Generalized Relativistic Equation of Arbitrary Mass and Spin and Basis Sets of Spinor Functions for Its Solution in Position, Momentum and Four-Dimensional Spaces

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Abstract

Using condition of relativistic covariance, group theory and Clifford algebra the $2(2s+1)$-component Lorentz invariance generalized relativistic wave equation for a particle with arbitrary mass m and spin s is suggested, where $m \geq 0$ and $s = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, ...$ It is shown that the charged scalar ($e \neq 0$ *and* $s = 0$) and noncharged scalar ($e = 0$ *and* $s = 0$) particles with $m \neq 0$ are described by two-component relativistic equations. Accordingly, the noncharged scalar fermi particles ($m \neq 0, e = 0$ *and* $s = 0$) can be used as an elementary particle of the Standard Model of particle physics. In the case of arbitrary integral spin $(s = 1, 2, ...)$, the relativistic equation for $m = 0$ leads to the equation of massless boson particles. For the solution of presented in this work generalized relativistic equation in the linear combination of atomic orbitals approximation, the 2(2s+1)-component orthogonal basis sets of spinor functions for the arbitrary mass and spin are suggested in position, momentum and four-dimensional spaces.

Keywords: Relativistic covariance, Clifford algebra, Lorentz invariance, Exponential type spinor orbitals, Slater type spinor orbitals

I. Introduction

It is well known that the form of relativistic or nonrelativistic wave equations of motion depends on the spin of the particles. The usual 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. The spin-1/2 particles are governed by the relativistic Dirac equation which, in the nonrelativistic limit, leads to the Schrödinger-Pauli equation [1-4]. For particles with spin-1 or higher, only relativistic equations are usually considered [5].

The first higher spin equations have been proposed by Dirac in [6]. These equations in the presence of an external electromagnetic field, as was shown by Fierz and Pauli [7], led to the inconsistencies. They have suggested the equations for the special cases of $s=\frac{3}{2}$ and $s=2$. Rarita and Schwinger [8] have developed theory of spin $\frac{3}{2}$ free particles which contains many of the features of the Dirac theory. The theory of spin-s free particles has been also developed by Proca [9], Kemmer [10] and Bargmann and Wigner [11]. All of these formalisms for spin-s free particles have many intrinsic contradictions and difficulties when an electromagnetic field interaction is introduced (see [12] and references therein). It should be noted that the mathematical structure of our study, based on the case of new definition of Bose-Fermion theory (see [13] and references therein), is different from all of the approaches which are available in the literature. Therefore, the generalized relativistic equation presented in this work can not be reduced to them. By the use of group theory and Clifford algebra, we have shown in [14] that the generalized relativistic equation for the particles with arbitrary half-integral spin is consistent and causal in the presence of an electromagnetic field interaction. The aim of this work is, using the method set out in [14, 15], to establish the generalized relativistic equation for fermions and bosons with arbitrary values of parameters. For the solution of this equation by the use of linear combination of atomic orbitals (LCAO) approach, the orthogonal basis sets of spinor functions are presented in position, momentum and four-dimensional spaces.

II. Generalized relativistic equation of arbitrary mass and spin

The arguments given for the solution of this problem are based on three completely different points of view, namely, the application of group theory, and making use of the conditions of relativistic covariance and Lorentz invariance.

II-1. Use of group theory and Clifford algebra

For a single particle of charge e and mass m the relativistic Hamilton operator is given by

$$\hat{H}=\sqrt{c^2(\hat{\vec{p}}-\tfrac{e}{c}\vec{A})^2+m^2c^4}+eA_0\,, \tag{II-1}$$

where $m\neq 0$ *and* $s=0,\frac{1}{2},\frac{3}{2},...$ for fermions, $m=0$ *and* $s=1,2,...$ for bosons, A_0 is the scalar potential, $\vec{A}$ the vector potential and $\hat{\vec{p}}=\frac{\hbar}{i}\vec{\nabla}$ the momentum operator.

The new arguments in presented approach based on the use of group theory and Clifford algebra. It is well known, in accordance with the postulates of quantum mechanics the Hamilton operator $\hat{H}$ has to be linear and Hermitian. One can immediately see that the condition of linearity cannot be fulfilled, since the square root is not a linear operator. Therefore, the relativistic problem for arbitrary mass and spin can be viewed in terms of a special polynomial algebra [16, 17]. In a previous work [14], for the linearization of the square root in the case of half-integral spin we have used the group theory and Clifford algebra. The generalized relativistic problem for arbitrary mass and spin can be solved in a similar way. Using the method set out in [14], we obtain for the order of the Clifford algebraic Dirac group the following relation:

$$g_s = 8(2s+1)^2, \qquad \text{(II-2)}$$

where $s = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, ...$ This group has $\frac{1}{2}g_s + 1$ classes, therefore, $\frac{1}{2}g_s + 1$ irreducible representations. The dimensions n_i for these representations are determined by

$$\sum_{i=1}^{\frac{1}{2}g_s+1} n_i^2 = g_s, \qquad \text{(II-3)}$$

where

$$n_i = \begin{cases} 1 & for\, 1 \le i \le \frac{1}{2}g_s \\ 2(2s+1) & for\, i = \frac{1}{2}g_s + 1 \end{cases}. \qquad \text{(II-4)}$$

The one-dimensional representations do not satisfy the conditions of Clifford, therefore, only the $2(2s+1)$ dimensional irreducible representations can be used. The results are presented in Table 1.

II-2. Generalized relativistic equation

Making use of Table 1 obtained from the application of group theory and condition of relativistic covariance we introduce the following $2(2s+1) \times 2(2s+1)$ Hermitian and unitary matrices:

$$\vec{\alpha}^s = \begin{pmatrix} 0 & 0 & . & . & . & 0 & \vec{\sigma} \\ 0 & 0 & . & . & . & \vec{\sigma} & 0 \\ . & . & . & . & \vec{\sigma} & 0 & 0 \\ . & . & 0 & \vec{\sigma} & . & . & . \\ . & . & \vec{\sigma} & 0 & . & . & . \\ 0 & \vec{\sigma} & 0 & . & . & . & . \\ \vec{\sigma} & 0 & . & . & . & 0 & 0 \end{pmatrix} \tag{II-5}$$

and

$$\beta^s = \begin{cases} \begin{pmatrix} I^s & 0^s \\ 0^s & -I^s \end{pmatrix} & for\ s = 0, \frac{1}{2}, \frac{3}{2}, ...\ and\ m \neq 0 \quad (II-6) \\ \begin{pmatrix} 0^s & 0^s \\ 0^s & 0^s \end{pmatrix} & for\ s = 1, 2, ...\ and\ m = 0. \quad (II-7) \end{cases}$$

These matrices satisfy

$$\alpha_k^s \beta^s + \beta^s \alpha_k^s = 0 \tag{II-8}$$

$$\alpha_k^s \alpha_l^s + \alpha_l^s \alpha_k^s = 2\delta_{kl} I^s. \tag{II-9}$$

It should be noted that, in the case of integral values of s the matrices β^s in the form $\beta^s = \begin{pmatrix} I^s & 0^s \\ 0^s & -I^s \end{pmatrix}$ do not satisfy the condition (II-8), i.e.,

$$\alpha_k^s \beta^s + \beta^s \alpha_k^s \neq 0 \qquad for\ s = 1, 2, ... \tag{II-10}$$

Therefore, Eq. (II-7) correspondences to the case of massless particles for $s = 1, 2, ...$.

The generalized relativistic equation corresponding to the matrices (II-5), (II-6) and (II-7) is defined as

$$i\hbar \frac{\partial \Psi^s}{\partial t} = \hat{H}^s \Psi^s \tag{II-11}$$

$$\hat{H}^s = c\vec{\alpha}^s (\hat{\vec{p}} - \tfrac{e}{c}\vec{A}) + mc^2 \beta^s + eA_0 \tag{II-12}$$

$$\Psi^s = \begin{pmatrix} \phi^s \\ \tilde{\phi}^s \end{pmatrix}, \quad \text{(II-13)}$$

where for integral spin (s=0,1,2,…)

$$\phi^s = \begin{pmatrix} \varphi^{s0} \\ \varphi^{s1} \\ \cdot \\ \cdot \\ \cdot \\ \varphi^{s,2s-1} \\ \varphi^{s,2s} \end{pmatrix} \quad \text{(II-14a)}$$

$$\tilde{\phi}^s = \begin{pmatrix} \tilde{\varphi}^{s,2s} \\ \tilde{\varphi}^{s,2s-1} \\ \cdot \\ \cdot \\ \cdot \\ \tilde{\varphi}^{s1} \\ \tilde{\varphi}^{s0} \end{pmatrix}, \quad \text{(II-14b)}$$

for half-integral spin $\left(s = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, ... \right)$

$$\phi^s = \begin{pmatrix} \chi^{s0} \\ \chi^{s2} \\ \cdot \\ \cdot \\ \cdot \\ \chi^{s,2s-3} \\ \chi^{s,2s-1} \end{pmatrix} \quad \text{(II-15a)}$$

$$\tilde{\phi}^{s} = \begin{pmatrix} \tilde{\chi}^{s,2s-1} \\ \tilde{\chi}^{s,2s-3} \\ . \\ . \\ . \\ \tilde{\chi}^{s2} \\ \tilde{\chi}^{s0} \end{pmatrix} \tag{II-15b}$$

Here, $\varphi^{s\lambda}$, $\tilde{\varphi}^{s\lambda}$ *and* $\chi^{s\lambda}, \tilde{\chi}^{s\lambda}$ are the single- and two-component matrices, respectively. The two-component matrices are defined as

$$\chi^{s\lambda} = \begin{pmatrix} u^{s\lambda} \\ u^{s,\lambda+1} \end{pmatrix} \tag{II-16a}$$

$$\tilde{\chi}^{s\lambda} = \begin{pmatrix} \tilde{u}^{s,\lambda+1} \\ \tilde{u}^{s\lambda} \end{pmatrix}, \tag{II-16b}$$

where $0 \le \lambda(1) \le 2s$ and $0 \le \lambda(2) \le 2s-1$ for s=0,1,2,… and $s = \frac{1}{2}, \frac{3}{2}, \frac{5}{2} \ldots$, respectively.

By the use of procedure described in Dirac's papers [18, 19] it is easy to show that the generalized relativistic equation (II-11) satisfies the condition of Lorentz invariance.

In the special case of scalar particles (s=0), the generalized relativistic equation (II-11) has the form:

$$i\hbar \frac{\partial \Psi^{0}}{\partial t} = \hat{H}^{0} \Psi^{0} \tag{II-17}$$

$$\hat{H}^{0} = c\vec{\alpha}^{0}(\hat{\vec{p}} - \tfrac{e}{c}\vec{A}) + mc^{2}\beta^{0} + eA_{0} \tag{II-18}$$

$$\Psi^{0} = \begin{pmatrix} \varphi^{00} \\ \tilde{\varphi}^{00} \end{pmatrix}, \tag{II-19}$$

where

$$\vec{\alpha}^{0} = \vec{\sigma}, \quad \beta^{0} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{II-20}$$

Here, $\vec{\sigma}$ is formed by the Pauli matrices $\sigma_1, \sigma_2, \sigma_3$ and

$$\vec{\sigma}\hat{\vec{p}} = \frac{\hbar}{i}\begin{pmatrix} \frac{\partial}{\partial z} & \frac{\partial}{\partial x} - i\frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} + i\frac{\partial}{\partial y} & -\frac{\partial}{\partial z} \end{pmatrix}. \qquad \text{(II-21)}$$

In the case of free particle for e=0, s=0 and $m \neq 0$, the two-component relativistic equation becomes

$$\hat{H}^0\Psi^0 = \varepsilon\Psi^0, \qquad \text{(II-22)}$$

$$\hat{H}^0 = c\left(\vec{\sigma}\hat{\vec{p}}\right) + mc^2\sigma_3. \qquad \text{(II-23)}$$

As can easily be seen that the Eq.(II-17) for relativistic scalar particles is a first-order differential equation, while the Klein-Cordon equation forms a second-order differential equation. Therefore, one has to arrive immediately at the conclusion that the Klein-Cordon equation does not meet the requirement of the condition of relativistic covariance, namely, the condition of linearity for a relativistic Hamiltonian. The Klein-Gordon equation only partially satisfies the postulates of (relativistic) quantum mechanics.

III. Basis sets of spinor functions in position, momentum and four-dimensional spaces

The elaboration of algorithms for the solution of the generalized relativistic equation for the particles with arbitrary mass and spin in linear combination of atomic orbitals (LCAO) approach [20-22] necessitates progress in the development of theory for complete orthonormal basis sets of relativistic spinor functions of multiple orders. The method for constructing in position, momentum and four-dimensional spaces the complete orthonormal basis sets for (2s+1)-component relativistic tensor wave functions and Slater tensor orbitals has been suggested in previous article [23]. Extending this approach to the case of spinors of multiple order and using the method set out in [24], we construct in this study the relevant complete orthonormal basis sets of 2(2s+1)-component relativistic $\Psi^{\alpha s}$-exponential type spinor orbitals ($\Psi^{\alpha s}$ -ETSO) for particles with arbitrary mass and spin in position, momentum and four-dimensional spaces through the sets of one- and two-component spinor type tensor spherical harmonics and radial parts of the complete orthonormal sets of nonrelativistic ψ^{α}-exponential type orbitals (ψ^{α} -ETO) [25] the angular parts of which are the scalar spherical harmonics. The indices α occurring in the radial parts of ψ^{α} -ETO is the self-frictional quantum number [26]. It should be noted that the nonrelativistic ψ^{α}-ETO are the special cases of $\Psi^{\alpha s}$-ETSO for s=0, i.e., $\Psi^{\alpha 0} \equiv \psi^{\alpha}$. The basis sets of relativistic spinors of multiple order obtained might be useful for solution of generalized relativistic equation of arbitrary mass and spin particles when the complete orthonormal relativistic $\Psi^{\alpha s}$-ETSO basis sets in LCAO approximation are employed. We notice that the definition of phases in this work for the scalar spherical harmonics $\left(Y^{*}_{lm_l} = Y_{l-m_l}\right)$ differs from the Condon-Shortley phases [27] by the sing factor $\left(Y^{*}_{lm_l} = i^{|m_l|+m_l} Y_{l-m_l}\right)$.

III-1. Relativistic spinor type tensor spherical harmonics

In order to construct the complete orthonormal basis sets of relativistic $\Psi^{\alpha s}$-ETSO and X^{s}-Slater type spinor orbitals (X^{s}-STSO) of 2(2s+1) order in position, momentum and four-dimensional spaces we introduce the following formulae for the independent spinor type tensor (STT) spherical harmonics of (2s+1) order (see Ref. [23]):

for integral spin:

$$H^{s}_{ljm}(\theta,\varphi) = \begin{bmatrix} H^{s0}_{ljm}(\theta,\varphi) \\ H^{s1}_{ljm}(\theta,\varphi) \\ \vdots \\ H^{s,2s-1}_{ljm}(\theta,\varphi) \\ H^{s,2s}_{ljm}(\theta,\varphi) \end{bmatrix} \tag{III-1a}$$

$$\mathcal{H}^{s}_{ljm}(\theta,\varphi) = \begin{bmatrix} \mathcal{H}^{s,2s}_{ljm}(\theta,\varphi) \\ \mathcal{H}^{s,2s-1}_{ljm}(\theta,\varphi) \\ \vdots \\ \mathcal{H}^{s1}_{ljm}(\theta,\varphi) \\ \mathcal{H}^{s0}_{ljm}(\theta,\varphi) \end{bmatrix} \tag{III-1b}$$

for half-integral spin

$$Y_{ljm}^{s}(\theta,\varphi)=\begin{bmatrix} Y_{ljm}^{s0}(\theta,\varphi) \\ Y_{ljm}^{s2}(\theta,\varphi) \\ \vdots \\ Y_{ljm}^{s,2s-3}(\theta,\varphi) \\ Y_{ljm}^{s,2s-1}(\theta,\varphi) \end{bmatrix} \tag{III-2a}$$

$$\Upsilon_{ljm}^{s}(\theta,\varphi)=\begin{bmatrix} \Upsilon_{ljm}^{s,2s-1}(\theta,\varphi) \\ \Upsilon_{ljm}^{s,2s-3}(\theta,\varphi) \\ \vdots \\ \Upsilon_{ljm}^{s2}(\theta,\varphi) \\ \Upsilon_{ljm}^{s0}(\theta,\varphi) \end{bmatrix} \tag{III-2b}$$

These STT spherical harmonics are eigenfunctions of operators $\hat{j}^2, \hat{j}_z, \hat{l}^2$ and $\hat{s}^2$. The one- and two-component basis sets of STT spherical harmonics $H_{ljm}^{s\lambda}(\theta,\varphi)$, $\mathcal{H}_{ljm}^{s\lambda}(\theta,\varphi)$ and $Y_{ljm}^{s\lambda}(\theta,\varphi)$, $\Upsilon_{ljm}^{s\lambda}(\theta,\varphi)$ occurring in Eqs. (III-1a), (III-1b) and (III-2a), (III-2b), respectively, can be expressed through the scalar spherical harmonics:

$$H_{ljm}^{s\lambda}(\theta,\varphi)=a_{ljm}^{s}(\lambda)\beta_{m(\lambda)}Y_{lm(\lambda)}(\theta,\varphi) \tag{III-3a}$$

$$\mathcal{H}_{ljm}^{s\lambda}(\theta,\varphi)=-ia_{ljm}^{s}(\lambda)\beta_{m(\lambda)}Y_{lm(\lambda)}(\theta,\varphi) \tag{III-3b}$$

$$Y_{ljm}^{s\lambda}(\theta,\varphi)=\begin{bmatrix} a_{ljm}^{s}(\lambda)\beta_{m(\lambda)}Y_{lm(\lambda)}(\theta,\varphi) \\ a_{ljm}^{s}(\lambda+1)\beta_{m(\lambda+1)}Y_{lm(\lambda+1)}(\theta,\varphi) \end{bmatrix} \tag{III-4a}$$

$$\Upsilon_{ljm}^{s\lambda}(\theta,\varphi)=\begin{bmatrix} -ia_{ljm}^{s}(\lambda+1)\beta_{m(\lambda+1)}Y_{lm(\lambda+1)}(\theta,\varphi) \\ -ia_{ljm}^{s}(\lambda)\beta_{m(\lambda)}Y_{lm(\lambda)}(\theta,\varphi) \end{bmatrix}, \tag{III-4b}$$

where

for integral spin

$$0\le\lambda(1)\le 2s, \qquad |l-s|\le j\le j+s,\ -j\le m\le j, \qquad j=l+\frac{1}{2}t, \qquad t=2(j-l)=0,\pm 2,\ldots,\pm 2s,$$

$$m_l=m(\lambda)=m-s+\lambda \ \ and \ \ \beta_{m(\lambda)}=(-1)^{[|m(\lambda)|-m(\lambda)]/2},$$

for half-integral spin

$$0 \le \lambda(2) \le 2s-1,\ |l-s| \le j \le j+s,\ -j \le m \le j,\ j = l + \frac{1}{2}t,$$

$$t = 2(j-l) = \pm1, \pm3, \ldots, \pm2s,\ \ m_l = m(\lambda) = m - s + \lambda,\ \ \beta_{m(\lambda)} = (-1)^{[|m(\lambda)|-m(\lambda)]/2}.$$

Here, $a^s_{ljm}(\lambda)$ are the modified Clebsch-Gordan coefficients defined as

$$a^s_{ljm}(\lambda) = \left(lsm(\lambda)s-\lambda \middle| lsjm\right). \qquad \text{(III-5)}$$

See Ref. [27] for the definition of Clebsch-Gordan coefficients $\left(lsm_l m-m_l \middle| lsjm\right)$.

The STT spherical harmonics $H^s_{ljm}(\theta,\varphi)$, $\mathcal{H}^s_{ljm}(\theta,\varphi)$ and $Y^s_{ljm}(\theta,\varphi)$, $\Upsilon^s_{ljm}(\theta,\varphi)$ for fixed s satisfy the following orthonormality relations:

$$\int_0^{\pi}\int_0^{2\pi} H^{s^*}_{ljm}(\theta,\varphi) H^s_{l'j'm'}(\theta,\varphi) Sin\theta d\theta d\varphi = \sum_{\lambda=0}^{2s}\int_0^{\pi}\int_0^{2\pi} H^{s\lambda^*}_{ljm}(\theta,\varphi) H^{s\lambda}_{l'j'm'}(\theta,\varphi) Sin\theta d\theta d\varphi = \delta_{ll'}\delta_{jj'}\delta_{mm'} \qquad \text{(III-6a)}$$

$$\int_0^{\pi}\int_0^{2\pi} \mathcal{H}^{s^*}_{ljm}(\theta,\varphi) \mathcal{H}^s_{l'j'm'}(\theta,\varphi) Sin\theta d\theta d\varphi = \sum_{\lambda=0}^{2s}\int_0^{\pi}\int_0^{2\pi} \mathcal{H}^{s\lambda^*}_{ljm}(\theta,\varphi) \mathcal{H}^{s\lambda}_{l'j'm'}(\theta,\varphi) Sin\theta d\theta d\varphi = \delta_{ll'}\delta_{jj'}\delta_{mm'} \qquad \text{(III-6b)}$$

$$\int_0^{\pi}\int_0^{2\pi} Y^{s^\dagger}_{ljm}(\theta,\varphi) Y^s_{l'j'm'}(\theta,\varphi) Sin\theta d\theta d\varphi = \sum_{\lambda=0}^{2s-1}\int_0^{\pi}\int_0^{2\pi} Y^{s\lambda^\dagger}_{ljm}(\theta,\varphi) Y^{s\lambda}_{l'j'm'}(\theta,\varphi) Sin\theta d\theta d\varphi = \delta_{ll'}\delta_{jj'}\delta_{mm'} \qquad \text{(III-7a)}$$

$$\int_0^{\pi}\int_0^{2\pi} \Upsilon^{s^\dagger}_{ljm}(\theta,\varphi) \Upsilon^s_{l'j'm'}(\theta,\varphi) Sin\theta d\theta d\varphi = \sum_{\lambda=0}^{2s-1}\int_0^{\pi}\int_0^{2\pi} \Upsilon^{s\lambda^\dagger}_{ljm}(\theta,\varphi) \Upsilon^{s\lambda}_{l'j'm'}(\theta,\varphi) Sin\theta d\theta d\varphi = \delta_{ll'}\delta_{jj'}\delta_{mm'}\ . \qquad \text{(III-7b)}$$

III-2. Basis sets of relativistic $\Psi^{\alpha s}$-ETSO and X^s-STSO functions

To construct the basis sets of 2(2s+1)-component relativistic spinors from STT spherical harmonics and radial parts of nonrelativistic orbitals we use the method set out in a previous paper [14]. Then, we obtain for the complete basis sets of relativistic spinor wave functions $\Psi^{\alpha s}$, $\bar{\Psi}^{\alpha s}$ and Slater spinor orbitals X^s in position space the following relations:

for integral spin

$$\Psi^{\alpha s}_{nljm}\left(r,\theta,\varphi\right)=\frac{1}{\sqrt{2}}\begin{bmatrix} R^{\alpha}_{nl}\left(r\right)H^{s}_{ljm}\left(\theta,\varphi\right)\\ \tilde{R}^{\alpha}_{\tilde{n}l}\left(r\right)\mathcal{H}^{s}_{ljm}\left(\theta,\varphi\right)\end{bmatrix}=\frac{1}{\sqrt{2}}\begin{bmatrix} a^{s}_{ljm}\left(0\right)\beta_{m(0)}\psi^{\alpha}_{nlm(0)}\left(r,\theta,\varphi\right)\\ a^{s}_{ljm}\left(1\right)\beta_{m(1)}\psi^{\alpha}_{nlm(1)}\left(r,\theta,\varphi\right)\\ \vdots\\ a^{s}_{ljm}\left(2s-1\right)\beta_{m(2s-1)}\psi^{\alpha}_{nlm(2s-1)}\left(r,\theta,\varphi\right)\\ a^{s}_{ljm}\left(2s\right)\beta_{m(2s)}\psi^{\alpha}_{nlm(2s)}\left(r,\theta,\varphi\right)\\ -ia^{s}_{ljm}\left(2s\right)\beta_{m(2s)}\psi^{\alpha}_{\tilde{n}lm(2s)}\left(r,\theta,\varphi\right)\\ -ia^{s}_{ljm}\left(2s-1\right)\beta_{m(2s-1)}\psi^{\alpha}_{\tilde{n}lm(2s-1)}\left(r,\theta,\varphi\right)\\ \vdots\\ -ia^{s}_{ljm}\left(1\right)\beta_{m(1)}\psi^{\alpha}_{\tilde{n}lm(1)}\left(r,\theta,\varphi\right)\\ -ia^{s}_{ljm}\left(0\right)\beta_{m(0)}\psi^{\alpha}_{\tilde{n}lm(0)}\left(r,\theta,\varphi\right)\end{bmatrix} \qquad \text{(III-8a)}$$

$$\bar{\Psi}^{\alpha s}_{nljm}\left(r,\theta,\varphi\right)=\frac{1}{\sqrt{2}}\begin{bmatrix} \bar{R}^{\alpha}_{nl}\left(r\right)H^{s}_{ljm}\left(\theta,\varphi\right)\\ \tilde{\bar{R}}^{\alpha}_{\tilde{n}l}\left(r\right)\mathcal{H}^{s}_{ljm}\left(\theta,\varphi\right)\end{bmatrix}=\frac{1}{\sqrt{2}}\begin{bmatrix} a^{s}_{ljm}\left(0\right)\beta_{m(0)}\bar{\psi}^{\alpha}_{nlm(0)}\left(r,\theta,\varphi\right)\\ a^{s}_{ljm}\left(1\right)\beta_{m(1)}\bar{\psi}^{\alpha}_{nlm(1)}\left(r,\theta,\varphi\right)\\ \vdots\\ a^{s}_{ljm}\left(2s-1\right)\beta_{m(2s-1)}\bar{\psi}^{\alpha}_{nlm(2s-1)}\left(r,\theta,\varphi\right)\\ a^{s}_{ljm}\left(2s\right)\beta_{m(2s)}\bar{\psi}^{\alpha}_{nlm(2s)}\left(r,\theta,\varphi\right)\\ -ia^{s}_{ljm}\left(2s\right)\beta_{m(2s)}\bar{\psi}^{\alpha}_{\tilde{n}lm(2s)}\left(r,\theta,\varphi\right)\\ -ia^{s}_{ljm}\left(2s-1\right)\beta_{m(2s-1)}\bar{\psi}^{\alpha}_{\tilde{n}lm(2s-1)}\left(r,\theta,\varphi\right)\\ \vdots\\ -ia^{s}_{ljm}\left(1\right)\beta_{m(1)}\bar{\psi}^{\alpha}_{\tilde{n}lm(1)}\left(r,\theta,\varphi\right)\\ -ia^{s}_{ljm}\left(0\right)\beta_{m(0)}\bar{\psi}^{\alpha}_{\tilde{n}lm(0)}\left(r,\theta,\varphi\right)\end{bmatrix} \qquad \text{(III-8b)}$$

$$X^{s}_{nljm}\left(r,\theta,\varphi\right)=\frac{1}{\sqrt{2}}\begin{bmatrix} R_{n}\left(r\right)H^{s}_{ljm}\left(\theta,\varphi\right)\\ R_{n}\left(r\right)\mathcal{H}^{s}_{ljm}\left(\theta,\varphi\right)\end{bmatrix}=\frac{1}{\sqrt{2}}\begin{bmatrix} a^{s}_{ljm}\left(0\right)\beta_{m(0)}\chi_{nlm(0)}\left(r,\theta,\varphi\right)\\ a^{s}_{ljm}\left(1\right)\beta_{m(1)}\chi_{nlm(1)}\left(r,\theta,\varphi\right)\\ \vdots\\ a^{s}_{ljm}\left(2s-1\right)\beta_{m(2s-1)}\chi_{nlm(2s-1)}\left(r,\theta,\varphi\right)\\ a^{s}_{ljm}\left(2s\right)\beta_{m(2s)}\chi_{nlm(2s)}\left(r,\theta,\varphi\right)\\ -ia^{s}_{ljm}\left(2s\right)\beta_{m(2s)}\chi_{\tilde{n}lm(2s)}\left(r,\theta,\varphi\right)\\ -ia^{s}_{ljm}\left(2s-1\right)\beta_{m(2s-1)}\chi_{\tilde{n}lm(2s-1)}\left(r,\theta,\varphi\right)\\ \vdots\\ -ia^{s}_{ljm}\left(1\right)\beta_{m(1)}\chi_{\tilde{n}lm(1)}\left(r,\theta,\varphi\right)\\ -ia^{s}_{ljm}\left(0\right)\beta_{m(0)}\chi_{\tilde{n}\tilde{l}m(0)}\left(r,\theta,\varphi\right)\end{bmatrix}, \qquad \text{(III-9)}$$

for half-integral spin

$$\Psi^{\alpha s}_{nljm}(r,\theta,\varphi)=\frac{1}{\sqrt{2}}\begin{bmatrix} R^{\alpha}_{nl}(r)Y^{s}_{ljm}(\theta,\varphi) \\ R^{\alpha}_{\tilde{n}l}(r)\Upsilon^{s}_{ljm}(\theta,\varphi)\end{bmatrix}=\frac{1}{\sqrt{2}}\begin{bmatrix} a^{s}_{ljm}(0)\beta_{m(0)}\psi^{\alpha}_{nlm(0)}(r,\theta,\varphi) \\ a^{s}_{ljm}(2)\beta_{m(2)}\psi^{\alpha}_{nlm(2)}(r,\theta,\varphi) \\ \vdots \\ a^{s}_{ljm}(2s-3)\beta_{m(2s-3)}\psi^{\alpha}_{nlm(2s-3)}(r,\theta,\varphi) \\ a^{s}_{ljm}(2s-1)\beta_{m(2s-1)}\psi^{\alpha}_{nlm(2s-1)}(r,\theta,\varphi) \\ -ia^{s}_{ljm}(2s-1)\beta_{m(2s-1)}\psi^{\alpha}_{\tilde{n}lm(2s-1)}(r,\theta,\varphi) \\ -ia^{s}_{ljm}(2s-3)\beta_{m(2s-3)}\psi^{\alpha}_{\tilde{n}lm(2s-3)}(r,\theta,\varphi) \\ \vdots \\ -ia^{s}_{ljm}(2)\beta_{m(2)}\psi^{\alpha}_{\tilde{n}lm(2)}(r,\theta,\varphi) \\ -ia^{s}_{ljm}(0)\beta_{m(0)}\psi^{\alpha}_{\tilde{n}lm(0)}(r,\theta,\varphi) \end{bmatrix} \quad \text{(III-10a)}$$

$$\bar{\Psi}^{\alpha s}_{nljm}(r,\theta,\varphi)=\frac{1}{\sqrt{2}}\begin{bmatrix} \bar{R}^{\alpha}_{nl}(r)Y^{s}_{ljm}(\theta,\varphi) \\ \tilde{\bar{R}}^{\alpha}_{\tilde{n}l}(r)\Upsilon^{s}_{ljm}(\theta,\varphi)\end{bmatrix}=\frac{1}{\sqrt{2}}\begin{bmatrix} a^{s}_{ljm}(0)\beta_{m(0)}\bar{\psi}^{\alpha}_{nlm(0)}(r,\theta,\varphi) \\ a^{s}_{ljm}(2)\beta_{m(2)}\bar{\psi}^{\alpha}_{nlm(2)}(r,\theta,\varphi) \\ \vdots \\ a^{s}_{ljm}(2s-3)\beta_{m(2s-3)}\bar{\psi}^{\alpha}_{nlm(2s-3)}(r,\theta,\varphi) \\ a^{s}_{ljm}(2s-1)\beta_{m(2s-1)}\bar{\psi}^{\alpha}_{nlm(2s-1)}(r,\theta,\varphi) \\ -ia^{s}_{ljm}(2s-1)\beta_{m(2s-1)}\bar{\psi}^{\alpha}_{\tilde{n}lm(2s-1)}(r,\theta,\varphi) \\ -ia^{s}_{ljm}(2s-3)\beta_{m(2s-3)}\bar{\psi}^{\alpha}_{\tilde{n}lm(2s-3)}(r,\theta,\varphi) \\ \vdots \\ -ia^{s}_{ljm}(2)\beta_{m(2)}\bar{\psi}^{\alpha}_{\tilde{n}lm(2)}(r,\theta,\varphi) \\ -ia^{s}_{ljm}(0)\beta_{m(0)}\bar{\psi}^{\alpha}_{\tilde{n}lm(0)}(r,\theta,\varphi) \end{bmatrix} \quad \text{(III-10b)}$$

$$X^{s}_{nljm}(r,\theta,\varphi)=\frac{1}{\sqrt{2}}\begin{bmatrix} R_{n}(r)Y^{s}_{ljm}(\theta,\varphi) \\ \tilde{R}_{\tilde{n}}(r)\Upsilon^{s}_{ljm}(\theta,\varphi)\end{bmatrix}=\frac{1}{\sqrt{2}}\begin{bmatrix} a^{s}_{ljm}(0)\beta_{m(0)}\chi_{nlm(0)}(r,\theta,\varphi) \\ a^{s}_{ljm}(2)\beta_{m(2)}\chi_{nlm(2)}(r,\theta,\varphi) \\ \vdots \\ a^{s}_{ljm}(2s-3)\beta_{m(2s-3)}\chi_{nlm(2s-3)}(r,\theta,\varphi) \\ a^{s}_{ljm}(2s-1)\beta_{m(2s-1)}\chi_{nlm(2s-1)}(r,\theta,\varphi) \\ -ia^{s}_{ljm}(2s-1)\beta_{m(2s-1)}\chi_{\tilde{n}lm(2s-1)}(r,\theta,\varphi) \\ -ia^{s}_{ljm}(2s-3)\beta_{m(2s-3)}\chi_{\tilde{n}lm(2s-3)}(r,\theta,\varphi) \\ \vdots \\ -ia^{s}_{ljm}(2)\beta_{m(2)}\chi_{\tilde{n}lm(2)}(r,\theta,\varphi) \\ -ia^{s}_{ljm}(0)\beta_{m(0)}\chi_{\tilde{n}lm(0)}(r,\theta,\varphi) \end{bmatrix}, \quad \text{(III-11)}$$

where $n \geq 1,\ s \leq j \leq s+n-1,\ \ j-s \leq l \leq \min(j+s,\ n-1)$ and

$$\tilde{R}_{\tilde{n}}(r)=R_{\tilde{n}}(\zeta,r)=\frac{(2\zeta)^{\tilde{n}+\frac{1}{2}}}{\sqrt{(2\tilde{n})!}}r^{\tilde{n}-1}e^{-\zeta r}. \quad \text{(III-12)}$$

The relativistic spinor wave functions ($K^{\alpha s}_{nljm}, \bar{K}^{\alpha s}_{nljm}$) and Slater spinor orbitals K^{s}_{nljm} in position, momentum and four-dimensional spaces are defined as

$$K^{\alpha s}_{nljm}\equiv\Psi^{\alpha s}_{nljm}(\zeta,\vec{r}),\Phi^{\alpha s}_{nljm}(\zeta,\vec{k}),Z^{\alpha s}_{nljm}(\zeta,\beta\theta\varphi) \quad \text{(III-13)}$$

$$\bar{K}^{\alpha s}_{nljm}\equiv\bar{\Psi}^{\alpha s}_{nljm}(\zeta,\vec{r}),\bar{\Phi}^{\alpha s}_{nljm}(\zeta,\vec{k}),\bar{Z}^{\alpha s}_{nljm}(\zeta,\beta\theta\varphi) \quad \text{(III-14)}$$

$$K^{s}_{nljm}\equiv X^{s}_{nljm}(\zeta,\vec{r}),U^{s}_{nljm}(\zeta,\vec{k}),V^{s}_{nljm}(\zeta,\beta\theta\varphi). \quad \text{(III-15)}$$

Here, the $k^{\alpha}_{nlm(\lambda)}$, $\bar{k}^{\alpha}_{nlm(\lambda)}$ and $k_{nlm(\lambda)}$ are the nonrelativistic complete basis sets of orbitals. They are determined through the corresponding nonrelativistic functions in position, momentum and four-dimensional spaces by

$$k^{\alpha}_{nlm(\lambda)}\equiv\psi^{\alpha}_{nlm(\lambda)}(\zeta,\vec{r}),\phi^{\alpha}_{nlm(\lambda)}(\zeta,\vec{k}),z^{\alpha}_{nlm(\lambda)}(\zeta,\beta\theta\varphi) \quad \text{(III-16)}$$

$$\bar{k}^{\alpha}_{nlm(\lambda)}\equiv\bar{\psi}^{\alpha}_{nlm(\lambda)}(\zeta,\vec{r}),\bar{\phi}^{\alpha}_{nlm(\lambda)}(\zeta,\vec{k}),\bar{z}^{\alpha}_{nlm(\lambda)}(\zeta,\beta\theta\varphi) \quad \text{(III-17)}$$

$$k_{nlm(\lambda)}\equiv\chi_{nlm(\lambda)}(\zeta,\vec{r}),u_{nlm(\lambda)}(\zeta,\vec{k}),v_{nlm(\lambda)}(\zeta,\beta\theta\varphi). \quad \text{(III-18)}$$

See Ref. [28] for the exact definition of functions occurring in Eqs. (III-13) - (III-18).

The relativistic spinor orbitals satisfy the following orthogonality relations:

$$\int K^{\alpha s^{\dagger}}_{nljm}(\zeta,\vec{x})\bar{K}^{\alpha s}_{n'l'j'm'}(\zeta,\vec{x})\,d\vec{x}=\delta_{nn'}\delta_{ll'}\delta_{jj'}\delta_{mm'} \quad \text{(III-19)}$$

$$\int K^{s^{\dagger}}_{nljm}(\zeta,\vec{x})K^{s}_{n'l'j'm'}(\zeta,\vec{x})\,d\vec{x}=\frac{(n+n')!}{\left[(2n)!(2n')!\right]^{1/2}}\delta_{ll'}\delta_{jj'}\delta_{mm'}. \quad \text{(III-20)}$$

Using the relation $a^{0}_{ljm}(\lambda)=\delta_{jl}\delta_{mm_l}\delta_{\lambda 0}$ and formulae

$$H^{0}_{ljm}(\theta,\varphi)=\beta_{m_l}Y_{lm_l}(\theta,\varphi) \quad \text{(III-21a)}$$

$$\mathcal{H}^{0}_{ljm}(\theta,\varphi)=-i\beta_{m_l}Y_{lm_l}(\theta,\varphi) \quad \text{(III-21b)}$$

for the scalar particles it is easy to show that the relativistic spinor functions

$K^{\alpha s}_{nljm}$, $\bar{K}^{\alpha s}_{nljm}$ and relativistic Slater spinor orbitals K^{s}_{nljm} for particles with spin s=0 are reduced to the corresponding quantities for nonrelativistic complete basis sets in positon, momentum and four-dimensional spaces, i.e., $K^{\alpha s}_{nljm} \equiv k^{\alpha}_{nlm_l}, \bar{K}^{\alpha s}_{nljm} \equiv \bar{k}^{\alpha}_{nlm_l}$ and $K^{s}_{nljm} \equiv k_{nlm_l}$, where $s=0,\ j=l,\ t=0,\ m(\lambda)=m_l\delta_{\lambda 0}$ and $m = m_l$. Thus, the nonrelativistic and relativistic scalar particles can be also described by wave functions $K^{\alpha s}_{nljm}, \bar{K}^{\alpha s}_{nljm}$ and K^{s}_{nljm} for s=t=0, $j=l$ and $m=m_l$, i.e.,

$$K^{\alpha 0}_{nlm_l} = \frac{1}{\sqrt{2}}\begin{bmatrix} k^{\alpha}_{nlm_l} \\ -ik^{\alpha}_{nlm_l} \end{bmatrix} \qquad \text{(III-22a)}$$

$$\bar{K}^{\alpha 0}_{nlm_l} = \frac{1}{\sqrt{2}}\begin{bmatrix} \bar{k}^{\alpha}_{nlm_l} \\ -i\bar{k}^{\alpha}_{nlm_l} \end{bmatrix} \qquad \text{(III-22b)}$$

$$K^{0}_{nlm_l} = \frac{1}{\sqrt{2}}\begin{bmatrix} k_{nlm_l} \\ -ik_{nlm_l} \end{bmatrix}. \qquad \text{(III-23)}$$

The 2-, 6-,10- and 4-, 8-component complete orthonormal basis sets of relativistic $\Psi^{\alpha s}$-ETSO through the nonrelativistic ψ^{α}-ETO in position space for $s=0,\ s=1,\ s=2$ *and* $s=\frac{1}{2},\ s=\frac{3}{2}$, respectively, are given in Tables 2, 3, 4 and 5, 6.

III-3. Derivatives of $\Psi^{\alpha s}$-ETSO in position space

Now, we evaluate the derivatives of $\Psi^{\alpha s}$-ETSO with respect to Cartesian coordinates that can be used in the solution of reduced relativistic equations when the LCAO approach is employed. For this purpose we use the $\Psi^{\alpha s}$-ETSO in the following form:

for integral spin

$$\Psi_{nljm}^{\alpha s}=\frac{1}{\sqrt{2}}\begin{bmatrix}\phi_{nljm}^{\alpha s}\\ \tilde{\phi}_{\tilde{n}ljm}^{\alpha s}\end{bmatrix}=\frac{1}{\sqrt{2}}\begin{bmatrix}\phi_{nljm}^{\alpha s,0}\\ \phi_{nljm}^{\alpha s,1}\\ \vdots\\ \phi_{nljm}^{\alpha s,2s}\\ \tilde{\phi}_{\tilde{n}ljm}^{\alpha s,2s}\\ \vdots\\ \tilde{\phi}_{\tilde{n}ljm}^{\alpha s,1}\\ \tilde{\phi}_{\tilde{n}ljm}^{\alpha s,0}\end{bmatrix}, \tag{III-24}$$

for half integral spin

$$\Psi_{nljm}^{\alpha s}=\frac{1}{\sqrt{2}}\begin{bmatrix}\varphi_{nljm}^{\alpha s}\\ \tilde{\varphi}_{\tilde{n}ljm}^{\alpha s}\end{bmatrix}=\frac{1}{\sqrt{2}}\begin{bmatrix}\varphi_{nljm}^{\alpha s,0}\\ \varphi_{nljm}^{\alpha s,2}\\ \vdots\\ \varphi_{nljm}^{\alpha s,2s-1}\\ \tilde{\varphi}_{\tilde{n}ljm}^{\alpha s,2s-1}\\ \vdots\\ \tilde{\varphi}_{\tilde{n}ljm}^{\alpha s,2}\\ \tilde{\varphi}_{\tilde{n}ljm}^{\alpha s,0}\end{bmatrix}, \tag{III-25}$$

where $\phi^{\alpha s,\lambda}$, $\tilde{\phi}^{\alpha s,\lambda}$ and $\varphi^{\alpha s,\lambda},\tilde{\varphi}^{\alpha s,\lambda}$ are the one- and two-component spinors, respectively, are defined by

$$\phi_{nljm}^{\alpha s,\lambda}=R_{nl}^{\alpha}\left(r\right)H_{ljm}^{s\lambda}\left(\theta,\varphi\right) \tag{III-26a}$$

$$\tilde{\phi}_{\tilde{n}ljm}^{\alpha s,\lambda}=\tilde{R}_{\tilde{n}l}^{\alpha}\left(r\right)\mathcal{H}_{ljm}^{s\lambda}\left(\theta,\varphi\right) \tag{III-26b}$$

$$\varphi_{nljm}^{\alpha s,\lambda}=R_{nl}^{\alpha}\left(r\right)Y_{ljm}^{s\lambda}\left(\theta,\varphi\right) \tag{III-27a}$$

$$\tilde{\varphi}_{\tilde{n}ljm}^{\alpha s,\lambda}=\tilde{R}_{\tilde{n}l}^{\alpha}\left(r\right)\Upsilon_{ljm}^{s\lambda}\left(\theta,\varphi\right). \tag{III-27b}$$

Here, $0\le\lambda(1)\le 2s$ and $0\le\lambda(2)\le 2s-1$ for integral and half-integral spin, respectively.

To obtain the derivatives of $\Psi^{\alpha s}$-ETSO we use the following relations [15]:

$$\frac{\partial}{\partial z}(f\beta_m Y_{lm})=\sum_{k=-1}^{1}{}' \left[\frac{df}{dr}+\left(\delta_{k,-1}-kl\right)\frac{f}{r}\right]b_k^{lm}\beta_m Y_{l+k,m} \tag{III-28}$$

$$\left(\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right)\left(f\beta_m Y_{lm}\right)=\sum_{k=-1}^{1}{}'\left[\frac{df}{dr}+\left(\delta_{k,-1}-kl\right)\frac{f}{r}\right]d_k^{lm}\beta_{m-1}Y_{l+k,m-1} \tag{III-29}$$

$$\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)\left(f\beta_m Y_{lm}\right)=\sum_{k=-1}^{1}{}'\left[\frac{df}{dr}+\left(\delta_{k,-1}-kl\right)\frac{f}{r}\right]c_k^{lm}\beta_{m+1}Y_{l+k,m+1}, \tag{III-30}$$

where f is any function of the radial distance r and

$$b_k^{lm}=\left[(l+m+\delta_{k1})(l-m+\delta_{k1})/\left(2(l+1)+k\right)(2l+k)\right]^{1/2} \tag{III-31}$$

$$d_k^{lm}=-k\left[(l-km+2\delta_{k1})(l-k\left(m-1\right))/(2\left(l+1\right)+k)(2l+k)\right]^{1/2} \tag{III-32}$$

$$c_k^{lm}=k\left[(l+km+2\delta_{k1})(l+k\left(m+1\right))/\left(2(l+1)+k\right)(2l+k)\right]^{1/2}=-d_k^{l,-m}. \tag{III-33}$$

The symbol $\sum'$ in Eqs. (III-28), (III-29) and (III-30) indicates that the summation is to be performed in steps of two. These formulae can be obtained by the use of method set out in Ref.[29].

Using Eqs. (III-28), (III-29) and (III-30) we obtain for the derivatives of two-component spinors of half-integral spin the following relations:

$$c(\vec{\sigma}\hat{\vec{p}})\varphi^{\alpha s\lambda}=c(\vec{\sigma}\hat{\vec{p}})\left[R_{nl}^{\alpha}Y_{ljm}^{s\lambda}\right]=\frac{c\hbar}{i}\sum_{k=-1}^{1}{}'\left[\frac{dR_{nl}^{\alpha}}{dr}+\left(\delta_{k,-1}-kl\right)\frac{R_{nl}^{\alpha}}{r}\right]\times$$
$$\times\begin{bmatrix}{}_kB_{ljm}^{s}\left(\lambda;\theta,\varphi\right)+{}_kD_{ljm}^{s}\left(\lambda+1;\theta,\varphi\right)\\ {}_kC_{ljm}^{s}\left(\lambda;\theta,\varphi\right)-{}_kB_{ljm}^{s}\left(\lambda+1;\theta,\varphi\right)\end{bmatrix} \tag{III-34}$$

$$c(\vec{\sigma}\hat{\vec{p}})\tilde{\varphi}^{\alpha s\lambda}=c(\vec{\sigma}\hat{\vec{p}})\left[\tilde{R}_{\tilde{n}l}^{\alpha}\Upsilon_{ljm}^{s\lambda}\right]=-c\hbar\sum_{k=-1}^{1}{}'\left[\frac{d\tilde{R}_{\tilde{n}l}^{\alpha}}{dr}+\left(\delta_{k,-1}-kl\right)\frac{\tilde{R}_{\tilde{n}l}^{\alpha}}{r}\right]\times$$
$$\times\begin{bmatrix}{}_kB_{ljm}^{s}\left(\lambda+1;\theta,\varphi\right)+{}_kD_{ljm}^{s}\left(\lambda;\theta,\varphi\right)\\ {}_kC_{ljm}^{s}\left(\lambda+1;\theta,\varphi\right)-{}_kB_{ljm}^{s}\left(\lambda;\theta,\varphi\right)\end{bmatrix}, \tag{III-35}$$

where,

$$ {}_{k}B^{s}_{ljm}\left(\lambda;\theta,\varphi\right)=a^{s}_{ljm}\left(\lambda\right)b^{lm(\lambda)}_{k}\beta_{m(\lambda)}Y_{l+k,m(\lambda)}\left(\theta,\varphi\right) \qquad \text{(III-36)} $$

$$ {}_{k}C^{s}_{ljm}\left(\lambda;\theta,\varphi\right)=a^{s}_{ljm}\left(\lambda\right)c^{lm(\lambda)}_{k}\beta_{m(\lambda)+1}Y_{l+k,m(\lambda)+1}\left(\theta,\varphi\right) \qquad \text{(III-37)} $$

$$ {}_{k}D^{s}_{ljm}\left(\lambda;\theta,\varphi\right)=a^{s}_{ljm}\left(\lambda\right)d^{lm(\lambda)}_{k}\beta_{m(\lambda)-1}Y_{l+k,m(\lambda)-1}\left(\theta,\varphi\right). \qquad \text{(III-38)} $$

The formulae presented in this work show that all of the 2(2s+1)-component relativistic basis spinor wave functions and Slater basis spinor orbitals are expressed through the sets of one- and two-component basis spinors. The radial parts of these basis spinors are determined from the corresponding nonrelativistic basis functions defined in position, momentum and four-dimensional spaces. Thus, the expansion and one-range addition theorems established in [28] for the nonrelativistic $k^{\alpha}_{nlm_l}$ and k_{nlm_l} basis sets in position, momentum and four-dimensional spaces can be also used in the case of relativistic basis spinor functions $K^{\alpha 0}_{nlm_l}$ and $K^{0}_{nlm_l}$. Accordingly, the electronic structure properties of arbitrary mass and spin relativistic systems can be investigated with the help of corresponding nonrelativistic calculations.

IV. Conclusions

In this study, we have generalized the Dirac's $spin-1/2$ theory to a relativistic theory for particles with arbitrary mass and integral and half-integral spin. The relativistic basis sets of spinor orbitals for the arbitrary spin particles in position, momentum and four-dimensional spaces are also constructed. It is shown that this theory has the following properties:

(1) The generalized relativistic matrices are irreducible and Clifford algebraic.

(2) The generalized relativistic wave functions and matrices possess the $2\left(2s+1\right)$ independent components.

(3) The generalized relativistic equation satisfies the condition of Lorentz invariance.

(4a) The relativistic scalar particles for $e\geq 0$ *and* $m\neq 0$ satisfy the two-component relativistic equation.

(4b) The free particle with e=0, s=0 and m≠0 is described by two-component relativistic equation.

(5) The integral spin $(s=1,2,\ldots)$ satisfies the $2(2s+1)$ component generalized relativistic equation for massless particles.

(6) The half-integral spin $\left(s=\frac{1}{2},\frac{3}{2},\ldots\right)$ satisfies the 2(2s+1)-component generalizes relativistic equation for particle with m≠0.

(7) The relativistic basis sets of spinor orbitals for the arbitrary mass and spin particles in position, momentum and four-dimensional spaces are expressed through the corresponding quantities of nonrelativistic spinor functions.

The generalized relativistic theory presented in this work can be used in the solution of different problems of describing particles with arbitrary mass and spin within the framework of relativistic quantum mechanics when the position, momentum and the four-dimensional spaces are employed.

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Table 1. Summary of the generalized Dirac group properties for $0 \le s \le \frac{7}{2}$

s	Group Order	No. of Classes	No. of 1-D irred	No. of 2-D irred	No. of 4-D irred	No. of 6-D irred	No. of 8-D irred	No. of 10-D irred	No. of 12-D irred	No. of 14-D irred	No. of 16-D irred
0	8	5	4	1	0	0	0	0	0	0	0
$1/2$	32	17	16	0	1	0	0	0	0	0	0
1	72	37	36	0	0	1	0	0	0	0	0
$3/2$	128	65	64	0	0	0	1	0	0	0	0
2	200	101	100	0	0	0	0	1	0	0	0
$5/2$	288	145	144	0	0	0	0	0	1	0	0
3	392	197	196	0	0	0	0	0	0	1	0
$7/2$	512	257	256	0	0	0	0	0	0	0	1

Note: irred-irreducible representation

Table 2. The exponential type spinor orbitals in position space for $s = 0$, $1 \le n \le 2$, $0 \le l \le n-1$, and $-l \le m_l \le l$

n	l	m_l	$\Psi^{\alpha 0}_{nlm_l}$
1	0	0	$\frac{1}{\sqrt{2}}\begin{bmatrix} \psi^{\alpha 0}_{100} \\ -i\psi^{\alpha 0}_{100} \end{bmatrix}$
2	0	0	$\frac{1}{\sqrt{2}}\begin{bmatrix} \psi^{\alpha 0}_{200} \\ -i\psi^{\alpha 0}_{200} \end{bmatrix}$
	1	1	$\frac{1}{\sqrt{2}}\begin{bmatrix} \psi^{\alpha 0}_{211} \\ -i\psi^{\alpha 0}_{211} \end{bmatrix}$
		0	$\frac{1}{\sqrt{2}}\begin{bmatrix} \psi^{\alpha 0}_{210} \\ -i\psi^{\alpha 0}_{210} \end{bmatrix}$
		-1	$\frac{1}{\sqrt{2}}\begin{bmatrix} \psi^{\alpha 0}_{21-1} \\ -i\psi^{\alpha 0}_{21-1} \end{bmatrix}$

Table 3. The exponential type spinor orbitals in position space for $s=1$, $1 \le n \le 2$, $0 \le l \le n-1$, $|l-s| \le j \le l+s$, $-j \le m \le j$, $t=2(j-l)$ and $\tilde{n}=n+|t|$

n	l	j	t	$\tilde{n}$	m	$\tilde{\Psi}^{\alpha 1}_{nljm}$					
1	0	1	2	3	1	$\frac{\psi^{\alpha}_{100}}{\sqrt{2}}$	0	0	0	0	$-\frac{i\psi^{\alpha}_{300}}{\sqrt{2}}$
					0	0	$\frac{\psi^{\alpha}_{100}}{\sqrt{2}}$	0	0	$-\frac{i\psi^{\alpha}_{300}}{\sqrt{2}}$	0
					-1	0	0	$\frac{\psi^{\alpha}_{100}}{\sqrt{2}}$	$-\frac{i\psi^{\alpha}_{300}}{\sqrt{2}}$	0	0
2	0	1	2	4	1	$\frac{\psi^{\alpha}_{200}}{\sqrt{2}}$	0	0	0	0	$-\frac{i\psi^{\alpha}_{400}}{\sqrt{2}}$
					0	0	$\frac{\psi^{\alpha}_{200}}{\sqrt{2}}$	0	0	$-\frac{i\psi^{\alpha}_{400}}{\sqrt{2}}$	0
					-1	0	0	$\frac{\psi^{\alpha}_{200}}{\sqrt{2}}$	$-\frac{i\psi^{\alpha}_{400}}{\sqrt{2}}$	0	0
	1	1	0	2	1	$-\frac{1}{2}\psi^{\alpha}_{210}$		0	0	$-\frac{1}{2}i\psi^{\alpha}_{211}$	
					0		0		$-\frac{1}{2}i\psi^{\alpha}_{211}$	0	$-\frac{1}{2}i\psi^{\alpha}_{21-1}$
					-1	0			$-\frac{1}{2}i\psi^{\alpha}_{210}$	$-\frac{1}{2}i\psi^{\alpha}_{21-1}$	0
		2	2	4	2	$\frac{\psi^{\alpha}_{211}}{\sqrt{2}}$	0	0	0	0	$-\frac{i\psi^{\alpha}_{411}}{\sqrt{2}}$
					1			0	0	$-\frac{i\psi^{\alpha}_{411}}{2}$	$-\frac{i\psi^{\alpha}_{410}}{2}$
					0	$-\frac{\psi^{\alpha}_{21-1}}{2\sqrt{3}}$	$\frac{\psi^{\alpha}_{210}}{\sqrt{3}}$	$\frac{\psi^{\alpha}_{211}}{2\sqrt{3}}$	$-\frac{i\psi^{\alpha}_{411}}{2\sqrt{3}}$	$-\frac{i\psi^{\alpha}_{410}}{\sqrt{3}}$	$-\frac{i\psi^{\alpha}_{41-1}}{2\sqrt{3}}$
					-1	0	$-\frac{1}{2}\psi^{\alpha}_{21-1}$		$-\frac{1}{2}i\psi^{\alpha}_{410}$		0
					-2	0	0	$-\frac{\psi^{\alpha}_{21-1}}{\sqrt{2}}$	$\frac{i\psi^{\alpha}_{41-1}}{\sqrt{2}}$	0	0

Table 4. The exponential type spinor orbitals in position space for $s=2$, $1\le n\le 2,\ 0\le l\le n-1,$ $\left|l-s\right|\le j\le l+s,\ -j\le m\le j,\ t=2\left(j-l\right)$ and $\tilde{n}=n+\left|t\right|$

n	l	j	t	$\tilde{n}$	m	$\tilde{\Psi}^{\alpha 2}_{nljm}$									
1	0	2	4	5	2	$\frac{\psi^{\alpha}_{100}}{\sqrt{2}}$	0	0	0	0	0	0	0	0	$-\frac{i\psi^{\alpha}_{500}}{\sqrt{2}}$
					1	0	$\frac{\psi^{\alpha}_{100}}{\sqrt{2}}$	0	0		0	0	0	$-\frac{i\psi^{\alpha}_{500}}{\sqrt{2}}$	0
					0	0	0	$\frac{\psi^{\alpha}_{100}}{\sqrt{2}}$	0	0	0	0	$-\frac{i\psi^{\alpha}_{500}}{\sqrt{2}}$	0	0
					-1	0	0	0	$\frac{\psi^{\alpha}_{100}}{\sqrt{2}}$	0	0	$-\frac{i\psi^{\alpha}_{500}}{\sqrt{2}}$	0	0	0
					-2	0	0	0	0	$\frac{\psi^{\alpha}_{100}}{\sqrt{2}}$	$-\frac{i\psi^{\alpha}_{500}}{\sqrt{2}}$	0	0	0	0
2	0	2	4	6	2	$\frac{\psi^{\alpha}_{200}}{\sqrt{2}}$	0	0	0	0	0	0	0	0	$-\frac{i\psi^{\alpha}_{600}}{\sqrt{2}}$
					1	0	$\frac{\psi^{\alpha}_{200}}{\sqrt{2}}$	0	0	0	0	0	0	$-\frac{i\psi^{\alpha}_{600}}{\sqrt{2}}$	0
					0	0	0	$\frac{\psi^{\alpha}_{200}}{\sqrt{2}}$	0	0	0	0	$-\frac{i\psi^{\alpha}_{600}}{\sqrt{2}}$	0	0
					-1		0	0	$\frac{\psi^{\alpha}_{200}}{\sqrt{2}}$	0		$-\frac{i\psi^{\alpha}_{600}}{\sqrt{2}}$	0	0	0
					-2	0	0	0	0	$\frac{\psi^{\alpha}_{200}}{\sqrt{2}}$	$-\frac{i\psi^{\alpha}_{600}}{\sqrt{2}}$	0	0	0	0
	1	2	2	4	2	$-\frac{\psi^{\alpha}_{210}}{\sqrt{3}}$	$\frac{\psi^{\alpha}_{211}}{\sqrt{6}}$	0	0	0	0	0	0	$-\frac{i\psi^{\alpha}_{411}}{\sqrt{6}}$	$-\frac{i\psi^{\alpha}_{410}}{\sqrt{3}}$

					1	$\frac{\psi^{\alpha}_{21-1}}{\sqrt{6}}$	$-\frac{\psi^{\alpha}_{210}}{2\sqrt{3}}$	$\frac{\psi^{\alpha}_{211}}{2}$	0	0	0	0	$-\frac{i\psi^{\alpha}_{411}}{2}$	$\frac{i\psi^{\alpha}_{410}}{2\sqrt{3}}$	$-\frac{i\psi^{\alpha}_{41-1}}{\sqrt{6}}$
					0	0		0		0	0	$-\frac{i\psi^{\alpha}_{411}}{2}$	0	0	$-\frac{i\psi^{\alpha}_{41-1}}{2}$
					-1	0	0		$\frac{\psi^{\alpha}_{210}}{2\sqrt{3}}$	$\frac{\psi^{\alpha}_{211}}{\sqrt{6}}$	$-\frac{i\psi^{\alpha}_{411}}{\sqrt{6}}$	$-\frac{i\psi^{\alpha}_{410}}{2\sqrt{3}}$	$-\frac{i\psi^{\alpha}_{41-1}}{2}$	0	0
					-2	0	0	0	$\frac{\psi^{\alpha}_{21-1}}{\sqrt{6}}$	$\frac{\psi^{\alpha}_{210}}{\sqrt{3}}$	$-\frac{i\psi^{\alpha}_{410}}{\sqrt{3}}$	$-\frac{i\psi^{\alpha}_{41-1}}{\sqrt{6}}$	0	0	0

Table 5. The exponential type spinor orbitals in position space for $s=\frac{1}{2}$,

$1 \le n \le 2,\ 0 \le l \le n-1,\ |l-s| \le j \le l+s,\ -j \le m \le j,\ t=2(j-l)$ and $\tilde{n}=n+|t|$

n	l	j	t	$\tilde{n}$	m	$\tilde{\Psi}^{\alpha 1/2}_{nljm}$			
1	0	1/2	1	2	1/2	$\frac{\psi^{\alpha}_{100}}{\sqrt{2}}$	0	0	$-\frac{i\psi^{\alpha}_{200}}{\sqrt{2}}$
					-1/2	0	$\frac{\psi^{\alpha}_{100}}{\sqrt{2}}$	$-\frac{i\psi^{\alpha}_{200}}{\sqrt{2}}$	0
2	0	1/2	1	3	1/2	$\frac{\psi^{\alpha}_{200}}{\sqrt{2}}$	0	0	$-\frac{i\psi^{\alpha}_{300}}{\sqrt{2}}$
					-1/2	0	$\frac{\psi^{\alpha}_{200}}{\sqrt{2}}$	$-\frac{i\psi^{\alpha}_{300}}{\sqrt{2}}$	0
	1	1/2	-1	3	1/2	$-\frac{\psi^{\alpha}_{210}}{\sqrt{6}}$	$\frac{\psi^{\alpha}_{211}}{\sqrt{3}}$	$-\frac{i\psi^{\alpha}_{311}}{\sqrt{3}}$	$\frac{i\psi^{\alpha}_{310}}{\sqrt{6}}$
					-1/2	$\frac{\psi^{\alpha}_{21-1}}{\sqrt{3}}$	$\frac{\psi^{\alpha}_{210}}{\sqrt{6}}$	$-\frac{i\psi^{\alpha}_{310}}{\sqrt{6}}$	$-\frac{i\psi^{\alpha}_{31-1}}{\sqrt{3}}$
		3/2	1	3	3/2	$\frac{\psi^{\alpha}_{211}}{\sqrt{2}}$	0	0	$-\frac{i\psi^{\alpha}_{311}}{\sqrt{2}}$
					1/2	$\frac{\psi^{\alpha}_{210}}{\sqrt{3}}$	$\frac{\psi^{\alpha}_{211}}{\sqrt{6}}$	$-\frac{i\psi^{\alpha}_{311}}{\sqrt{6}}$	$-\frac{i\psi^{\alpha}_{310}}{\sqrt{3}}$
					-1/2	$-\frac{\psi^{\alpha}_{21-1}}{\sqrt{6}}$	$\frac{\psi^{\alpha}_{210}}{\sqrt{3}}$	$-\frac{i\psi^{\alpha}_{310}}{\sqrt{3}}$	$\frac{i\psi^{\alpha}_{31-1}}{\sqrt{6}}$
					-3/2	0	$-\frac{\psi^{\alpha}_{21-1}}{\sqrt{2}}$	$\frac{i\psi^{\alpha}_{31-1}}{\sqrt{2}}$	0

Table 6. The exponential type spinor orbitals in position space for $s=\frac{3}{2}$, $1\le n\le 2,\ 0\le l\le n-1,\ |l-s|\le j\le l+s,\ -j\le m\le j,\ t=2(j-l)$ and $\tilde{n}=n+|t|$

n	l	j	t	$\tilde{n}$	m	$\tilde{\Psi}^{\alpha 3/2}_{nljm}$							
1	0	3/2	3	4	3/2	$\frac{\psi^{\alpha}_{100}}{\sqrt{2}}$	0	0	0	0	0	0	$-\frac{i\psi^{\alpha}_{400}}{\sqrt{2}}$
					1/2		$\frac{\psi^{\alpha}_{100}}{\sqrt{2}}$	0	0	0	0	$-\frac{i\psi^{\alpha}_{400}}{\sqrt{2}}$	0
					-1/2	0	0	$\frac{\psi^{\alpha}_{100}}{\sqrt{2}}$			$-\frac{i\psi^{\alpha}_{400}}{\sqrt{2}}$	0	0
					-3/2	0	0	0	$\frac{\psi^{\alpha}_{100}}{\sqrt{2}}$	$-\frac{i\psi^{\alpha}_{400}}{\sqrt{2}}$	0	0	0
2	0	3/2	3	5	3/2	$\frac{\psi^{\alpha}_{200}}{\sqrt{2}}$	0	0	0	0	0	0	$-\frac{i\psi^{\alpha}_{500}}{\sqrt{2}}$
					1/2	0	$\frac{\psi^{\alpha}_{200}}{\sqrt{2}}$	0	0	0	0	$-\frac{i\psi^{\alpha}_{500}}{\sqrt{2}}$	0
					-1/2	0	0	$\frac{\psi^{\alpha}_{200}}{\sqrt{2}}$	0	0	$-\frac{i\psi^{\alpha}_{500}}{\sqrt{2}}$	0	0
					-3/2	0	0	0	$\frac{\psi^{\alpha}_{200}}{\sqrt{2}}$	$-\frac{i\psi^{\alpha}_{500}}{\sqrt{2}}$	0	0	0
	1	3/2	1	3	3/2	$-\sqrt{\frac{3}{10}}\psi^{\alpha}_{210}$	$\frac{\psi^{\alpha}_{211}}{\sqrt{5}}$	0	0	0	0	$-\frac{i\psi^{\alpha}_{311}}{\sqrt{5}}$	$\sqrt{\frac{3}{10}}i\psi^{\alpha}_{310}$

					1/2	$\frac{\psi^{\alpha}_{21-1}}{\sqrt{5}}$	$-\frac{\psi^{\alpha}_{210}}{\sqrt{30}}$		0	0	$-\frac{2i\psi^{\alpha}_{311}}{\sqrt{15}}$	$\frac{i\psi^{\alpha}_{310}}{\sqrt{30}}$	$-\frac{i\psi^{\alpha}_{31-1}}{\sqrt{5}}$
					-1/2	0		$\frac{\psi^{\alpha}_{210}}{\sqrt{30}}$	$\frac{\psi^{\alpha}_{211}}{\sqrt{5}}$	$-\frac{i\psi^{\alpha}_{311}}{\sqrt{5}}$	$-\frac{i\psi^{\alpha}_{310}}{\sqrt{30}}$	$-\frac{2i\psi^{\alpha}_{31-1}}{\sqrt{15}}$	0
					-3/2	0	0	$\frac{\psi^{\alpha}_{21-1}}{\sqrt{5}}$	$\sqrt{\frac{3}{10}}i\psi^{\alpha}_{210}$	$-\sqrt{\frac{3}{10}}i\psi^{\alpha}_{310}$	$-\frac{i\psi^{\alpha}_{31-1}}{\sqrt{5}}$	0	0
		5/2	3	5	5/2	$\frac{\psi^{\alpha}_{211}}{\sqrt{2}}$	0	0	0	0	0	0	$-\frac{i\psi^{\alpha}_{511}}{\sqrt{2}}$
					3/2	$\frac{\psi^{\alpha}_{210}}{\sqrt{5}}$	$\sqrt{\frac{3}{10}}\psi^{\alpha}_{211}$	0	0	0	0	$-\sqrt{\frac{3}{10}}i\psi^{\alpha}_{511}$	$-\frac{i\psi^{\alpha}_{510}}{\sqrt{5}}$
					1/2	$-\frac{\psi^{\alpha}_{21-1}}{2\sqrt{5}}$	$\sqrt{\frac{3}{10}}\psi^{\alpha}_{210}$		0	0	$-\sqrt{\frac{3}{20}}i\psi^{\alpha}_{511}$	$-\sqrt{\frac{3}{10}}i\psi^{\alpha}_{510}$	$\frac{i\psi^{\alpha}_{51-1}}{2\sqrt{5}}$
					-1/2	0	$-\sqrt{\frac{3}{20}}\psi^{\alpha}_{21-1}$	$\sqrt{\frac{3}{10}}\psi^{\alpha}_{210}$	$\frac{\psi^{\alpha}_{211}}{2\sqrt{5}}$	$-\frac{i\psi^{\alpha}_{511}}{2\sqrt{5}}$	$-\sqrt{\frac{3}{10}}i\psi^{\alpha}_{510}$		0
					-3/2	0	0	$-\sqrt{\frac{3}{10}}\psi^{\alpha}_{21-1}$	$\frac{\psi^{\alpha}_{210}}{\sqrt{5}}$	$-\frac{i\psi^{\alpha}_{510}}{\sqrt{5}}$	$\sqrt{\frac{3}{10}}i\psi^{\alpha}_{51-1}$	0	0
					-5/2	0	0	0	$-\frac{\psi^{\alpha}_{21-1}}{\sqrt{2}}$	$\frac{i\psi^{\alpha}_{51-1}}{\sqrt{2}}$	0	0	0