Derivation of the Pauli Exclusion Principle and Meaning Simplification of the Dirac Theory of the Hydrogen Atom

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Abstract: In general, the Pauli Exclusion Principle follows from the spectroscopy whereas its origin is not good understood. To understand fully this principle, most important is the origin of quantization of the azimuthal quantum number i.e. of the angular momentum quantum number. Here, applying the theory of ellipse and starting from very simple physical condition, we quantized the azimuthal quantum number. The presented model leads directly to the eigenvalue of the square of angular momentum and to the additional potential energy that appears in the equation for the modified wave function. We formulated also a very simple semiclassical analog to the Dirac and Sommerfeld theories of the hydrogen atom. The constancy of the base of the natural logarithm for the quantum fields is the reason that the three theories are equivalent.

1. Introduction

The Pauli Exclusion Principle says that no two identical half-integer-spin fermions may occupy the same quantum state simultaneously. For example, no two electrons in an atom can have the same four quantum numbers. They are the principal quantum number n that denotes the number of the de Broglie-wave lengths λ in a quantum state, the azimuthal quantum number l (i.e. the angular momentum quantum number), the magnetic quantum number m and the spin s.

On the base of the spectrums of atoms, placed in magnetic field as well, follows that the quantum numbers take the values:

$n = 1, 2, 3, \ldots$
$l = 0, 1, 2, \ldots, n - 1$
$m = -l, \ldots, +l$
$s = \pm 1 / 2$.

The three first quantum numbers n, l, and m are the integer numbers and define a state in which can be maximum two electrons with opposite spins.

The magnetic quantum number m determines the projection of the azimuthal quantum number l on the arbitrary chosen axis. This axis can overlap with a diameter of the circle $l = 0$.

To understand fully the Pauli Exclusion Principle we must answer following questions concerning the azimuthal quantum number l:

1.
What is physical meaning of this quantum number?
2.
Why the l numbers are the natural numbers only?
3.
Why the zero is the lower limit?
4.
Why the $n - 1$ is the upper limit?

To answer these questions we must apply the theory of ellipse, especially the formula for its circumference C and eccentricity e. When we use the complete elliptic integral of the second kind and the Carlson symmetric form [1], we obtain for circumference C of an ellipse following formula

$$C = 2\,\pi\,a\,[1 - (1/2)^2 e^2/1 - (1{\cdot}3/(2{\cdot}4))^2 e^4/3 - (1{\cdot}3{\cdot}5/(2{\cdot}4{\cdot}6))^2 e^6/5 - \ldots], \quad (1)$$

where a is the major radius and e is the eccentricity defined as follows

$$e = [sqrt(a^2 - b^2)]/a, \quad (2)$$

where b is the minor radius.

Here, we formulated as well the very simple semiclassical analog to the Dirac and Sommerfeld theories of the hydrogen atom and proved that these three theories are equivalent.

2. Calculations
2.1 Angular momentum quantum number

In the figure, the circumference of the ellipse $C_{de\text{-}Broglie}$ is $C_{de\text{-}Broglie} = n\,\lambda = 2\,\pi\,n\,\lambdabar,$ where the n is the principal quantum number whereas the $\lambdabar$ is the reduced de Broglie-wave length. Assume that there are allowed only ellipses that circumference is the arithmetic mean of the circumferences of two circles that radii are equal to the major and minor radii of the ellipse.
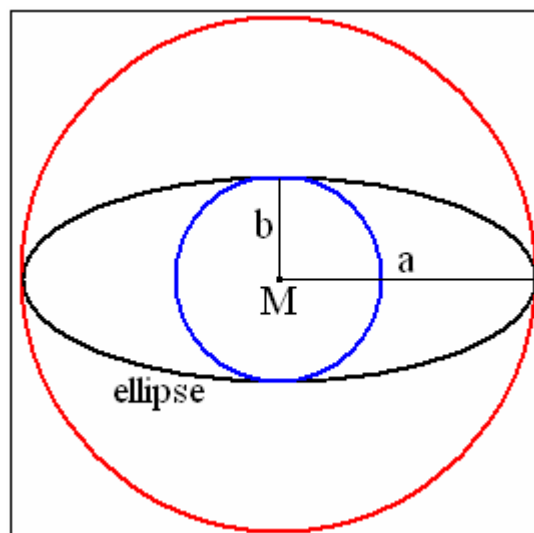
ellipse

Similarly as for the circumference of the ellipse, the circumferences of the circles must be equal to a natural number multiplied by the de Broglie-wave length. This leads to following definitions

$$a = j\,\lambda \text{ and } b = k\,\lambda. \tag{3}$$

Notice that $j = k = 0$ has no sense.
Then, we can rewrite formula (2) as follows

$$e = [sqrt(j^2 - k^2)]\,/\,j. \tag{4}$$

It is the natural assumption that the allowed circumferences of the ellipse should be the arithmetic mean of the sum of the circumferences of the two circles. It leads to following conclusion

$$(j + k)\,/\,2 = n. \tag{5}$$

Define some number l as follows

$$(j - k)\,/\,2 = l. \tag{6}$$

Formulae (5) and (6) lead to following relations

$$j = n + l, \tag{7}$$
$$k = n - l. \tag{8}$$

Since the j, k and n are the integers so the number l must be an integer as well.
Applying formulae (7) and (8) we can rewrite formula (4) as follows

$$e = 2\,[sqrt(n\,l)]\,/\,(n + l). \tag{9}$$

We can see that due to the square root, this formula has no real sense for $l < 0$. Since the l cannot be negative then from formulae (5) and (6) follows that $l < n$.
Applying formulae (3) and (7), we can rewrite formula (1) as follows

$$C_K = 2\pi(n + l)\lambda[1 - (1/2)^2 e^2/1 - (1\cdot3/(2\cdot4))^2 e^4/3 - (1\cdot3\cdot5/(2\cdot4\cdot6))^2 e^6/5 - \ldots]. \tag{10}$$

Notice that for $n = l$ is $e = 1$ and then $C_{de\text{-}Broglie} > C_K$ i.e. l cannot be equal to n. For $l = 0$ is $C_{de\text{-}Broglie} = C_K$ and because l cannot be negative then the $l = 0$ is the lower limit for l.
Some recapitulation is as follows. We proved that the azimuthal quantum number l
  1) is associated with transitions between the states j and k,
  2) is the integer,
  3) cannot be negative and the lower limit is zero,
  4) the $n - 1$ is the upper limit.
Some abbreviation of it is as follows
$l = 0, 1, 2, \ldots, n - 1.$

The Quantum Physics is timeless because a quantum particle disappears in one region of a field or spacetime and appears in another one, and so on. There are no trajectories of individual quantum particles. Quantum Physics concerns the statistical shapes and their allowed orientations. Such procedure simplifies considerably the Quantum Physics.

2.2 Eigenvalue of the square of angular momentum

An ellipse/electron-state we can resolve into two circles that radii are defined by the semi-axes of the ellipse. The two circles in a pair are entangled due to the exchanges of the binary systems of the closed strings (of the entanglons [2A]) the Einstein-spacetime components (from which are built all the Principle-of-Equivalence particles) consist of [2A]. Spin of the entanglons is 1 [2A] and they are responsible for the infinitesimal transformations that lead to the commutators [3]. Calculate a change in the azimuthal quantum number l when the smaller circle or one of identical two circles emits one entanglon (since in this paper is $j \geq k$ so there is the transition $k \to k - 1$) whereas the second circle in the pair almost simultaneously absorbs the emitted entanglon (there is the transition $j \to j + 1$). Such transition causes that ratio of the major radius to the minor radius of the ellipse (or circle) increases. From formula (5) follows that such emission-absorption does not change the principal quantum number n whereas from formula (6) follows that there is following transition for the azimuthal quantum number l: $l \to l + 1$. The geometric mean is $sqrt(\ l\ (l\ +\ 1))$ and this expression multiplied by $\hbar$ is the mean angular momentum L for the described transition. This leads to conclusion that eigenvalue of the square of angular momentum $\boldsymbol{L}^2$ is $l(l\ +\ 1)\hbar^2$.

The eigenvalue of the square of angular momentum leads to the additional potential energy E_A (it follows from the radial transitions i.e. from the changes in shape of the ellipses) equal to

$$E_A = L^2 / (2\ m\ r^2) = l\ (l\ +\ 1)\ \hbar^2 / (2\ m\ r^2). \tag{11}$$

The energy E_A appears in the equation for the modified wave function.

The theory of baryons [2A] shows that inside the baryons are only the $l = 0$ states (i.e. there are only the circles) so the quantum mechanics describing baryons is much simpler than for atoms.

2.3 The very simple semiclassical analog to the Dirac and Sommerfeld theories of the hydrogen atom

Since the fermions consist, at least for period of spinning, of the stable/classical structures/bare-fermions and of the quantum fields so the semiclassical theories are simplest, most fruitful and contain least parameters. And such method is not a mathematical trick – just in such a way behaves Nature.

Gravity is associated with the inverse square law. It is because gravitational fields are the gradients produced in the superluminal non-gravitating Higgs field by masses [2A]. There are the divergently moving classical tachyons so there appears the inverse square law

$$F \sim 1 / r^2. \tag{12}$$

Today, in the Higgs field cannot be created any virtual pairs as it is in the Einstein spacetime [2A]. The produced structures in the Einstein spacetime and associated with them virtual pairs cause that field ψ of the virtual pairs changes according following function [4]

$$\psi = \psi_o\, e^{-r}, \tag{13}$$

where $e \approx 2.718\ldots$ is close to the base of the natural logarithm. In reality, this formula is more complicated for $r \to 0$ because there appears torus/charge/spin and central condensate [2A]. It causes that the quantum physics is the incomplete theory. Notice that, for example, we define mean-lifetime in such a way that after this time there does not decay $1 / e$ particles. Amplitude ψ_o should be in proportion to coupling constant characteristic for a field i.e. $\psi_o \sim \alpha$. On the other hand, a physical meaning has following expression

$$\psi_o\, \psi_o \sim \alpha^{\,2}. \tag{14}$$

   Formulae (12) and (13) and associated with them the sets of applied methods differ very much so unification of gravity and quantum physics within one of the two sets is impossible.
   Due to the gluons→photons transitions on edges of the nuclear strong fields, there leaks the strong and weak structure of nucleons [2A]. Due to the quantum phenomena i.e. due to the disappearance of electric charge of electron in one place and appearance in another one, and so on, there as well leaks the weak structure of electrons [2A]. But, of course, there must be replaced the coupling constants of the nuclear strong and weak interactions for the fine-structure constant. The coupling constant at low energy for the strong interactions of pions is $\alpha_S = 1$, for weak interactions of baryons is $\alpha_{W(proton)} = 0.0187228615\ldots$, for the weak interactions of electrons is $\alpha'_{W(electron)} = 1.11943581\cdot10^{-5}$, whereas the fine-structure constant is $\alpha_{em} = 1/137.036001$ [2A]. On the other hand, due to the atom-like structure of baryons, [2A], and due to the structures that can appear in the Einstein spacetime due to the entanglement of the Einstein-spacetime components, there can arise wave functions in which the base of the natural logarithm should be replaced by two values $e_{ET,1} = 2.71954252$ or $e_{ET,2} = 2.71666667$ [4]. The geometric mean is $e_{ET,mean} = sqrt(e_{ET,1} \cdot e_{ET,2}) = 2.718104213$. Value of the $e_{ET,1}$ follows from formula $e_{ET,1} = 2 + B / A$, [4], where $A = 0.6974425..$ fm and $B = 0.5018395..$ fm and A and B define the atom-like structure of baryons $R = A + dB$, where $d = 1, 2, 4$ (all states are the $l = 0$ states) [2A]. Physical meaning of $e_{ET,1}$ and $e_{ET,2}$ is described here [4]. Value of the $e_{ET,2}$ follows from formula $e_{ET,2} = 1 + 1 + 1/2 + 1/6 + 1/24 + 1/120$.
   The above remarks show that instead the e we should apply $e_{ET,mean} = (fe)$, where $f = 0.9999347..$. Using these results calculate following expression

$$X = e_{ET,mean}^{\,-1}(\alpha_S + \alpha_{W(proton)} + \alpha'_{W(electron)}) = 0.374795805\ldots. \tag{15}$$

Can we quantize the value X i.e. can we write an expression that leads to X? Notice that

$$\boldsymbol{Y = m\ (1 - 1 / 2 - 1 / 8) / m_{electron}} = 0.374795880\ldots, \tag{16}$$

where m is the reduced mass of electron i.e. $m / m_{electron} = m_{proton} / (m_{proton} + m_{electron}) = 0.99945568\ldots$ [2A].
   It leads to following expression

$$Y = m\ [1 - \Sigma_{d=1,2}\ 1 / (2^{2d-1})] / m_{electron} = 0.374795880\ldots \tag{17}$$

From the leaking the nuclear strong and weak virtual energies are produced the virtual electron-positron pairs – in places of their annihilations are produced unstable holes in the Einstein spacetime. If in such a hole is electron then its binding energy increases i.e. absolute value of the negative potential electromagnetic energy is higher.

Calculate the ratio of electromagnetic energy of a virtual electron-positron pair (on assumption that the components of the pair are in distance equal to the reduced Compton length of electron) to internal energy of the electron which creates the virtual pair:

$E_{em,pair} / (m_{electron} c^2) = [(c^2 e^2) / (10^7 \lambda)] / (m_{electron} c^2) = \alpha_{em}$.

This leads to conclusion that each virtual electron-positron pair in a group of virtual pairs decreases the initial energy the α_{em} times i.e., for example, four successively created pairs decrease the initial energy α_{em}^4 times.

Energy associated with a loop is inversely proportional to length of wave which is in proportion to the principal quantum number n: $E \sim 1 / \lambda \sim 1 / n$.

It leads to conclusion that each virtual electron-positron pair produced in state defined by n decreases energy (α_{em} / n) times.

Formula (16) can be realized by Nature via creations and annihilations of the virtual electron-positron pairs. The first component in the brackets represents a fermion without virtual pairs. The second component is associated with the weak mass of the proton. Since it is the condensate/scalar, [2A], so there must be created simultaneously two virtual pairs with antiparallel spins (the pairs are the vectors). The third component is associated with the weak mass of the electron. Since it is as well the condensate/scalar, [2A], but carrying lower energy so there is created a group containing 4 virtual pairs. We can write column matrix for the field composed of the virtual pairs. To obtain formula for energy, we must multiple the quantized base of the exponential wave function rewritten as a matrix by the column matrix

$$mc^2 \begin{bmatrix} 1 & -1/2 & -1/8 \end{bmatrix} \cdot \begin{bmatrix} \left\{\dfrac{\alpha_{em}}{n}\right\}^0 = 1 \\ \left\{\dfrac{\alpha_{em}}{n}\right\}^2 \\ \left\{\dfrac{\alpha_{em}}{n}\right\}^4 \end{bmatrix}$$

On the other hand, in the Quantum Theory of Fields (QTF) we apply Lagrangians (energy) in which as well appear products of two generators and each generator is proportional to coupling constant i.e. there are components for which energy is proportional to α^2. This remark and formula (14) suggests as well that we should expand energy into series of type $(\alpha/n)^{2d}$, where $d = 0, 1, 2$, whereas $n = 1, 2, 3,...$ defines the basic standing waves in the exponentially changing field.

For the hydrogen atom we obtain

$$E = m c^2 [1 - (\alpha_{em} / n)^2 / 2 - (\alpha_{em} / n)^4 / 8], \tag{18}$$

where $mc^2 = 0.5107208$ MeV is the reduced mass of electron, n is the principal quantum number whereas $\alpha_{em} = 1 / 137.036001$ is the fine-structure constant.

The first component $E_R = mc^2$ is the internal energy concerning the reduced mass of electron.

The second component

$$E_{B,n} = -m\,c^2\,(\alpha_{em}/n)^2\,/\,2 \qquad (19)$$

is equal to the energies of the Bohr orbits in the hydrogen atom and $E_{B,n=1} = -13.598$ eV.

The third component is the fine structure energy

$$E_{FS,n} = -m\,c^2\,(\alpha_{em}/n)^4\,/\,8. \qquad (20)$$

This component depends on classical and quantum structure of electron so we must write it in such a way to interpret it correctly. Write the factor $1/8$ as follows

$$1\,/\,8 = (1 - 3\,/\,4)\,/\,2. \qquad (21)$$

The $3/4$ represents the classical mass of electron ([2A]: see Fig.; the factor $3/4$ follows from the internal structure of the bare electron – there is the torus/electric-charge) whereas the value 1 represents the quantum mass of electron. We can see that we separated the two very different masses.

The torus/electric-charge of electron it is only the polarized Einstein spacetime so it is very difficult to detect it [2A]. There is the torus and weak condensate in point B [2A]. The tori that appear due to the phase transitions of the non-gravitating Higgs field have the inner radius BC three times smaller than the outer radius BD – such tori are most stable [2A]. The Einstein-spacetime components, the torus is built of, are exchanged in such a way that points A and D are in the same phase whereas the point C has the opposite phase. The distance AD is the length of the electromagnetic waves, $\lambda_{em,electron}$, that appear in the classical theory of electron. In the point B is the weak condensate [2A] so the quantum radius of the electron, so the length of the quantum wave as well, $\lambda_{electron}$, is equal to BD.
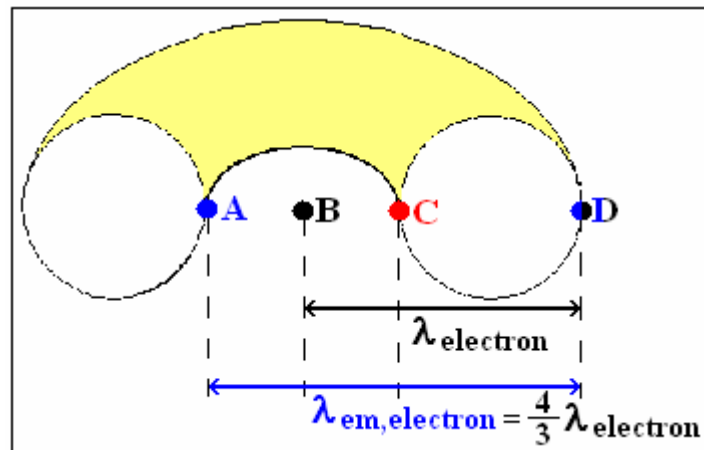
The $\lambda_{em,electron}$ defines the classical electromagnetic mass of electron (these quantities are inversely proportional) whereas the $\lambda_{electron}$ defines the quantum mass of the bare electron. We can see that we cannot separate these two masses – they are the different descriptions of the same structure. The formula for the total momentum $\boldsymbol{p}$ obtained within the M. Abraham

classical theory of electron [5] $p = (m_{electron} + 4\ m_{em,electron}\ /\ 3)v$ is incorrect. The correct formula looks as follows $p = m_{electron}\ v = 4\ m_{em,electron}\ v\ /\ 3 = 4\cdot3\ m_{electron}\ v\ /\ (3\cdot4)$.

The formula for momentum of the Coulomb electron field moving with velocity v, i.e. $p_{em} = 4\ m_{em,electron}\ v\ /\ 3$, is consistent with the Newtonian definition $p = m\ v$. **Emphasize that the difference in the descriptions of electron within the classical and quantum theories lead to the torus of the bare electron**. Most important is following formula $m_{em,electron} = 3\ m_{electron}\ /\ 4$. In the further calculations, we will use the factor $3/4$ that appears in the classical theory of electron.

We know that maximum azimuthal quantum number l is $l_{max} = n - 1$ so $n\ /\ (l_{max} + 1) = 1$. This means that we can rewrite formula (21) as follows

$$1\ /\ 8 = [n\ /\ (l_{max} + 1) - 3\ /\ 4]\ /\ 2. \tag{22}$$

The n and $(l_{max}+1)$ define the lengths of the de Broglie waves but the additional potential energy $E_A = l\ (l\ +\ 1)\ \hbar^2\ /\ (2\ m\ r^2)$ suggests that for defined n there can appear spontaneously as well the other standing waves defined by $l + 1$. For smaller l waves are shorter so corresponding absolute energy is greater. Since in formula (20) is the sign "– " so the levels defined by smaller and smaller l are closer and closer to the ground state $n = 1$. Finally, we can rewrite formula (20) as follows

$$E_{FS,n} = -m\ c^2\ (\alpha_{em}/\ n)^4\ [n\ /\ (l\ +\ 1) - 3\ /\ 4]\ /\ 2. \tag{23}$$

The ground state is shifted by $E_{FS,n=1} = -m\ c^2\ \alpha_{em}^4\ [1 - 3\ /\ 4]\ /\ 2 = -1.81\cdot10^{-4}$ eV.

Calculate the energy distance between the states $l = 0, 1$ for $n = 2$. The general solution for the energy distance between the extreme levels for defined n is as follows

$$\Delta E_{FS,n} = -m\ c^2\ (\alpha_{em}/\ n)^4\ (n - 1)\ /\ 2. \tag{24}$$

From it is $\Delta E_{FS,n=2} = -m\ c^2\ (\alpha_{em}/\ 2)^4\ (2 - 1)\ /\ 2 = -m\ c^2\ \alpha_{em}^4\ /\ 32 = -4.53\cdot10^{-5}$ eV.

Why we obtained results the same as in the Sommerfeld theory [6]? Why we obtained results the same as in the Dirac theory [7] neglecting the relativistic effects, the spin-orbit interactions, and so on? **It follows from the fact that for the quantum fields is $X \approx Y$. It follows from the constancy of the base of the natural logarithm for the quantum fields (more precisely, from constancy of the product fe)**. It is due to the applied methods – just the standing waves defined by the quantum numbers cannot be changed by any phenomena. Just the quantum numbers define the total picture and must be conserved. The three theories are equivalent because the numbers n_θ in the Sommerfeld theory, $j + 1/2$ in the Dirac theory (the j is not the j in this paper) and $l + 1$ in presented here theory, are the integers and change from 1 to n. But only presented here theory of hydrogen atom proves equivalence of the three theories and describes in all respects the physical origin of the final equation.

The Lamb-Retherford shift is associated with the internal structure of proton and we calculated it here [2A]. Since the all levels inside baryons are the $l = 0$ states so the Lamb-Retherford shift, due to the resonance, concerns only the $l = 0$ states in atoms. This shift is the energy distance between the $l = 0$ and $l = 1$ states for the same n and j. This shift decreases binding energy in the $l = 0$ state.

Notice that absolute value of the second component (the Bohr theory of atoms) for coupling constant for the nuclear strong interactions of pions ($\alpha = 1$) is $E_{B,n=1,\alpha=1} = 0.25536$ MeV and it is in approximation the mass of the torus/electric-charge inside the bare electron whereas for the coupling constant for the nuclear strong interactions of the nucleons at very low energy ($\alpha = 14.4$ [2A]) we obtain $E_{B,n=1,\alpha=14.4} = 52.95$ MeV and it is in approximation the mass of the torus/electric-charge of muon [2A].

3. Summary

In general, the Pauli Exclusion Principle follows from the spectroscopy whereas its origin is not good understood. To understand fully this principle, most important is the origin of quantization of the azimuthal quantum number i.e. the angular momentum quantum number. Here, on the base of the theory of ellipse and starting from very simple physical condition, we quantized the azimuthal quantum number. The presented model leads directly to the eigenvalue of the square of angular momentum and to the additional potential energy that appears in the equation for the modified wave function.

The Quantum Physics is timeless because a quantum particle disappears in one region of a field or spacetime and appears in another one, and so on. There are no trajectories of individual quantum particles. Quantum Physics concerns the statistical shapes and their allowed orientations. Such procedure simplifies considerably the Quantum Physics.

We formulated as well the very simple semiclassical analog to the Sommerfeld and Dirac theories of the hydrogen atom. Due to the constancy of the base of the natural logarithm for the quantum fields, the Sommerfeld, Dirac and presented here theories of hydrogen atom are equivalent. The standing waves defined by the quantum numbers cannot by changed by any phenomena. Just the quantum numbers define the total picture and must be conserved. The three theories are equivalent because the numbers n_θ in the Sommerfeld theory, $j + 1/2$ in the Dirac theory (the j is not the j in this paper) and $l + 1$ in presented here theory, change from 1 to n. But only presented here theory of hydrogen atom proves equivalence of the three theories and describes in all respects the physical origin of the final equation.

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