the hydrogen atom with the following parameters: The value of the quantum number $l = -\frac{1}{2}$. State energy value $E_0 = -510785.13388932$ eV. The value of the orbital radius $r_0 = 0.006726620641 \times 10^{-12}$ M.In the formation of the state of energy is released $E = mc^2 \approx 511$ keV, that supports the hypothesis of J.Va'vra [5] about the origin of the annihilation peak associated with the formation of a compact hydrogen atom.

Numerical solution in cylindrical coordinates

As in the previous time [2], when applying the non-standard value of the quantum number $l = -\frac{1}{2}$, it is desirable to further evidence obtained analytical solutions. In a previous paper [2], this question is set out in detail. Therefore, we write the equation immediately M2 in cylindrical coordinates with the value of the energy E = 0, and with the value of the quantum number m = 0. This means that the binding energy is equal to $E_0 = -510785.13388932$ eV. For hydrogen Z = 1.

$$\frac{\partial^2 R}{\partial r^2} + \frac{1}{r} \frac{\partial R}{\partial r} + \frac{\partial^2 R}{\partial z^2} - \left[\frac{c^6}{\left(\frac{Z}{\sqrt{r^2 + z^2}}\right)^2} - c^2 \right] R = 0 \quad (5.1)$$

To solve the equation (5.1) we will use a software package for the numerical solution of systems of differential equations **FlexPDE**<u>http://www.pdesolutions.com/</u>

As a result, the numerical solution we got the following values of the parameters of the hydrogen in the state E = 0. Binding energy $E_0 = -510744.2 \text{ eV}$, orbital radius $r_0 = 0.007460784*10^{-12} \text{ M}$.

Which has a good agreement with the analytical solution.

Numerical solution revealed:

- 1. The equation for the hydrogen state with a binding energy $E_0 = -510785.13388932 \text{ eV}$ has sufficiently high convergence.
- 2. Concerns about the singular behavior of the angular part of the wave function are groundless.
- 3. Therefore, there are sufficient grounds for the expediency of an experimental hydrogen research in the state c $E_0 = -510785.13388932 \text{ eV}$ and $r_0 = 0.006726620641*10^{-12} \text{ M}.$

Below we present the results of the decision in the form of two-dimensional and three-dimensional graphs of the radial probability density.



M2Z=1: Grid#6 p2 Nodes=18691 Cells=9240 RMS Err= 9.4e-7 E0 eV= -510785.1 E eV= -510744.2 Orbital Radius*52.9 (pm)= 7.460784e-3 Surf_Integral= 1.648877e-4

Pic.8 The two-dimensional graph of the radial probability density





Pic.9 The three-dimensional graph of the radial probability density



M2Z=1: Grid#6 p2 Nodes=18691 Cells=9240 RMS Err= 9.4e-7 E0 eV= -510785.1 E eV= -510744.2 Orbital Radius*52.9 (pm)= 7.460784e-3 Vol_Integral= 1.633578e-7

Pic.10 The projection of the three-dimensional radial probability density

Results and discussion

It was found and fixed a mistake in the Klein-Gordon equation. As a result, it was confirmed the correctness of the equation M2. Consequently, the subject of perennial debate about the controversy SRT and quantum mechanics, can be considered exhausted.

The use of equation M2 for the hydrogen atom, revealed additional subtleties in the behavior of the electron. It was found a family of strongly localized states with high binding energy. The values of energy, depending on the quantum numbers. In many works [5],[6],[7],[8], were presented similar solutions of the Dirac's equation. However, in the second section, it was shown that the Dirac's equation does not have this behavior. And without further manipulation of the Coulomb potential, such solutions will not work. Further analytical and numerical solution of the equation M2 was proved the hypothesis J.Va'vra [5] about the origin of the annihilation peak associated with the formation of a compact hydrogen atom. The parameters of this state have been obtained: the binding energy $E_0 = -510785.13388932 \,\text{eV}$ and orbital radius $r_0 = 0.006726620641*10^{-12} \,\text{M}$.

I think there were represented enough theoretical bases for the organization of experimental research described states of the hydrogen atom.

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