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# An attempt of 2-electrons Dirac equation in Minkowski space

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**Abstract.** Quantum mechanics describes multi-electronic systems by using probabilistic theories. All of these theories are approximations and provide a probabilistic conception of quantum mechanics, which prevents it to be compatible with general relativity. Indeed, the real observable world is for us a 3D+time Minkowski space but quantum mechanics is expressed in multi-dimensional Hilbert space: which is not physical but purely mathematical. In this article we try to make a relativistic equation that gives a correct description of atomic physics in the real space for 2 electrons systems: i.e a 2-electrons Dirac equation. The starting point is to use the wave mechanics concept of De Broglie and Schrödinger: considering the electron as a matter-wave. For this we start from the Hartree equation, which gives already a 3D space description of each electron wave function. Then we switch to Hartree-Fock representation, which gives birth to the exchange potential, which can be also expressed in 3D. By extended the concept of exchange potential in relativistic 4-exchange: we obtain a relativistic 2-electrons real space Dirac-Hartree-Fock (RSDHF) equation, in Minkowski space. That equation takes into account relativistic effects but not correlation effects, which is the difficulty of this study. We will show the equivalence of the 2-electrons RSDHF equation with the Hartree-Fock equation in non-relativistic, stationary and scalar regime. Electron correlation issues will be discussed as well.

## 1 Introduction

Quantum mechanics is expressed in probabilistic subspaces instead of real 3D space. The real space-time expression of quantum mechanics would imply also a deterministic nature of microscopic physics. The probabilistic expression forbids to solve the big physical challenge of almost 100 years: to find the bridge between quantum mechanics and general relativity. Nobel prized physicists from Schrödinger in late 1920's [1] to Gerard't Hooft in 2020's [2] have suggested or studied a deterministic interpretation of quantum mechanics. But unnatural probabilistic interpretation remains: this is due to the conclusion of the Solvay conference in 1927, led by Niels Bohr. However the probabilistic interpretation of quantum mechanics was discarded by

$\alpha = q^2/(4\pi\epsilon_0\hbar c)$	Fine structure constant
$\hbar$	Reduced Planck constant
$k_0 = \frac{1}{\alpha a_0}$	Electron's Compton wave number, $a_0$ Bohr radius
$c$	Speed of light
$\hat{\gamma} = (\hat{\gamma}_0, \hat{\gamma}_1, \hat{\gamma}_2, \hat{\gamma}_3)$	Gamma matrices vector
$\hat{\sigma} = \hat{\sigma}_1\mathbf{e}_1 + \hat{\sigma}_2\mathbf{e}_2 + \hat{\sigma}_3\mathbf{e}_3$	Pauli vector in 3D basis
$\hat{\gamma}_0 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}$	First (time-like) Gamma matrix
$\hat{\gamma}_\mu = \begin{pmatrix} 0 & -\hat{\sigma}_\mu \\ \hat{\sigma}_\mu & 0 \end{pmatrix}$	The three spatial Gamma matrices
$\hat{\alpha}_\mu = -\hat{\gamma}_0\hat{\gamma}_\mu = \begin{pmatrix} 0 & \hat{\sigma}_\mu \\ \hat{\sigma}_\mu & 0 \end{pmatrix}$	The three spatial Alpha matrices
$\langle \mathbf{A}   \mathbf{B} \rangle = \int \mathbf{A}^\dagger \mathbf{B} d^3r$	Scalar product
$\mathbf{A}^\dagger \mathbf{B}$	Matrix product between $\mathbf{A}^\dagger$ and $\mathbf{B}$
$\mathbf{A} \cdot \mathbf{B} = \sum_i A_i B_i$	Dot product

Table 1: Used physical constants, mathematical tools and notations

Einstein, De Broglie and Schrödinger himself who has discovered the equation of the same name back in 1926. In 1929 the Hylleraas solution [3] of the Helium's ground state (in the frame of the many-body Hamiltonian theory [4]), using a correlated wave function (joint probability density of the two electrons), has permitted to find the most accurate value among others theory (mainly Hartree theory [5]): this result has pushed the probabilistic interpretation as the right one. Since the Hylleraas method is computationally greedy [6], the Hartree-Fock approximation was used instead (introduced in 1928 [7]) for almost every atoms and molecules with a really good accuracy. The limitations of Hartree-Fock approximation remain the relativistic effects and the electron correlation, which become important for big atoms or molecules [8]. To take into account the electron correlation, which is a hard to define concept, several method are employed beyond Hartree-Fock theory. However these methods use a degree of freedom to fit to the experimental data: the wave function in the case of many-body theory [4] and the "exchange-correlation" potential in the case of the density functional theory (DFT) [9].

We have recalled in our last paper that Hartree theory can be expressed in real space [10] and, using the Slater-Condon rules, even Hartree-Fock theory can also be expressed in 3D [11]. In this paper we will go a bit further: we will propose a relativistic 2-electrons real space Dirac-Hartree-Fock (RSDHF) equation in real space. First we will remind the basics about atomic physics with Hartree and Hartree-Fock approximations. Then we will define the relativistic potentials felt by every electrons in a system using Maxwell equations. After that, we will present the 2-electrons RSDHF equation, its equivalence to Hartree-Fock in a special regime and the need to modify it to take into account correlations.

## 2 Reminder of actual quantum theories

We can make a distinction between quantum theories with the many-body Hamiltonian and the density functional theory. These two theories are probabilistic that means the electron wave function is interpreted as a probability density. The first one is an ab-initio theory with an undefined total electrons wave function and the second one, DFT, is an approximation since it tends to reproduce exchange and correlation effects via fictitious potentials. DFT won't be discussed in this paper.

## 2.1 Two-body Hamiltonian theory

2.1.1 *Non-relativistic case* The non-relativistic two-body Hamiltonian of an atom of  $Z$  protons and 2 electrons is written as:

$$\hat{H} = -\frac{\hbar^2 \Delta_1}{2m} - \frac{\hbar^2 \Delta_2}{2m} - \frac{Z}{4\pi\epsilon_0 r_1} - \frac{Z}{4\pi\epsilon_0 r_2} + \frac{1}{4\pi\epsilon_0 r_{12}} \quad (1)$$

with  $r_{12} = \|\mathbf{r}_1 - \mathbf{r}_2\|$ ,  $m$  the electron mass (protons are too heavy to move: Born-Oppenheimer approximation),  $\epsilon_0$  vacuum permittivity and  $q$  electron charge. This Hamiltonian is used in the many-body eigenvalue equation:

$$\hat{H}\Psi(\mathbf{r}_1, \mathbf{r}_2) = E\Psi \quad (2)$$

with  $\Psi$  the undefined total wave function of  $3 \times 2$  coordinates of the electrons and  $E$  the electronic energy of the atom. The problem is that the form of  $\Psi$  is unrestricted by the theory of the many-body Hamiltonian [4] so we have to make an approximation on its form. Then, these different assumptions lead to Hartree theory, Hartree-Fock theory, correlated Hylleraas-type [6] wave functions or multi-configuration Hartree-Fock [12]. All of these theories are just convenient to find atomic ground state but do not have a clear physical foundation except for Hartree-Fock which includes the Pauli's principle in its formulation [8].

2.1.2 *Approximately relativistic case* Instead of using the many-body Hamiltonian (1) we use the Dirac-Coulomb-Breit Hamiltonian [13] which is only approximately relativistic (it includes indeed some relativistic effects) and the wave function  $\Psi$  is a  $4 \times 2$  spinor of  $3 \times 2$  coordinates. This theory is not used in practice because it is computationally greedy due to the structure of the multi-particles spinor wave function [14].

2.1.3 *Approximations on the total wave function form* The form of the wave function in the many-body Hamiltonian theory is a degree of freedom because it is undetermined. We will just evoke these theories here to have an overview and then we will focus on Hartree-Fock which is the best starting point at our sens (because it is related to Pauli's principle):

- Hartree approximation (individual product of wave functions):  $\Psi \simeq \Phi_1(\mathbf{r}_1)\Phi_2(\mathbf{r}_2)$
- Hartree-Fock approximation (Slater determinant):  $\Psi \simeq \frac{1}{\sqrt{2}} \begin{vmatrix} \Phi_1(\mathbf{r}_1) & \Phi_2(\mathbf{r}_1) \\ \Phi_1(\mathbf{r}_2) & \Phi_2(\mathbf{r}_2) \end{vmatrix}$ , it reduces to zero if  $\Phi_1 = \Phi_2$ , so two electrons cannot have the same state (Pauli's principle)
- Multi-configuration Hartree-Fock approximation:  $\Psi \simeq \sum_i C_i \begin{vmatrix} \Phi_{1i}(\mathbf{r}_1) & \Phi_{2i}(\mathbf{r}_1) \\ \Phi_{1i}(\mathbf{r}_2) & \Phi_{2i}(\mathbf{r}_2) \end{vmatrix}$  with  $C_i$  coefficients to adjust with variational principle and  $\Phi_{ji}(\mathbf{r}_k)$  is the spin-orbital of the electron  $j$  in the configuration  $i$  with the coordinates of the electron  $k$
- Hylleraas-type approximation (mix of coordinates):  $\Psi \simeq \Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_{12})$  with  $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$

All of this mathematical manipulation can arrange the energy functional  $E$  to achieve the ground state, in some way. We will focus on Hartree-Fock theory, which includes the important Pauli's principle, to develop the 2-electrons RSDHF equation (in real space). We will not use the total wave function, which has too many degrees of freedom but a Dirac 4-spinor for each electron: that is a healthy starting point in our sens.

### 3 Basics, construction of real space atomic physics

#### 3.1 Stationary states

In the following we will define implicitly the non-relativistic wave function of an electron  $i$  in stationary state as  $\Psi_i(\mathbf{r}, t)$  :

$$\Psi_i(\mathbf{r}, t) = \Phi_i(\mathbf{r})e^{-iE_it/\hbar} \quad (3)$$

where  $t$  is the time and  $\mathbf{r}$  the position of an observer. So we have trivially:

$$|\Psi_i(\mathbf{r}, t)|^2 = |\Phi_i(\mathbf{r})|^2 \quad (4)$$

The atomic total energy  $E_a$  is defined by (for two electrons):

$$E_a = \sum_{i=1}^2 E_i = E_1 + E_2 \quad (5)$$

#### 3.2 Hartree equation

Let an atom of  $Z$  protons located at the origin and 2 electrons. In the Hartree approximation, we have each electron  $i$  represented by a scalar wave function  $\Phi_i(\mathbf{r})$  and submitted to the following equation (S.I units  $i \neq j$ ) [5]:

$$H_i(\mathbf{r})\Phi_i(\mathbf{r}) = E_i\Phi_i(\mathbf{r}) \quad (6)$$

with:

$$H_i(\mathbf{r}) = -\frac{\hbar^2\Delta}{2m} - \frac{Zq^2}{4\pi\epsilon_0 r} + \frac{q^2}{8\pi\epsilon_0} \int d^3r' \frac{|\Phi_j(\mathbf{r}')|^2}{\|\mathbf{r} - \mathbf{r}'\|} \quad (7)$$

Then we divide by  $\hbar c$  to get:

$$h_i(\mathbf{r})\Phi_i(\mathbf{r}) = k_i\Phi_i(\mathbf{r}) \quad (8)$$

with:

$$h_i = \frac{H_i}{\hbar c} = -\frac{\Delta}{2k_0} - \frac{Z\alpha}{r} + \frac{\alpha}{2} \int d^3r' \frac{|\Phi_j(\mathbf{r}')|^2}{\|\mathbf{r} - \mathbf{r}'\|} \quad (9)$$

the Hamiltonian (containing kinetic energy, proton electrostatic attraction and electrostatic electron-electron repulsion), with  $k_i = E_i/(\hbar c)$ , energy of electron  $i$  (in wave numbers) and  $k_0 = mc/\hbar$  the electron's Compton wave number.

This equation works pretty well for light elements like the first five (Hydrogen up to Boron) [10, 15]. However, things get more complicated for heavier atoms [15, 7] and here comes the so-called electron exchange energy introduced by the Hartree-Fock approximation.

#### 3.3 Hartree-Fock equation

The Hartree-Fock model in probabilistic quantum mechanics indeed uses a determinant of spin-orbitals approach (scalar wave functions multiplied by a Pauli Cartesian 2-spinor) inside the multi-electronic Schrödinger equation to fit with the Pauli exclusion principle. The result of this, using Slater-Condon orthogonality rules, leads to the canonical Hartree-Fock equation for electron  $i$  [11] (it is just the Hartree equation with a new potential,  $i \neq j$ ):

$$h_i\Phi_i(\mathbf{r}) - v_{ij}(\mathbf{r})\Phi_j(\mathbf{r}) = k_i\Phi_i(\mathbf{r}) \quad (10)$$

with:

$$v_{ij}(\mathbf{r}) = \frac{\alpha}{2} \int d^3r' \frac{\Phi_j^*(\mathbf{r}')\Phi_i(\mathbf{r}')\delta_{s_i s_j}}{\|\mathbf{r} - \mathbf{r}'\|} \quad (11)$$

the exchange potential [7] with  $(s_i, s_j)$  magnetic spin numbers of electron  $i$  and  $j$ . We notice also that:

$$v_{ij}^* = v_{ji} \quad (12)$$

This is no longer a scalar eigenvalue equation (like the Hartree equation is:  $h_i\Phi_i = k_i\Phi_i$ ). But now equation (10) can be written explicitly in matrix form (equivalent to Fock matrix) as

$$\widehat{h}\Phi = \widehat{k}\Phi \quad (13)$$

which is a sort of vector eigenvalue equation with:

$$\begin{pmatrix} h_1 & -v_{1,2} \\ -v_{1,2}^* & h_2 \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} = \begin{pmatrix} k_1 & 0 \\ 0 & k_2 \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} \quad (14)$$

and  $\widehat{h}^\dagger = \widehat{h}$  (real energy eigenvalues). In this theory each electron's energy  $k_i$  is given by:

$$k_i = \int \Phi_i^*(\mathbf{r}) (h_i\Phi_i(\mathbf{r}) - v_{ij}(\mathbf{r})\Phi_j(\mathbf{r})) d^3r \quad (15)$$

**Remark:**

Hartree stated originally in 1928 the Hartree equation [5], in the idea of Schrodinger's interpretation, i.e each wave functions are considered as an electron cloud: it was the deterministic real space interpretation. But in 1930 [16], Slater and Gaunt rediscovered the Hartree equation using the multi-electron probabilistic wave function: so they found it back but starting from the Borh's point of view. The canonical Hartree-Fock equation (10) has been discovered using the multi-electronic anti-symmetric wave function, i.e the Slater determinant. In this article we are doing the opposite process of Slater and Gaunt: we start in the probabilistic interpretation to come back in the real space.

*3.4 The example of Helium atom in Hartree-Fock theory*

The ground state of the Helium atom is known to be a singlet state [17], i.e the 2 electrons have opposite spins ( $s_1 = -s_2$ ):

$$\delta_{s_1 s_2} = 0 \quad (16)$$

That means the exchange potential is zero and so the Hartree-Fock equation reduces to an Hartree equation for each wave functions which are equal (we can prove that  $\Phi_1 = \Phi_2 = \Phi$  and  $k_1 = k_2 = k$ ):

$$\left( -\frac{\Delta}{2k_0} - \frac{2\alpha}{r} + \frac{\alpha}{2} \int d^3r' \frac{|\Phi(\mathbf{r}')|^2}{\|\mathbf{r} - \mathbf{r}'\|} \right) \Phi = k\Phi \quad (17)$$

Switching in atomic units ( $a_0 \equiv 1$  and  $k/\alpha \equiv k$ ) that gives:

$$\left( -\frac{\Delta}{2} - \frac{2}{r} + \frac{1}{2} \int d^3r' \frac{|\Phi(\mathbf{r}')|^2}{\|\mathbf{r} - \mathbf{r}'\|} \right) \Phi = k\Phi \quad (18)$$

Using the Hartree self-consistent field procedure, which allows us to find the "best"  $\Phi$  that solves the non-linear eigenvalue equation above, we obtain [18]:

$$k_a = 2k \simeq -2.8616 \quad (19)$$

and the Helium ground state is  $-2.9037$  a.u, so it is an error of 1.45%, which is still important. This is the minimum energy that the Hartree-Fock theory can reach for Helium. The remaining energy can be calculated exactly with the many-body Hamiltonian [17] and is called the "correlation energy". This is the hardest problem in this study at our sens, that we will discuss briefly in section 8.

## 4 Electrons 4-spinor

### 4.1 Relativistic stationary states

We choose to extend the Dirac theory of the electron. The wave function of each electron  $i$  is a 4-spinor  $\Psi_i(\mathbf{r}, t)$  defined in stationary state by:

$$\Psi_i(\mathbf{r}, t) = \Phi_i(\mathbf{r})e^{-iE_it/\hbar} \quad (20)$$

with  $\Phi_i(\mathbf{r})$  4-spinors. In this case we have also  $\|\Psi_i\| = \|\Phi_i\|$ .

### 4.2 Spinor orthogonality and Pauli exclusion principle

**4.2.1 Introduction** The exclusion principle stated by Pauli is at the origin very practical. It is good to recall that the Pauli exclusion principle was stated to avoid big computational mistakes in quantum mechanics like taking for instance three  $1s$  (i.e spherically symmetric) wave functions to describe the three electrons of the Lithium atom in its ground state [11]: the obtained energy using Hartree equation is much lower than the experimental one, which is of course a big issue. So the principle forbids to get the 3 same states: two electrons can share the non-relativistic  $1s$  function at the condition they have opposite spin and because there is only two spin number ( $\pm 1/2$ ) the third electron should have a different wave function from  $1s$ .

**4.2.2 Statement** Still in stationary states (an atom for instance), for a system of 2 electrons we define the total cross charge density  $n$  by:

$$n = \left\| \sum_{i=1}^2 \Psi_i(\mathbf{r}, t) \right\|^2 = \|\Psi_1\|^2 + \|\Psi_2\|^2 + \Psi_1^\dagger \Psi_2 + \Psi_2^\dagger \Psi_1 \quad (21)$$

Then the number of electrons is given by:

$$\int n(\mathbf{r}, t) d^3r = 2 \quad (22)$$

Then we have the normalization condition (or "localized matter distribution" condition) for each electron  $i$ :

$$\int \|\Psi_i\|^2 d^3r = 1 \quad (23)$$

which means:

$$\int (\Psi_1^\dagger \Psi_2 + \Psi_2^\dagger \Psi_1) d^3r = 0 \quad (24)$$

In order to vanish the cross terms, we assume that the 4-spinors are orthogonal (this is equivalent to Slater-Condon rules in Hartree-Fock theory, i.e orthogonality of spin-orbitals):

$$\int \Psi_i^\dagger \Psi_j d^3r = \delta_{ij} \quad (25)$$

That means that 2 electrons in the same system (an atom for instance) cannot have the same spinor (or quantum state, in non-relativistic theory): this is the expression of the Pauli exclusion principle, explained here by the conservation of the electrons number using the total cross charge density concept and spinors orthogonality.

## 5 Electromagnetic 4-potentials

### 5.1 The 4-repulsion

*5.1.1 Scalar potential: electrostatic Coulomb repulsion* Each electron  $i$  feels the effect of the repulsive potential which is created by the other electrons charge densities  $\|\Psi_j\|^2$ . The relativistic expression just follows Maxwell equations:

$$\square V_i(\mathbf{r}, t) = \frac{q^2}{2\epsilon_0} \sum_{j \neq i} \|\Psi_j(\mathbf{r}, t)\|^2 \quad (26)$$

with  $\square = \partial_t^2/c^2 - \Delta$ . Then we pose  $v_i = V_i/\hbar c$  to obtain the more convenient unit (in wave number):

$$\square v_i(\mathbf{r}, t) = 2\pi\alpha \sum_{j \neq i} \|\Psi_j(\mathbf{r}, t)\|^2 \quad (27)$$

In stationary states ( $\Psi_j = \Phi_j e^{-iE_j t/\hbar}$ ) that gives only:

$$\Delta v_i(\mathbf{r}) = -2\pi\alpha \sum_{j \neq i} \|\Phi_j(\mathbf{r})\|^2 \quad (28)$$

which is the classical electrostatic Poisson's equation that we find already in Hartree equation (8).

*5.1.2 Vector potential: magnetic-like repulsion* Starting from the Dirac 3-current (the 3 dimensional space current), spatial part of the Dirac conserved 4-current, of each electron  $j$  defined by:

$$\mathbf{J}_j = qc (\hat{\gamma}_0 \Psi_j)^\dagger \hat{\Gamma} \Psi_j \quad (29)$$

with  $\hat{\Gamma} = (\hat{\gamma}_1, \hat{\gamma}_2, \hat{\gamma}_3)$ . We can define the magnetic vector potential felt by electron  $i$  as:

$$\square \mathbf{A}_i(\mathbf{r}, t) = \frac{\mu_0}{2} \sum_{j \neq i} \mathbf{J}_j \quad (30)$$

The factor 2 comes from the magnetic energy shared by electron  $i$  and electron  $j$  (same factor 2 than in Coulomb repulsion in equation (26)). Then we define  $\mathbf{a}_i = \frac{q}{\hbar} \mathbf{A}_i$  to get:

$$\square \mathbf{a}_i(\mathbf{r}, t) = 2\pi\alpha \sum_{j \neq i} (\hat{\gamma}_0 \Psi_j)^\dagger \hat{\Gamma} \Psi_j \quad (31)$$

Then in stationary states this reduces to:

$$\Delta \mathbf{a}_i(\mathbf{r}) = -2\pi\alpha \sum_{j \neq i} (\hat{\gamma}_0 \Phi_j)^\dagger \hat{\Gamma} \Phi_j \quad (32)$$

## 5.2 4-repulsion compact expression

We have for both scalar and vector repulsion potential:

$$\square \begin{pmatrix} v_i \\ \mathbf{a}_i \end{pmatrix} = 2\pi\alpha \sum_{j \neq i} \begin{pmatrix} \|\Psi_j\|^2 \\ (\hat{\gamma}_0 \Psi_j)^\dagger \hat{\Gamma} \Psi_j \end{pmatrix} \quad (33)$$

Using index notation we get the more compact expression (we use  $(\hat{\gamma}_0 \Psi_j)^\dagger \hat{\gamma}_0 \Psi_j = \|\Psi_j\|^2$ ):

$$\square a_{i\mu} = 2\pi\alpha \sum_{j \neq i} (\hat{\gamma}_0 \Psi_j)^\dagger \hat{\gamma}_\mu \Psi_j \quad (34)$$

with  $a_{i0} = v_i$ . This expression can be seen also in relativistic DFT [19]. The source of the right side of the equation is just the usual Dirac 4-current.

## 5.3 The 4-exchange

**5.3.1 Scalar potential: Hartree-Fock exchange** Taking the equation (11) we can make it relativistic by considering the Maxwell equation and the cross charge  $\Psi_j^\dagger \Psi_i$  as its source:

$$\square V_{ij}(\mathbf{r}, t) = \frac{q^2}{2\epsilon_0} \Psi_j^\dagger \Psi_i \quad (35)$$

Again we pose  $v_{ij} = V_{ij}/(\hbar c)$  and we get:

$$\square v_{ij}(\mathbf{r}, t) = 2\pi\alpha \Psi_j^\dagger \Psi_i \quad (36)$$

In stationary states that gives:

$$\square v_{ij}(\mathbf{r}, t) = 2\pi\alpha \Phi_j^\dagger \Phi_i e^{i(E_j - E_i)t/\hbar} \quad (37)$$

which is still time-dependent (when we add it to  $v_{ji}$ , it gives the potential created by an oscillating charge).

**5.3.2 Vector potential: electromagnetic exchange** In this part we will use the Dirac transition 4-currents, already used to define classical radiation in some textbooks [20, 21]. First, similarly to the Dirac 3-current, we introduce the Dirac transition 3-current:

$$\mathbf{J}_{ij} = qc (\hat{\gamma}_0 \Psi_j)^\dagger \hat{\Gamma} \Psi_i \quad (38)$$

Then we can define the vector potential felt by electron  $j$  due to electron  $i$  by:

$$\square \mathbf{A}_{ij}(\mathbf{r}, t) = \frac{\mu_0}{2} \mathbf{J}_{ij} \quad (39)$$

Then we pose  $\mathbf{a}_{ij} = q\mathbf{A}_{ij}/\hbar$  and we obtain:

$$\square \mathbf{a}_{ij}(\mathbf{r}, t) = 2\pi\alpha (\hat{\gamma}_0 \Psi_j)^\dagger \hat{\Gamma} \Psi_i \quad (40)$$

**5.3.3 4-exchange compact expression** As we did for the 4-repulsion we can express the 4-exchange as:

$$\square \begin{pmatrix} v_{ij} \\ \mathbf{a}_{ij} \end{pmatrix} = 2\pi\alpha \begin{pmatrix} \Psi_j^\dagger \Psi_i \\ (\hat{\gamma}_0 \Psi_j)^\dagger \hat{\Gamma} \Psi_i \end{pmatrix} \quad (41)$$

In index notation that gives:

$$\square a_{ij\mu} = 2\pi\alpha (\hat{\gamma}_0 \Psi_j)^\dagger \hat{\gamma}_\mu \Psi_i \quad (42)$$

### Remark:

The Dirac transition current is used to describe atomic transitions and electromagnetic radiations in Hydrogen atom [21]. In non-relativistic case (using the Gordon decomposition of the 4-current) we can even derive the Einstein's spontaneous emission coefficient [22, 23].

## 6 Dirac equation

### 6.1 Without external potential

We know that the one electron Dirac equation is written as (we use the Einstein's summation convention, then the  $\mu$  go from 0 to 3):

$$i\hbar c \hat{\gamma}^\mu \partial_\mu \Psi = mc^2 \Psi \quad (43)$$

with  $\hat{\gamma}^\mu = (\hat{\gamma}_0, -\hat{\gamma}_1, -\hat{\gamma}_2, -\hat{\gamma}_3)$ . Divided by  $\hbar c$  the above equation gives:

$$i\hat{\gamma}^\mu \partial_\mu \Psi = k_0 \Psi \quad (44)$$

with  $\mu = \{0, 1, 2, 3\}$  and  $\partial_0 = \partial_t/c$ . Written without the index notation that gives:

$$i \left[ \hat{\gamma}_0 \frac{\partial_t}{c} - \hat{\gamma} \cdot \nabla \right] \Psi = k_0 \Psi \quad (45)$$

with  $\hat{\gamma} \cdot \nabla = \hat{\gamma}_1 \nabla_1 + \hat{\gamma}_2 \nabla_2 + \hat{\gamma}_3 \nabla_3$ .

### 6.2 With an external potential: minimal coupling

In case of an external electromagnetic 4-potential  $a_{e\mu}$  (we differentiate potentials due to an external source, like the Coulomb's attraction by a positively charged nucleus, than those due to others electrons) we have the usual electromagnetic minimal coupling:

$$i\partial_\mu \rightarrow i\partial_\mu - a_{e\mu} \quad (46)$$

That gives for the Dirac equation:

$$\hat{\gamma}^\mu (i\partial_\mu - a_{e\mu}) \Psi = k_0 \Psi \quad (47)$$

with:

$$a_{e\mu} = \begin{pmatrix} a_{e0} \\ \mathbf{a}_e \end{pmatrix} \quad (48)$$

Without the index notation we write it as:

$$\left[ \hat{\gamma}_0 \left( i \frac{\partial_t}{c} - a_{e0} \right) - \hat{\gamma} \cdot (i\nabla - \mathbf{a}_e) \right] \Psi = k_0 \Psi \quad (49)$$

## 7 Approaching of 2-electrons Dirac equation

### 7.1 General case

**7.1.1 Without external potential** By taking the analog to the Hartree-Fock equation we only have to add the 4-repulsion and the 4-exchange to the Dirac equation for each electron spinor  $\Psi_i(\mathbf{r}, t)$ . That gives a sort of 2-electron RSDHF equation  $\Psi_i$  ( $i \neq j$ ):

$$[\hat{\gamma}^\mu (i\partial_\mu - a_{i\mu}) - k_0] \Psi_i + \hat{\gamma}^\mu a_{ij\mu} \Psi_j = 0 \quad (50)$$

which can constitute a base to work on. With the 4-potentials, which are not external but internal because these are due to other electrons, given by:

$$\square a_{i\mu} = 2\pi\alpha (\hat{\gamma}_0 \Psi_j)^\dagger \hat{\gamma}_\mu \Psi_j \quad (51)$$

$$\square a_{ij\mu} = 2\pi\alpha (\hat{\gamma}_0 \Psi_j)^\dagger \hat{\gamma}_\mu \Psi_i \quad (52)$$

7.1.2 *Minimal coupling* To include an external potential  $a_{e\mu}$ , we apply again the minimal coupling to get:

$$[\hat{\gamma}^\mu (i\partial_\mu - a_{i\mu} - a_{e\mu}) - k_0] \Psi_i + \hat{\gamma}^\mu a_{ij\mu} \Psi_j = 0 \quad (53)$$

## 7.2 Atomic stationary states

7.2.1 *Statement of the problem* In case of stationary states ( $\Psi_i(\mathbf{r}, t) = \Phi_i(\mathbf{r})e^{-iE_i t/\hbar}$ ) we have:

$$[\hat{\gamma}_0(k_i - a_{e0} - a_{i0}) - \hat{\gamma} \cdot (i\nabla - \mathbf{a}_e - \mathbf{a}_i) - k_0] \Phi_i e^{-ik_i ct} + (\hat{\gamma}_0 a_{ij0} - \hat{\gamma} \cdot \mathbf{a}_{ij}) \Phi_j e^{-ik_j ct} = 0 \quad (54)$$

with  $k_i = E_i/(\hbar c)$ , then the 4-potentials and external potential (here due to the nucleus of  $Z$  protons) are given by ( $i \neq j$ ):

$$\Delta a_{i\mu}(\mathbf{r}) = -2\pi\alpha (\hat{\gamma}_0 \Phi_j)^\dagger \hat{\gamma}_\mu \Phi_j \quad (55)$$

$$\square a_{ij\mu}(\mathbf{r}, t) = 2\pi\alpha (\hat{\gamma}_0 \Phi_j)^\dagger \hat{\gamma}_\mu \Phi_i \quad (56)$$

$$\Delta a_{e\mu} = 4\pi\alpha Z \delta(\mathbf{r}) \delta_{\mu 0} \quad (57)$$

So we have two electrostatic Poisson's equations and one wave equation (for the exchange). We can integrate these equations in free space:

$$a_{i\mu}(\mathbf{r}) = \frac{\alpha}{2} \int \frac{(\hat{\gamma}_0 \Phi_j(\mathbf{r}'))^\dagger \hat{\gamma}_\mu \Phi_j(\mathbf{r}')}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' \quad (58)$$

$$a_{ij\mu}(\mathbf{r}, t) = \frac{\alpha}{2} \int \frac{(\hat{\gamma}_0 \Phi_j(\mathbf{r}'))^\dagger \hat{\gamma}_\mu \Phi_i(\mathbf{r}') e^{ik_{ij}(\|\mathbf{r} - \mathbf{r}'\| - ct)}}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' \quad (59)$$

$$a_{e\mu} = -\frac{\alpha Z}{r} \delta_{\mu 0} \quad (60)$$

with  $k_{ij} = k_i - k_j$ . Now we should explicit a bit more the equations and for that we can multiply at left side the equation (54) by  $\hat{\gamma}_0$  and using the Dirac Alpha vector defined as:

$$\hat{\alpha} = -\hat{\gamma}_0 \hat{\gamma} = \begin{pmatrix} 0 & \hat{\sigma} \\ \hat{\sigma} & 0 \end{pmatrix} \quad (61)$$

we get:

$$[\hat{\alpha} \cdot (i\nabla - \mathbf{a}_e - \mathbf{a}_i) + k_i - a_{e0} - a_{i0} - k_0 \hat{\gamma}_0] \Phi_i e^{-ik_i ct} + (\hat{\alpha} \cdot \mathbf{a}_{ij} + a_{ij0}) \Phi_j e^{-ik_j ct} = 0 \quad (62)$$

with the potentials (these can be written with  $\hat{\alpha}$ , using  $\hat{\gamma} = -\hat{\gamma}_0 \hat{\alpha}$  and the fact that  $\hat{\gamma}_0$  is unitary):

$$a_{e0} = -\frac{\alpha Z}{r} \quad (63)$$

$$a_{i0} = \frac{\alpha}{2} \int \frac{\|\Phi_j(\mathbf{r}')\|^2}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' \quad (64)$$

$$\mathbf{a}_i = -\frac{\alpha}{2} \int \frac{\Phi_j^\dagger(\mathbf{r}') \hat{\alpha} \Phi_j(\mathbf{r}')}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' \quad (65)$$

$$a_{ij0} = \frac{\alpha}{2} \int \frac{\Phi_j(\mathbf{r}')^\dagger \Phi_i(\mathbf{r}') e^{ik_{ij}(\|\mathbf{r} - \mathbf{r}'\| - ct)}}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' \quad (66)$$

$$\mathbf{a}_{ij} = -\frac{\alpha}{2} \int \frac{\Phi_j(\mathbf{r}')^\dagger \hat{\alpha} \Phi_i(\mathbf{r}') e^{ik_{ij}(\|\mathbf{r} - \mathbf{r}'\| - ct)}}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' \quad (67)$$

We can now multiply equation (62) by  $e^{ik_i ct}$  to get (time-dependency disappears):

$$[\hat{\alpha} \cdot (i\nabla - \mathbf{a}_e - \mathbf{a}_i) + k_i - a_{e0} - a_{i0} - k_0 \hat{\gamma}_0] \Phi_i + (\hat{\alpha} \cdot \tilde{\mathbf{a}}_{ij} + \tilde{a}_{ij0}) \Phi_j = 0 \quad (68)$$

with:

$$\tilde{a}_{ij0} = \frac{\alpha}{2} \int \frac{\Phi_j(\mathbf{r}')^\dagger \Phi_i(\mathbf{r}') e^{ik_{ij}\|\mathbf{r} - \mathbf{r}'\|}}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' \simeq \frac{\alpha}{2} \int \frac{\Phi_j(\mathbf{r}')^\dagger \Phi_i(\mathbf{r}')}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' \quad (69)$$

$$\tilde{\mathbf{a}}_{ij} = -\frac{\alpha}{2} \int \frac{\Phi_j(\mathbf{r}')^\dagger \hat{\alpha} \Phi_i(\mathbf{r}') e^{ik_{ij}\|\mathbf{r} - \mathbf{r}'\|}}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' \simeq -\frac{\alpha}{2} \int \frac{\Phi_j(\mathbf{r}')^\dagger \hat{\alpha} \Phi_i(\mathbf{r}')}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' \quad (70)$$

in the dipole approximation (i.e  $k_{ij}\|\mathbf{r} - \mathbf{r}'\| \ll 1$ ).

**7.2.2 Atomic energy** The energy  $k_i$  of electron  $i$  is given by ( $j \neq i$ ):

$$k_i = \int \Phi_i^\dagger [a_{i0} + a_{e0} + k_0 \hat{\gamma}_0 - \hat{\alpha} \cdot (i\nabla - \mathbf{a}_i - \mathbf{a}_e)] \Phi_i d^3 r - \int \Phi_i^\dagger (\hat{\alpha} \cdot \tilde{\mathbf{a}}_{ij} + \tilde{a}_{ij0}) \Phi_j d^3 r \quad (71)$$

and the total electronic energy of the atom  $k_a$  is simply:

$$k_a = k_1 + k_2 \quad (72)$$

From the general stationary states equation (68), we can check now that this system of equations can indeed be reduced into Hartree-Fock equations (8) in the non-relativistic and scalar approximation. Exactly like the Dirac equation can be reduced into a Schrödinger equation in the non-relativistic regime [24].

**7.3 Stationary, non-relativistic and scalar approximation: the Hartree-Fock approximation**

To start, without loss of generality we can separate the stationary 4-spinors into two Pauli spinors as:

$$\Phi_i = \begin{pmatrix} \varphi_i \\ \chi_i \end{pmatrix} \quad (73)$$

7.3.1 *Non-relativistic approximation* In the non-relativistic approximation (i.e  $(Z\alpha)^2 \ll 1$ ) we have [24]:

$$\|\chi_i\| \ll \|\varphi_i\| \quad (74)$$

and  $\varphi_i$  is called the "large spinor" and  $\chi_i$  the "small spinor" in Dirac central field problem. The  $\hat{\alpha}$  matrices, which are anti-diagonal blocks (see table 1), mix the large and small spinors in the magnetic electron-electron potential  $\mathbf{a}_i$  and magnetic exchange potential  $\mathbf{a}_{ij}$ . So we can approximate it to zero in the non-relativistic limit:

$$\mathbf{a}_i \simeq 0 \quad (75)$$

$$\tilde{\mathbf{a}}_{ij} \simeq 0 \quad (76)$$

The only external potential we have is the nucleus charge attraction, so it is scalar only (i.e  $\mathbf{a}_e = 0$ ). Then the energy of each electron  $i$  is very close to its rest mass energy  $k_0$  (which is approximately  $1.9 \times 10^4$  a.u and  $\sim 0.1 - 1$  a.u for kinetic and electromagnetic energies). So we have:

$$k_i + k_0 \simeq 2k_0 \quad (77)$$

$$k_i - k_0 \simeq \kappa_i \quad (78)$$

$$k_0 \gg (\kappa_i, a_{e0}, a_{i0}) \quad (79)$$

with  $\kappa_i$  the kinetic and electromagnetic energy of electron  $i$ . Then we have:

$$a_{e0} = -\frac{\alpha Z}{r} \quad (80)$$

$$a_{i0} \simeq \frac{\alpha}{2} \int \frac{\|\varphi_j(\mathbf{r}')\|^2}{\|\mathbf{r} - \mathbf{r}'\|} d^3r' \quad (81)$$

$$\tilde{a}_{ij0} \simeq \frac{\alpha}{2} \int \frac{\varphi_j(\mathbf{r}')^\dagger \varphi_i(\mathbf{r}')}{\|\mathbf{r} - \mathbf{r}'\|} d^3r' \quad (82)$$

Now we can explicit the equation (68):

$$\begin{pmatrix} \kappa_i - a_{e0} - a_{i0} & i\hat{\sigma} \cdot \nabla \\ i\hat{\sigma} \cdot \nabla & 2k_0 \end{pmatrix} \begin{pmatrix} \varphi_i \\ \chi_i \end{pmatrix} + \tilde{a}_{ij0} \begin{pmatrix} \varphi_j \\ \chi_j \end{pmatrix} \simeq 0 \quad (83)$$

That gives the couple of differential equations for each 2-spinor components of electron  $i$  (Lévy-Leblond like equations):

$$(\kappa_i - a_{e0} - a_{i0}) \varphi_i + i\hat{\sigma} \cdot \nabla \chi_i + \tilde{a}_{ij0} \varphi_j = 0 \quad (84)$$

$$i\hat{\sigma} \cdot \nabla \varphi_i + 2k_0 \chi_i + \tilde{a}_{ij0} \chi_j = 0 \quad (85)$$

The second equation above can be approximated as:

$$\chi_i = -\frac{i\hat{\sigma} \cdot \nabla \varphi_i + \tilde{a}_{ij0} \chi_j}{2k_0} \simeq -\frac{i\hat{\sigma} \cdot \nabla \varphi_i}{2k_0} \quad (86)$$

because  $k_0 \gg \tilde{a}_{ij0}$ , that gives a kinetic balance equation [25]. Replacing the result above in the first equation in (84) we get:

$$(\kappa_i - a_{e0} - a_{i0}) \varphi_i + \frac{\Delta}{2k_0} \varphi_i + a_{ij0} \varphi_j = 0 \quad (87)$$

We rearrange it to get a spinor Hartree-Fock equation:

$$\left( -\frac{\Delta}{2k_0} + a_{e0} + a_{i0} \right) \varphi_i - a_{ij0} \varphi_j = \kappa_i \varphi_i \quad (88)$$

**7.3.2 Scalar approximation** In the scalar approximation, we consider that each 2-spinor  $\varphi_i$  can be reduced to a product of a scalar function and a Cartesian 2-spinor as:

$$\varphi_i = \varphi_i \begin{pmatrix} \delta_{s_i \frac{1}{2}} \\ \delta_{s_i -\frac{1}{2}} \end{pmatrix} \quad (89)$$

so we have the scalar equation:

$$\left( -\frac{\Delta}{2k_0} - \frac{\alpha Z}{r} + \frac{\alpha}{2} \int \frac{|\varphi_j(\mathbf{r}')|^2}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' \right) \varphi_i - \frac{\alpha}{2} \int \frac{\varphi_j(\mathbf{r}')^* \varphi_i(\mathbf{r}') \delta_{s_i s_j}}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' \varphi_j \simeq \kappa_i \varphi_i \quad (90)$$

which is the set of Hartree-Fock equations (10).

## 8 Lack of correlation terms: case of Helium ground state

We suppose we want to find the Helium ground state using the RSDHF equation. The intuitive thing is to consider a singlet (opposite spin)  $1s^2$  state in the non-relativistic (relativistic corrections are of the order of  $\alpha^2$  [17]) equation (88) for each electron 1 and 2 with:

$$\varphi_1 = Y_0^0 \begin{pmatrix} f(r) \\ g(r) \end{pmatrix} \quad (91)$$

$$\varphi_2 = Y_0^0 \begin{pmatrix} g(r) \\ f(r) \end{pmatrix} \quad (92)$$

$$\kappa_1 = \kappa_2 = \kappa \quad (93)$$

$$\int \|\varphi_1\|^2 d^3 r = \int \|\varphi_2\|^2 d^3 r = 1 \quad (94)$$

with  $\int_0^{+\infty} r^2 f g dr = 0$  and  $Y_0^0 = 1/\sqrt{4\pi}$  the first spherical harmonic. In this case we have a couple of equations to solve (atomic units):

$$\left( -\frac{\Delta}{2} - \frac{Z}{r} + \frac{1}{2} \int \frac{(Y_0^0)^2 (f(r')^2 + g(r')^2)}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' \right) f - \int \frac{(Y_0^0)^2 f(r') g(r')}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' g = \kappa f \quad (95)$$

$$\left( -\frac{\Delta}{2} - \frac{Z}{r} + \frac{1}{2} \int \frac{(Y_0^0)^2 (f(r')^2 + g(r')^2)}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' \right) g - \int \frac{(Y_0^0)^2 f(r') g(r')}{\|\mathbf{r} - \mathbf{r}'\|} d^3 r' f = \kappa g \quad (96)$$

which gives after integration of the potentials (using Laplace expansion):

$$\left( -\frac{\Delta}{2} - \frac{Z}{r} + \frac{1}{2} h_0(f^2 + g^2) \right) f - h_0(fg)g = \kappa f \quad (97)$$

$$\left( -\frac{\Delta}{2} - \frac{Z}{r} + \frac{1}{2} h_0(f^2 + g^2) \right) g - h_0(fg)f = \kappa g \quad (98)$$

with:

$$h_0(F) = \frac{1}{r} \int_0^r r'^2 F(r') dr' + \int_r^\infty r' F(r') dr' \quad (99)$$

Both  $f$  and  $g$  obey the same equation and using the property of variational principle (i.e Rayleigh-Ritz method): the ground state should be non-degenerate [26]. Then because of Pauli's principle, we should not have  $f = g$ . To avoid to take an orthogonal function to  $f$  which lead to a too high energy, we choose to take  $g = 0$ . In this case we have:

$$\left( -\frac{\Delta}{2} - \frac{Z}{r} + \frac{1}{2} h_0(f^2) \right) f = \kappa f \quad (100)$$

which is the Hartree equation (18) for Helium-like atom. So additional work must be done since the minimum energy reached by this equation is  $-2.8616$  [18] ( $-2.9037$  a.u. for exp. value).

#### Remark:

Many attempts have been done in this study to try to reach the ground state of Helium. The first one was to completely make symmetric the RSDHF equation (50) by extending the exchange to kinetic, rest mass and nucleus attraction exchange (i.e "crossing" the  $\Psi$ 's between operators). It appeared that it lowers down the energy too much (much below the  $-2.9037$  a.u energy of the Helium, the same for the He-like components) so we have dropped this idea.

## 9 Conclusion

The 2-electrons RSDHF equation (50) at this point is a good approximation that tends to Hartree-Fock in stationary, non-relativistic and scalar regime. The theory is relativistic, ab-initio and have clearly defined electrons wave functions as matter distributions. Then the theory remains in Minkowski space: so it is compatible with general relativity. This obviously lack of correlation terms and needs additional work, starting by determining the right ground state of Helium atom.

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