

Combined Open Shell Hartree-Fock Theory of Atomic and Molecular Systems Constructed from Noncharged Scalar Particles

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Abstract

By the use of condition of relativistic covariance, Dirac group theory, Clifford algebra and complete orthonormal sets of $\psi^{(\alpha^*)}$ -self-frictional exponential type orbitals ($\psi^{(\alpha^*)}$ -SFETOs) introduced by the author in standard convention, the Hartree-Fock (HF) theory is suggested for multideterminantal single configuration states with any number of open shells of atoms and molecules constructed from the Standard Model-Fermi (SM-F) particles with $m \neq 0, s \neq 0$ and $e \neq 0$ defined in the Standard Model of particle physics. It is shown that the origin of stability of these systems is the quantum damping or self-frictional forces produced by the SM-F particle itself. **As an application, we have presented the periodic table for the SM-F atomic elements using Pauli principle of spinless noncharged identical SM-F particles.**

Key words: Hartree-Fock theory, Standard Model, Relativistic covariance, Exponential type orbitals, Self-frictional fields

I. Introduction

According to the condition of relativistic covariance, for a single particle of mass m , charge e and spin s , the relativistic Hamilton operator is given by

$$\hat{H} = \sqrt{c^2(\hat{p} - \frac{e}{c}A)^2 + m^2c^4} + eA_0, \quad (1)$$

where $m \neq 0$ and $s = 0, \frac{1}{2}, \frac{3}{2}, \dots$ for fermions, $m = 0$ and $s = 1, 2, \dots$ for bosons, A_0 is the scalar

potential, A the vector potential and $\vec{p} = \frac{\hbar}{i} \vec{\nabla}$ the momentum operator. It is well-known that

the relativistic energy for a free particle is defined by Einstein's formula [1]:

$$E = \begin{cases} mc^2 & \text{for } m \neq 0 \text{ and } v < c \\ pc & \text{for } m = 0 \text{ and } v = c \end{cases} \quad (2a)$$

$$E = pc \quad (2b)$$

As we see that the particles with $m \neq 0, s \neq 0, e \neq 0$ and $v = c$ do not satisfy the condition of relativistic covariance and, therefore, these "particles" can not be observed in experiments.

Unfortunately, this kind of “particles” has been the target of a long search in Particle Physics (see Ref. [2] and references therein). Consequently, other theories **in or beyond** the Standard Model of particle physics are needed instead. The arguments of a new theory given in this work are based on completely different point of view, namely, making use of the condition of relativistic covariance, i.e., the condition of linearity for a relativistic Hamiltonian of SM-F particle (see Appendix). We note that the Schrödinger equation describes the motion of the spin-0 particles in the nonrelativistic domain, while the Klein-Gordon equation is the relativistic equation appropriate for spin-0 particles. As it was shown in the previous papers [3, 4], the wave function of Dirac equation for spin- $\frac{1}{2}$ particle satisfies the Klein-Gordon equation component-wise, and the relativistic wave functions of scalar particles are reduced to the nonrelativistic complete sets of orbitals. Therefore, the SM-F atomic-molecular systems can be also treated in the nonrelativistic way.

It should be noted that the SM-F particles **have non-zero rest mass and cannot move like photons**. Because of this, the situation is changed fundamentally. Therefore, one has to arrive immediately at the conclusion that the identical spinless noncharged SM-F particles can be studied by the use of two-component antisymmetric functions [4]. The aim of this paper is to suggest the new theory for open shell HF theory of SM-F atomic and molecular systems based on the use of condition of relativistic covariance, complete orthonormal sets of $\psi^{(\alpha^*)}$ - SFETOs in standard convention and self-frictional quantum fields which are analog of radiation damping or self-frictional fields introduced by Lorentz in classical electrodynamics [5, 6] (see. Refs. [7-9] and references therein to our papers). **We note that the presented approach in this work is an extension of suggested in a previous paper [10] to the case of atomic-molecular systems constructed from noncharged scalar particles. We believe that the presented theory will be of interest especially in the Standart Model of particles physics, astrophysics and Bose-Fermion theory.**

2. Definitions and basic formulas

According to the relativistic covariance, the identical scalar particles ($s = 0$) in position and momentum spaces with hyperspherical harmonics can be described by antisymmetric functions (see Eqs. (25) in Ref. [4]). This statement can also be used for a system consisting of an arbitrary number of identical SM-F particles. Therefore, we can write in position space

the antisymmetric wave function of SM-F particles in the form of a determinant (a so-called Slater determinant):

$$\begin{aligned}
 U^{(\alpha^*)} & \left(u_{n_{N-k}}^{(\alpha^*)} (x_{N-k}) u_{n_{N-k+1}}^{(\alpha^*)} (x_{N-k+1}) \dots u_{n_N}^{(\alpha^*)} (x_N) \right) \\
 & = \frac{1}{\sqrt{N!}} \begin{vmatrix} u_{n_1}^{(\alpha^*)} (x_1) & u_{n_2}^{(\alpha^*)} (x_1) & \dots & u_{n_{N-k}}^{(\alpha^*)} (x_1) & u_{n_{N-k+1}}^{(\alpha^*)} (x_1) & \dots & u_{n_N}^{(\alpha^*)} (x_1) \\ u_{n_1}^{(\alpha^*)} (x_2) & u_{n_2}^{(\alpha^*)} (x_2) & \dots & u_{n_{N-k}}^{(\alpha^*)} (x_2) & u_{n_{N-k+1}}^{(\alpha^*)} (x_2) & \dots & u_{n_N}^{(\alpha^*)} (x_2) \\ \vdots & \vdots & \dots & \vdots & \vdots & \dots & \vdots \\ u_{n_1}^{(\alpha^*)} (x_N) & u_{n_2}^{(\alpha^*)} (x_N) & \dots & u_{n_{N-k}}^{(\alpha^*)} (x_N) & u_{n_{N-k+1}}^{(\alpha^*)} (x_N) & \dots & u_{n_N}^{(\alpha^*)} (x_N) \end{vmatrix}, \quad (3)
 \end{aligned}$$

where $k=0$ and $1 \leq k \leq N$ for closed and open shells, respectively; n, nlm, x, xyz and α^* are the integer ($\alpha^* = \alpha, -\alpha \leq 2$) and noninteger ($\alpha^* = \alpha, -\alpha < 3$) self-frictional quantum numbers; the $u_{nlm}^{(\alpha^*)}$ are determined by

$$u_{nlm}^{(\alpha^*)} (\zeta, r) = g_{nl}^{(\alpha^*)} (\zeta, r) \beta_m Y_{lm} (\theta, \varphi). \quad (4)$$

The functions $u^{(\alpha^*)}, g^{(\alpha^*)}$ and $U^{(\alpha^*)}$ form the orthonormal sets,

$$u_{nlm}^{(\alpha^*)} (\zeta, \vec{r}) u_{n'l'm'}^{(\alpha^*)} (\zeta, \vec{r}) d^3 r = \delta_{nn'} \delta_{ll'} \delta_{mm'}, \quad (5)$$

$$g_{nl}^{(\alpha^*)} (\zeta, r) g_{n'l'}^{(\alpha^*)} (\zeta, r) r^2 dr = \delta_{nn'}, \quad (6)$$

$$U^{(\alpha^*)\dagger} (\zeta, \vec{r}) U^{(\alpha^*)} (\zeta, \vec{r}) d^3 \tau = \delta_{U^{(\alpha^*)} U^{(\alpha^*)}}, \quad (7)$$

where $d^3 \tau = d^3 r_1 d^3 r_2 \dots d^3 r_N$, $\beta_m = (-1)^{(|m|-m)/2}$ and ζ is the self-frictional parameter

($0 < \zeta < \infty$).

3. Periodic table of SM-F atomic elements

It has been shown in a previous paper [4] that the relativistic spinors with $s=0$ are reduced to the nonrelativistic complete sets of orbitals. Accordingly, it is completely relevant to

investigate the periodic table of SM-F atoms within the framework of nonrelativistic quantum mechanics. We notice that the stability of SM-F atomic-molecular systems is performed with the help of Lorentz damping or self-frictional quantum forces.

To construct the periodic table, we use the Hamiltonian of the system of N SM-F particles in the following form:

$$\hat{H}_{nl}^{(\alpha^*)} = \sum_{\mu=1}^N -\frac{1}{2} \frac{2}{\mu} + \sum_a V_{nl}^{(\alpha^*)}(\zeta, r_{a\mu}) + \sum_{\mu=1}^{N-1} \sum_{\nu=\mu+1}^N V_{nl}^{(\alpha^*)}(\zeta, r_{\mu\nu}), \quad (8)$$

where $V_{nl}^{(\alpha^*)}(\zeta, r)$ is the self-frictional potential determined as follows [7]:

$$V_{nl}^{(\alpha^*)}(\zeta, r) = -\frac{\zeta n}{r} G_{nl}^{(\alpha^*)}(\zeta, r) \quad (9)$$

$$G_{nl}^{(\alpha^*)}(\zeta, r) = 1 + (\alpha^* - 1) \frac{n-l-1}{2n} \frac{1}{\zeta r} R_{nl+1}^{(\alpha^*+1)}(\zeta, r) / R_{nl}^{(\alpha^*)}(\zeta, r). \quad (10)$$

It is easy to show that the function $G_{nl}^{(\alpha^*)}(\zeta, r)$ occurring in Eq (9), as is expected, has the following properties:

$$G_{nl}^{(\alpha^*)}(\zeta, r) = 1 \quad \text{for } r \rightarrow \infty. \quad (11)$$

As can be seen from Eqs.(9) and (10), the self-frictional properties disappear for $\zeta = \frac{Z}{n}$

and $n = l+1$, i.e.,

$$V_{nl}^{(\alpha^*)}(\zeta, r) = -\frac{Z}{r} \quad (12)$$

$$\mathcal{E}_n = -\frac{\zeta^2}{2} = -\frac{Z^2}{2n^2}, \quad (13)$$

where Z denotes the SM-F -nucleus number of elements in the periodic table. In this case, the $\psi^{(\alpha^*)}$ -SFETOs are reduced to the Schrödinger's wave function for the SM-F-like atoms and become the noncomplete, i.e., $\psi_{nlm}^{(\alpha^*)} = \psi_{nlm}^{(1)}$, where ψ_{nlm} is the Schrödinger wave function in nonstandard convention.

As can be seen from Eq. (8), the potential of the field acting upon a particle in a SM-F atom is the self-frictional. The state of a SM-F particle in such a field will be characterized by the four quantum numbers n, l, m and α^* . In SM-F atoms, we find that the energy depends on the three quantum numbers n, l and α^* ; these numbers are used to denote the corresponding energy states: $n l \alpha^*$.

In the ground state of SM-F atom, the particles fill, in accordance with the Pauli principle for spinless ($s = 0$) particles, the lowest energy states. No more than one particle can be in each s-state, no more than 3 in a p-state, and no more than 5 in a d-state;... The SM-F atoms with completed shells (H, He, B, C, F, Si, ...) are very stable, they have great difficulty in forming chemical compounds with other SM-F atoms and interact weakly with one another.

We show in Table 1 the SM-F configurations of the atoms for the first 14 elements of the periodic table. The rectangles indicate the open shells (the number of chemical valence) of SM-F atoms. As we see from this table that the total number of SM-F energy states corresponding to one principal quantum number n is equal to n^2 .

Table 1. Configurations of SM-F atoms

Z	SM-F Element	1s	2s	2p	3s	3p	3d	Terms
1	H	1						S
2	He	1	1					S
3	Li	1	1	1				P
4	Be	1	1	2				P
5	B	1	1	3				S
6	C	1	1	3	1			S
7	N	1	1	3	1	1		P
8	O	1	1	3	1	2		P
9	F	1	1	3	1	3		S
10	Ne	1	1	3	1	3	1	D
11	Na	1	1	3	1	3	2	P,F
12	Mg	1	1	3	1	3	3	P,F
13	Al	1	1	3	1	3	4	D
14	Si	1	1	3	1	3	5	D

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As an example, we study now the ground states of a system of two SM-F particles moving in the field of a SM-F -nucleus of $Z = 2$. The SM-F He atom is such a system, which has two SM-F particles and a SM-F -nucleus with $Z = 2$: other examples are the single “ionised” SM-F Li “ion”, the double “ionised” SM-F Be “ion”, and other multiply “ionised” SM-F He-like “ions”.

Now we obtain the independent determinantal wave functions and terms of SM-F atoms by the use of modified determinantal method introduced in a previous paper [10]. To make the argument concrete, let us consider the configuration Na $(1s^1 2s^1 2p^3 3s^1 3p^3 3d^2)$ in which two SM-F particles occur outside closed shells. The complete sets for these particles are classified by M_L values and the independent determinants obtained by modified determinantal method. It is easy to find the terms and the orthonormal sets of multideterminantal wave functions which are eigenfunctions of operators \hat{L}^2 and \hat{M}_z . The results are given in Table 2.

Table 2. The terms of SM-F configuration of Na $(1s^1 2s^1 2p^3 3s^1 3p^3 3d^2)$ and their multideterminantal wave functions

Terms	M_L	$U^{(\alpha^*)}$
P	1	$U^{(\alpha^*)} (321, 320)$
	0	$U^{(\alpha^*)} (321, 32-1)$
	-1	$U^{(\alpha^*)} (321, 32-2)$
F	3	$U^{(\alpha^*)} (322, 321)$
	2	$U^{(\alpha^*)} (322, 320)$
	1	$U^{(\alpha^*)} (322, 32-1)$
	0	$U^{(\alpha^*)} (322, 32-2)$
	-1	$U^{(\alpha^*)} (320, 32-1)$

-2	$U^{(\alpha^*)}(320,32-2)$
-3	$U^{(\alpha^*)}(32-1,32-2)$

4. Orbital-dependent energy expression for system of SM-F particles

By the use of method set out in [10], the postulated energy expectation value for a single configuration multideterminantal state of SM-F atomic-molecular systems with a given space symmetry can be written as follows:

$$E^{(\alpha^*)} = \sum_i^n f_i h_i^{(\alpha^*)} + \sum_{ij,kl}^n \frac{1}{2} A_{kl}^{(\alpha^*)ij} J_{kl}^{(\alpha^*)ij} - \frac{1}{2} B_{kl}^{(\alpha^*)ij} K_{kl}^{(\alpha^*)ij}, \quad (14)$$

where $A_{kl}^{(\alpha^*)ij} = 4A_{kl}^{ij}$, $B_{kl}^{(\alpha^*)ij} = 2B_{kl}^{ij}$, $n = n_c + n_o$ is the number of occupied orbitals belonging to the closed shells (n_c) and open shells (n_o), and $1 \leq i, j, k, l \leq n$. The Eq. (14) denotes the energy expectation value of SM-F atomic-molecular systems; f_i is the fractional occupancy of shell i determined by

$$f_i = \frac{N_i}{N_{0i}}. \quad (15)$$

Here, N_{0i} and N_i are number of states and SM-F particles in shell i , respectively.

The coefficients A_{kl}^{ij} and B_{kl}^{ij} are the coupling projection constants (see Ref. [10]). For closed-closed and closed-open shell interaction energies ($1 \leq i, j \leq n_c, 1 \leq k, l \leq n$ and $1 \leq i, j \leq n, 1 \leq k, l \leq n_c$) the coupling projection coefficients are determined as follows:

$$A_{kl}^{ij} = B_{kl}^{ij} = f_i f_k \delta_{ij} \delta_{kl}. \quad (16)$$

In the case of open-open shell interaction energies ($n_c + 1 \leq i, j \leq n$ and $n_c + 1 \leq k, l \leq n$) the values of coefficients A_{kl}^{ij} and B_{kl}^{ij} depend on the state under study.

We notice that the possibility of writing the energy of SM-F atomic-molecular systems in the form (14) is based on the assumption that the energy $E^{(\alpha^*)}$ is the average expectation

value for all degenerate total orthonormal sets of multideterminantal wave functions $U_{\Gamma M_\Gamma}^{(\alpha^*)}$ for state with the irreducible representation Γ :

$$E_\Gamma^{(\alpha^*)} = \frac{1}{N_\Gamma^{(\alpha^*)}} \sum_{M_\Gamma} U_{\Gamma M_\Gamma}^{(\alpha^*)\dagger} \hat{H}^{(\alpha^*)} U_{\Gamma M_\Gamma}^{(\alpha^*)} d^3\vec{\tau} , \quad (17)$$

where

$$E_L^{(\alpha^*)} = \frac{1}{N_L^{(\alpha^*)}} \sum_{M_L} U_{LM_L}^{(\alpha^*)\dagger} \hat{H}^{(\alpha^*)} U_{LM_L}^{(\alpha^*)} d^3\vec{\tau} \quad \text{for SM - F atoms} \quad (18)$$

$$E_\Lambda^{(\alpha^*)} = \frac{1}{N_\Lambda^{(\alpha^*)}} \sum_{M_\Lambda} U_{\Lambda M_\Lambda}^{(\alpha^*)\dagger} \hat{H}^{(\alpha^*)} U_{\Lambda M_\Lambda}^{(\alpha^*)} d^3\vec{\tau} \quad \text{for linear SM - F molecules} \quad (19)$$

$$E_\Gamma^{(\alpha^*)} = \frac{1}{N_\Gamma^{(\alpha^*)}} \sum_{M_\Gamma} U_{\Gamma M_\Gamma}^{(\alpha^*)\dagger} \hat{H}^{(\alpha^*)} U_{\Gamma M_\Gamma}^{(\alpha^*)} d^3\vec{\tau} \quad \text{for nonlinear SM - F molecules} . \quad (20)$$

The integrals $h_i^{(\alpha^*)}$, $J_{kl}^{(\alpha^*)ij}$ and $K_{kl}^{(\alpha^*)ij}$ occurring in Eq.(14) are determined by

$$h_i^{(\alpha^*)} = u_i^{(\alpha^*)*}(\vec{r}_1) \hat{h}^{(\alpha^*)} u_i^{(\alpha^*)}(\vec{r}_1) d^3\vec{r}_1$$

(21)

$$J_{kl}^{(\alpha^*)ij} = u_i^{(\alpha^*)*}(\vec{r}_1) \hat{J}_{kl}^{(\alpha^*)}(\vec{r}_1) u_j^{(\alpha^*)}(\vec{r}_1) d^3\vec{r}_1 \quad (22a)$$

$$= u_k^{(\alpha^*)*}(\vec{r}_2) \hat{J}_{ij}^{(\alpha^*)}(\vec{r}_2) u_l^{(\alpha^*)}(\vec{r}_2) d^3\vec{r}_2 \quad (22b)$$

$$K_{kl}^{(\alpha^*)ij} = u_i^{(\alpha^*)*}(\vec{r}_1) \hat{K}_{kl}^{(\alpha^*)}(\vec{r}_1) u_j^{(\alpha^*)}(\vec{r}_1) d^3\vec{r}_1 \quad (23a)$$

$$= u_k^{(\alpha^*)*}(\vec{r}_2) \hat{K}_{ij}^{(\alpha^*)}(\vec{r}_2) u_l^{(\alpha^*)}(\vec{r}_2) d^3\vec{r}_2 , \quad (23b)$$

where

$$\hat{h}^{(\alpha^*)} = -\frac{1}{2} \nabla^2 + \sum_a V_{nl}^{(\alpha^*)}(\zeta, r_{a1}) \quad (24)$$

$$\hat{J}_{kl}^{(\alpha^*)}(\vec{r}_1)\varphi(\vec{r}_1) = u_k^{(\alpha^*)}(\vec{r}_2)V_{nl}^{(\alpha^*)}(\zeta, r_{21})u_l^{(\alpha^*)}(\vec{r}_2)d^3r_2\varphi(\vec{r}_1) \quad (25)$$

$$\hat{K}_{kl}^{(\alpha^*)}(\vec{r}_1)\varphi(\vec{r}_1) = u_k^{(\alpha^*)}(\vec{r}_2)V_{nl}^{(\alpha^*)}(\zeta, r_{21})\varphi(\vec{r}_2)d^3r_2u_l^{(\alpha^*)}(\vec{r}_1) . \quad (26)$$

Here, $\hat{K}_{kl}^{(\alpha^*)}$ is the exchange operator.

In the single-determinantal closed shell case ($f_i = f_k = 1$ and $A_{kl}^{ij} = B_{kl}^{ij} = \delta_{ij}\delta_{kl}$), the formula for $E^{(\alpha^*)}$, Eq.(14), can be rewritten using 2-indexed integrals $J_{kk}^{(\alpha^*)ii}$ and $K_{kk}^{(\alpha^*)ii}$:

$$E^{(\alpha^*)} = \sum_i^n h_i^{(\alpha^*)} + \sum_{ik}^n \left(2J_{kk}^{(\alpha^*)ii} - K_{kk}^{(\alpha^*)ii} \right) . \quad (27)$$

It should be noted that the Eqs. (14) and (27) **are completely** general for a single configuration with arbitrary open and closed shells, respectively. These formulas have no spin. Accordingly, the HF and Combined Hartree-Fock-Roothaan (CHFR) equations presented in a previous paper [10] can be also used in the case of SM-F atomic-molecular systems.

5. Conclusion

In this paper, using complete orthonormal sets of $\psi^{(\alpha^*)}$ -SFETOs, condition of relativistic covariance and Pauli principle for fermions with $s=0$ and $e=0$, the periodic table for configurations of SM-F atoms has been constructed **up to Z=14. The suggested method successfully works also beyond Z=14.** The open shell HF and CHFR equations for SM-F atomic-molecular systems are also suggested. The presented formulas can be used in the study of different quantum mechanical problems in both the theory and practice of structure calculations dealing with SM-F atomic-molecular and solid systems with arbitrary values of quantum numbers, screening constants and location of SM-F orbitals.

We note that the suggested theory in this paper can be also used in the case of SM-F atomic-molecular and nuclear systems. This work and presented approach in Ref. [10] will do to help understand atomic and molecular systems within the domain of nuclear particles. An application of presented theory in this paper to the atomic-molecular and nuclear systems will be examined in future studies.

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Appendix

In accordance with the condition of relativistic covariance, the Hamilton operator of relativistic noncharged ($e = 0$) scalar ($s = 0$) particle

$$\hat{H} = \sqrt{c^2 \hat{p}^2 + m^2 c^4} + V \quad (\text{A1})$$

corresponding to the Hamilton function

$$H = \sqrt{c^2 \vec{p}^2 + m^2 c^4} + V \quad (\text{A2})$$

has to be linear and Hermitian, where V is the potential produced by the Lorentz self-frictional field (see Eq. (9)). For the linearization of the square root in Eq. (A1) one has to use the Dirac group theory and Clifford algebra. In the case of $\frac{1}{2}$ -spin theories, the groups with a Clifford algebraic structure are discussed in [11]. The self-frictional SM-F field problem can be solved in a similar way.

Using the method set out in [3] and [11], in the case of spinless particle ($s = 0$), one can **easily show** that, the order of the Dirac group is:

$$g = 8. \quad (\text{A3})$$

It has five classes, and therefore five irreducible representations of dimensions n_i such that

$$\sum_{i=1}^5 n_i^2 = g \quad (\text{A4})$$

of which four are one-dimensional and one is **four-dimensional**. **One-dimensional** representations are commutative, i.e., do not satisfy the conditions of Clifford algebra. Accordingly, only the **four-dimensional** representation is of help. The matrices for this irreducible representation are given in a previous paper [3]. The properties of the Dirac group **are summarized** in Table A.

Table A. Summary of Dirac group properties for $s = 0$

s	Group order	Number of classes	Number of 1-D irreps	Number of 2-D irreps
0	8	5	4	1

Note: irreps, irreducible representations