A Singular Solution for a Hydrogen Atom as a Way Toward Cold Nuclear Fusion

Ignatovich V. K.
Joint Institute for Nuclear Research, Dubna, Russia

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Abstract
The cold nuclear fusion (CNF) can be ensued by the usually rejected singular solution of the Schrödinger equation for an atom. This solution, when atom is confined inside matter, though singular, is normalizable. It can be an admixture to the standard solution. A possibility of CNF because of nucleus charge screening provided by the electron in the singular state is discussed.

Keywords
Quantum Mechanics, Hydrogen Atom, Cold nuclear Fusion, Singular Solutions, Coulomb Barrier, Charge Screening

1. Introduction
The last publications on real devices for CNF [1,2], existence of the European patent on some analogous device [3], a lot of recent reviews on experiments and theoretical researches [4-7], reproduction of the Rossi’s generator in Russia [8] and report [9] about huge isotopic changes in fuel of Rossi’s generator --- all that deeply impresses and makes thinking that there is some truth in CNF. The attitude toward it as a pathological science should be changed, though with some reservation, because it may happen, that all the activity in this area stems from a simple desire to get much money from venture capital or hedge funds.

Suppose that CNF reactions really take place. The common opinion of enthusiasts is that explanation of these reactions requires some new physics. However, it seems that the old physics also can be useful here. Under pressure of the new data it is only necessary to look carefully, what was missed in the old physics.

The presented here idea was induced by the paper [10], where a spectrum of an atom confined in a spherical well was calculated. The authors considered the well-known stationary Schrödinger equation for an atom, when it is confined in a spherical well with the infinitely high potential walls.

Such a model is not quite realistic. Here a more realistic model of an atom and its confinement is adopted. The potential of the confinement is described by a potential step at \( r=R_w \) of a finite height \( U_w \), as is shown in Fig.1. In the interval \( 0<r<R_w \) a solution of the Schrödinger equation in the Coulomb field is found. Earlier [11] it was attempted to find a localized singular radial eigen wave function \( \Psi_s \), which is matched to the exponentially decaying wave function of the type \( C \exp(-q(r-R_w))/r \) inside the wall at \( r>R_w \). The matching at \( R_w \) gives an equation for determination of the bound level of the singular solution. However calculations involved complicated hypergeometric functions [12], difficult for interpretations.

Here another approach is also used. In the next section in the Coulomb range \( r<R_w \) the common solution of lowest level hydrogen atom is accepted and the singular linear independent part is added to it. A possibility to match the superposition of the singular and nonsingular solutions to an exponentially decaying part is investigated. In the third part the possibility of a pure singular eigen state is studied. In [11] some relativistic corrections were considered. Here they will be omitted.

2. A Superposition of Singular and Normal Solutions
The Schrödinger equation for a confined atom looks

\[
\left( \frac{\hbar^2}{2m} \Delta + \Theta(r<R_w) - U_w \Theta(r>R_w) - E \right) \Psi(r) = 0,
\]  

where \( E>0 \), i.e. \( -E \) is the bound state energy, and \( \Theta \) is the step function equal to unity, when inequality in its argument is
satisfied, and to zero otherwise. The composite potential function looks as shown in Fig. 1.

Fig. 1. The total potential for the electron in presence of confinement.

After substitution of \( \Psi(r) = \Psi_L(r) \varphi_L(\theta, \phi) \) the Eq.(1) is transformed to

\[
\left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{L(L+1)}{r^2} + \frac{2m}{\hbar^2} \right) \left( \frac{Ze^2}{r} \Theta(r < R_w) - U_w \Theta(r > R_w) - E \right) \Psi_L(r) = 0, \tag{2}
\]

and after substitution

\[
\Psi_L(r) = u(r)/r \tag{3}
\]

Eq. (2) for \( L=0 \) and \( Z=1 \) is transformed to

\[
\left( \frac{d^2}{dr^2} + \frac{2m}{\hbar^2} \frac{e^2}{r} \Theta(r < R_w) - U_w \Theta(r > R_w) - E \right) u(r) = 0. \tag{4}
\]

The radial Schrödinger equation for \( u(r) \) can be rewritten in dimensionless units: \( r^* = r/a_0 \), \( E^* = E/E_h \), \( U^*_w = U_w/E_h \), where square brackets denote usual dimensional values, \( a_0 = \hbar^2 / me^2 = 0.525 \ \text{Å} \) is the Bohr radius, and \( E_h = e^2 / a_0 = 27.2 \ \text{eV} \) is the Hartree energy. In dimensionless units the equation is:

\[
\left( \frac{d^2}{dr^2} + \frac{2m}{\hbar^2} \frac{e^2}{r} \Theta(r < R_w) - 2U_w \Theta(r > R_w) - 2E \right) u(r) = 0. \tag{5}
\]

A solution of this equation for \( 0 < r < R_w \) can be found by Laplace method [13]:

\[
u(r) = \oint dt e^{r t} Z(t). \tag{6}\]

Substitution into (5) gives an equation for \( Z(t) \)

\[
\oint dt e^{r t} \left[ -\frac{d}{dt} (t^2 - 2E) + 2 \right] Z(t) = 0, \tag{7}
\]

which is equivalent to

\[
\frac{d}{dt} (t^2 - 2E) Z(t) = 2Z(t). \tag{8}\]

Solution of this equation is

\[
Z(t) = c e^{(t^2 - 2E) t} \tag{9}\]

where \( k = \sqrt{2E} \), and \( c \) is a constant, which is determined by a normalization. For now it will be put to \( c = 1 \). Substitution into (6) gives

\[
u(r) = \frac{1}{k} \oint dt e^{r t k} \frac{(t-1)^{1/k-1}}{(t+1)^{1/k+1}}. \tag{10}\]

For Hydrogen atoms it is accepted \( 2E = 1/n^2 \), where \( n \) is integer, therefore \( 1/k = n \), and

\[
u(r) = u_n(r) = n \oint dt e^{r t/n} \frac{(t-1)^{n-1}}{(t+1)^{n+1}}. \tag{11}\]

i.e. the expression under the integral has a simple pole, though, in general, when \( n \) is not integer, there are two branch points. Here it is accepted that \( n = 1 \). Then

\[
u_n(r) = e^{-r}. \tag{12}\]

The second independent solution \( u_s(r) \) is defined through Wronskian, which satisfies the equation

\[
u_s'(r)u_n(r) - u_s'(r)u_n(r) = c. \tag{13}\]

The constant \( c \) again is related to normalization and for convenience it is chosen to be \( c = -1 \). Therefore the equation for \( u_s \) becomes
The Schrödinger equation for Hydrogen has a constant which, seems, has no physical meaning. Let’s suppose that the total wave function is

\[ u(r) = A(-\alpha u_n(r) + u_n(r)), \]  

(19)

where \( A \) is a normalization constant. It can be shown that for some values of the constant \( \alpha \) the logarithmic derivative of \( u(r) \) in some range of \( r \) is negative. Therefore, choice of the confinement radius \( R_w \) in this range makes it possible to match \( u \) with the function

\[ u_n(r) = u(R_w) \exp(-q(r-R_w)) \]  

(20)
in the confinement wall, where \( q = \sqrt{2(E+U_n)} \). In the case of \( \alpha = 0.01 \) the logarithmic derivative is - 0.335, for instance, at \( r = 3 \). If \( R_w = 3 \) is accepted, then \( U_n = -0.44 \) of the Hartree energy, which is a little bit higher than the binding energy of the hydrogen ground state \( E = -0.5 \).

The full wave function (3) has asymptotics \( 1/r \). One of the reason to reject such a solution is that substitution of it in the Schrödinger equation creates a term [14]

\[ \Delta \frac{1}{r} = -4\pi\delta(r), \]  

(21)

which, seems, has no physical meaning.

Integration of this equation by parts 3 times gives

\[ C = \left( \frac{1}{r} - 2\ln r + 4r(\ln r - 1) \right) e^{2r} - 8\int_0^r dr'(ln r' - 1)e^{2r'}. \]  

(17)

The integral in the right hand side is numerically well integrable. With account of (16) the solution of (15) after substitution of (17) becomes

\[ u_\alpha(r) = \left( 1 - 2r \ln(1 - 2r) - 4r^2 \right) e^{2r} - 8re^{-r} \int_0^r dr' (\ln r' - 1)e^{2r'}. \]  

(18)

2) It is well known that there exist such a phenomenon as neutron-electron interaction [15], which can be described by the Fermi pseudo potential [16]

\[ 4\pi b_{ne}\delta(r), \]  

(22)

where \( b_{ne} \) is the point like neutron-electron scattering amplitude defined by quark or meson structure of the neutron. The similar amplitude should exist also in proton-electron scattering. Therefore such a term can be included in the Schrödinger equation for atoms. In fact, regular solution of the Schrödinger equation for Hydrogen has a constant amplitude of the electron field incident on the nucleus, therefore there should be the scattered field with asymptotics \( 1/r \).

The singular part of the wave function (3) increases probability of an electron to be near nucleus. With the function (19) and \( \alpha = 0.01 \) such a probability is

\[ Q = \int_0^{R_w} dr |\phi(r)|^2 \int_0^{R_w} dr |\psi(r)|^2 = 1.8 \times 10^{-8}, \]  

(23)

if \( R_N = 10^{-4} \). This parameter can be considered as a probability of complete screening of the nuclear charge or a probability of production of a compact hydrogen atom. Without the singular part the parameter \( Q \) is of the order \( 10^{-12} \), which is four orders of magnitude smaller.

In the usual circumstances the distance between atoms is of the order 5 – 6. The confinement with such a radius \( R_w \) can be achieved with much smaller parameter \( \alpha \) in the function (19), and there are almost no gain in screening comparing to a normal free atom without singular wave function. Therefore for a gain in screening atoms should be closer than in common circumstances. It means that the matter should be highly compressed or heated to sufficiently high temperatures. Then there is a probability that the hydrogen or deuterium atom transforms into a very compact neutral particle, which can easily penetrate a nucleus in its neighborhood. It can be imagined that the electron of the compact particle, penetrated into neighboring nucleus, becomes collectivized with electrons of this neighboring atom, therefore the nuclear reaction can proceed without radiation of neutrons and without \( \beta \) decay.

Fig. 2. Logarithmic derivative of the function (19) with \( \alpha = 0.01 \).
3. A Singular Eigen Solution Outside Hydrogen Spectrum

The Schrödinger equation (5) after definition of the parameter $\beta \neq n$ such that $E = 1/2\beta^2$, and change of variable $r = \beta \rho/2$, $U_w = 2V_w\beta^2$, $R_w = \beta \rho/2$ transforms to

$$
\left( \frac{d^2}{d \rho^2} + \frac{\beta}{\rho} \Theta(\rho < \rho_w) - V(\rho > \rho_w) - \frac{1}{4} \right) u(\rho) = 0. \tag{24}
$$

Solution of the Eq. (27) is usually represented by a regular in the origin confluent hypergeometric (Kummer) function $w(\rho) = M(1-\beta,2,\rho)$, where in the case of a free hydrogen-like atom parameter $\beta$ is a positive integer.

Another independent solution[12], $w(\rho) = U(1-\beta,2,\rho)$, of (27) is singular one and it behaves at the origin as

$$
w(\rho) \approx U(1-\beta,2,\rho)^{-1}. \tag{28}
$$

With account of the functional relations

$$
\Gamma(a) = \Gamma(a+n) \psi(z) = \Gamma(z) \tag{30}
$$

the formula (29) for $n = 1$ is reduced to

$$
U(1-\beta,2,\rho) = \sum_{k=0}^{\infty} \frac{\Gamma(k+1-\beta)}{k!(k+2)} \rho^k \ln \rho + \psi(1-\beta+k) - \psi(1+k) - \frac{1}{2} \ln \rho + \psi(1-\beta+k) - 2\psi(1+k) - \frac{1}{k+1} + \frac{1}{\rho}, \tag{32}
$$

where the factor $1/\Gamma(1-\beta)$ is excluded because it can be included in normalization.

3. At $\rho > \rho_w$ the solution of the equation is

$$
u(\rho) = C \exp(-q(\rho - \rho_w)), \tag{25}
$$

where $q = \sqrt{2(E - U_w)}$.

3. At $0 < \rho < \rho_w$ substitution of

$$
\rho(\rho - \rho_w) = \rho(\rho - \rho_w) \tag{26}
$$

into (24) gives

$$
\left( \rho \frac{d^2}{d \rho^2} + (2 - \rho) \frac{d}{d \rho} - [1 - \beta \Theta(\rho < \rho_w)] - \rho V_w(\rho > \rho_w) \right) u(\rho) = 0. \tag{27}
$$

Therefore $\Psi(\rho) = u(\rho)/\rho$ has asymptotic $1/\rho$ at the origin. Such a solution is usually rejected. Nevertheless this function is normalizable, and one must take it into account. When the atom is put inside matter the singular state can be even an eigen state of the atom.

The singular solution $U(a,b,\rho)$, according to[12], for positive integer $b = 1 + n$, where in our case $n = 1$, is representable as

$$
U(1-\beta,2,\rho) = \sum_{k=0}^{\infty} \frac{\Gamma(k+1-\beta)}{k!(k+2)} \rho^k \ln \rho + \psi(1-\beta+k) - \psi(1+k) - \frac{1}{2} \ln \rho + \psi(1-\beta+k) - 2\psi(1+k) - \frac{1}{k+1} + \frac{1}{\rho}, \tag{32}
$$

where the factor $1/\Gamma(1-\beta)$ is excluded because it can be included in normalization.

It is understandable, that this function can be matched with (25), if logarithmic derivative of $u(\rho) = \rho e^{-\rho} w(\rho)$ is negative. This derivative is presented in Fig.3 for different $\beta$.

It seems that the function (32) exponentially decays at infinity for any $\beta$. If so, then there is a continuous spectrum of singular normalizable states in hydrogen-like atoms. This suggestion should be studied further.

The contribution of the singular wave function to screening of the nuclear charge can be estimated by the ratio of integrals

$$
Q = \int_0^\infty dz u_1(a,b,z)^2 / \int_0^\infty dz u_0(a,b,z)^2 \tag{33}
$$

Fig. 3. Logarithmic derivative of the function (26) with $w = w(\rho)$ given by (32) for $\beta$ equal to 1) 0.8; 2) 0.6; 3) 1.2. It is seen that the singular states bound energy can be lower and higher than the normal hydrogen ground state energy with $\beta = 1$. 


where \( R_s = 10^{-4} \) and \( R_n = 6 \). Numerical calculations with the above parameters gives \( Q = 3.8 \times 10^5 \) for \( \beta = 0.8 \), \( 9.3 \times 10^5 \) for \( \beta = 0.6 \) and \( 8 \times 10^5 \) for \( \beta = 1.2 \). The parameter \( Q \) can be considered as a probability of complete screening of the nuclear charge or a probability of production of a compact hydrogen atom.

One can conclude that in the matter the atom can come to a state described by the singular wave function. Because of vibration of neighboring atoms the radius \( R \) of confinement and its potential are always changing, which affects the eigen values of the singular state and there is a probability that the hydrogen or deuterium atom transforms into a very compact neutral particle, which can easily penetrate a nucleus in its neighborhood. It can be imagined that the electron of the compact neutral particle, penetrated into neighboring nucleus, collectivizes with electrons of this neighboring atom, therefore the nuclear reaction can proceed without radiation of neutrons and without \( \beta \) decay. Of course, the resulted nucleus is excited, and can release its excitation to thermal degrees of freedom.

4. Some Ideas About Energy Release in CNF

There are several types of experiments in literature where CNF reactions were observed. Some of them are related to glow discharge in deuterium atmosphere, some others are related to electrolysis with deuterated electrolyte. In both types of experiments a Pd cathode saturated with deuterium is involved. Let’s imagine that \( Q = 10^{-5} \) of \( N_0 = 10^{23} \) density of deuterium atoms are in a compact state. A deuterium ion entering Pd of thickness \( d = 1 \) cm absorbs the compact atom with probability \( w = N_0 Q \sigma d \), where \( \sigma \) is the cross section, which can be of the order 10 barn. If every absorption releases 24 MeV energy, and the incident flux of ions corresponds to current 10 A, i.e. to \( 10^{20} \) ions/sec, then the total release of energy is \( 2.4 \times 10^{22} \) eV/s or 3.8 kW. Of course, the cross section can be 100 times larger, then the released power becomes 0.380 MW. It can be even higher, if other, not well known parameters are larger. It is seen that the field is worth of investigation.

5. Conclusion

A possibility to explain the so long discussed cold nuclear fusion is undertaken in this paper. Contrary to wide spread belief, that a new physics is required for the explanation, the old physics, as shown, can also be of use. It is only necessary to look for some features that were missed in the old physics. The most appropriate are singular states in hydrogen like atoms with zero angular momentum. These states lead to screening of nuclear charge with some probability, which in some circumstances can be essential. Here the singular states are considered and their contribution to heat release in CNF are estimated.

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