A Theory of Heavy Atoms: A New Relativistic Approach in Momentum Representation

B. K. Novosadov[*]

V. I. Vernadsky Institute of Geochemistry and Analytical Chemistry,
Russian Academy of Sciences,
Moscow, Russian Federation

Abstract

The development of high energy physics and chemistry leads to a necessity of seeking and employing many-particle relativistic equations. A goal of this paper is to suggest some relativistic models and to give methods of their solving for heavy atoms.

A new relativistic approach in the theory of heavy atoms has been suggested in momentum representation.

The method is in diagonalization of the kinematic c–momentum matrix and obtaining an integral equation system for many atomic electrons both in Clifford algebra of the Dirac-Pauli matrices, and in hypercomplex (quaternionic) algebra.

A scalar relativistic equation as an approximation to the equation system has been suggested, which takes into account the spin-relativistic kinematics of atomic electrons.

Keywords: many-particle relativistic quantum theory, quaternionic quantum models, hypercomplex algebra, momentum representation, heavy atoms

Aim and Background

The development of high energy physics and chemistry leads to a necessity of seeking for and employing many-particle relativistic equations.

A goal of this paper is to propose some relativistic models and to give methods of their solving for heavy atoms.

A new relativistic approach in the theory of heavy atoms has been suggested in momentum representation.

A scalar relativistic equation as an approximation to the equation system has been suggested, with taking into account the spin-relativistic kinematics of atomic electrons.

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[*] e-mail: bk.novosadov@mail.ru

INTRODUCTION

The problem of studies on the electronic structure of heavy atoms faces with some theoretical difficulties in describing physical behavior of many-particle system in accordance with the relativity theory. Spectroscopy of heavy atoms has got a large massive of data that needs in proper interpretation on the base of relativistic theoretical models. So far there do not exist many-electron relativistic approaches for Coulombic systems, from which one could obtain approximations (even Hartree-Fock models) for the purpose of systematical study in the field of atomic and molecular spectroscopy and quantum chemistry. The development of high energy physics and chemistry leads to a necessity of seeking and employing many-particle relativistic equations. A goal of this paper is to suggest some relativistic models and to give methods of their solving for heavy atoms. Some efforts will be made for obtaining asymptotical properties of wave functions and spectra of many-electron stationary systems.

1. RELATIVISTIC EQUATION SYSTEM IN COORDINATE SPACE OF PARTICLES

Classical energy for a system of free particles may be written as follows

$$E = \sum_{k=1}^{n} \sqrt{c^2 p_k^2 + m_k^2 c^4} \tag{1.1}$$

We may consider this expression like a root of some eigenvalue problem. For a system of non-interacting particles (electrons) this root is a sum of eigenvalues belonging to Dirac equations, or another one-particle relativistic equation system, for example, those in quaternionic representation. We use the both possibilities in our paper.

The main relation in relativistic physics connects energy and momentum with taking into account the twofold degeneracy by spin

$$\left(\frac{E^2}{c^2} - p^2 - m^2 c^2 \right)^2 = 0. \tag{1.2}$$

The one-particle Dirac system of four equations may be written as follows

$$\begin{pmatrix} c\boldsymbol{\sigma}\mathbf{p} & mc^2 \\ mc^2 & -c\boldsymbol{\sigma}\mathbf{p} \end{pmatrix} \begin{pmatrix} g(\mathbf{r}) \\ u(\mathbf{r}) \end{pmatrix} = E \begin{pmatrix} g(\mathbf{r}) \\ u(\mathbf{r}) \end{pmatrix}. \tag{1.3}$$

The kinematic matrix differs from the original Dirac one up to an orthogonal transformation of spinor components, but Eq. (1.3) is more convenient for deriving spin-relativistic members to non-relativistic expression for the particle energy. (We do not face fractions with singular denominators in the variable *r*, when a Coulombic potential is included.) Eq. (1.3) has four roots, of which two are negative and has no physical sense,

however the eigenvalue spectrum proves to be unlimited and there does not exist a lower limit to formulate a variational principle for the Dirac equation directly. This is one of the difficulties in numerical analysis of the relativistic equations for many-particle systems in quantum mechanics.

2. FOURIER-TRANSFORMATION TO MOMENTUM SPACE OF PARTICLES

The particle coordinates and momentum are conjugate variables in quantum mechanics. A transfer to the momentum representation for the wave equation can be made by the Fourier-transformation of the wave function and operators. One has

$$\varphi\left(\mathbf{p}_1,\ldots,\mathbf{p}_n\right)=\left(2\pi\right)^{-3n/2}\int\exp\left(-i\sum_{k=1}^{n}\mathbf{p}_k\mathbf{r}_k\right)\psi\left(\mathbf{r}_1,\ldots,\mathbf{r}_n\right)\prod_{k=1}^{n}d^3\mathbf{r}_k\,. \tag{2.1}$$

The Coulomb potential is transformed by the formula

$$\int e^{-i\mathbf{pr}}r^{-1}d^3\mathbf{r}=4\pi p^{-2}\,. \tag{2.2}$$

The inverse Fourier-transformation of the Coulomb potential is calculated as follows

$$2\pi^2 r^{-1}=\int e^{i\mathbf{pr}}p^{-2}d^3\mathbf{p}\,. \tag{2.3}$$

The convolution theorem allows one to calculate the Fourier-transformation of the two functions product

$$\int\exp\left(-i\mathbf{pr}\right)f\left(\mathbf{r}\right)g\left(\mathbf{r}\right)d^3\mathbf{r}=\int\overline{f}\left(\mathbf{k}\right)\overline{g}\left(\mathbf{p}-\mathbf{k}\right)d^3\mathbf{k}\,, \tag{2.4}$$

where

$$\overline{f}\left(\mathbf{k}\right)=\left(2\pi\right)^{-3/2}\int\exp\left(-i\mathbf{kr}\right)f\left(\mathbf{r}\right)d^3\mathbf{r}\,. \tag{2.5}$$

A proof of the formulae given can be made using the properties of the Dirac δ-function

$$\delta\left(\mathbf{r}\right)=\left(2\pi\right)^{-3}\int\exp\left(i\mathbf{pr}\right)d^3\mathbf{p}\,. \tag{2.6}$$

The Fourier-transformation of the Dirac equation converts the momentum into a c-number, while the product of the potential function and a bispinor turns into an integral in

which the first one becomes the kernel of the equation integral operator. Write down the integral Dirac equation for hydrogen atom (the proton is considered fixed).

$$\begin{pmatrix} c\boldsymbol{\sigma}\mathbf{p} & mc^2 \\ mc^2 & -c\boldsymbol{\sigma}\mathbf{p} \end{pmatrix} \begin{pmatrix} \overline{g}(\mathbf{p}) \\ \overline{u}(\mathbf{p}) \end{pmatrix} = \left(E - V(\mathbf{p},\mathbf{p}')\right) \begin{pmatrix} \overline{g}(\mathbf{p}) \\ \overline{u}(\mathbf{p}) \end{pmatrix}. \tag{2.7}$$

Here the product of the potential function and the bispinor ought to understand like the integral expression

$$V(\mathbf{p},\mathbf{p}') \begin{pmatrix} \overline{g}(\mathbf{p}) \\ \overline{u}(\mathbf{p}) \end{pmatrix} = \frac{1}{2\pi^2} \int \frac{-Ze^2}{(\mathbf{p}-\mathbf{p}')^2} \begin{pmatrix} \overline{g}(\mathbf{p}') \\ \overline{u}(\mathbf{p}') \end{pmatrix} d^3\mathbf{p}'. \tag{2.8}$$

An analogous Fourier-transformation allows one to write down in the momentum space many-particle relativistic equations, which will be given below.

3. EIGENVECTORS OF THE DIRAC KINEMATIC MATRIX IN THE MOMENTUM SPACE

The relationship (1.2) can be considered as a *determinant* of an eigenvalue problem with the Dirac matrix B and a column-function $\varphi(t)$ with 4 components

$$B\varphi = \frac{E}{c}\varphi, \tag{3.1}$$

where the matrix B is as follows

$$B = \begin{bmatrix} m_0c & 0 & p_z & p_- \\ 0 & m_0c & p_+ & -p_z \\ p_z & p_- & -m_0c & 0 \\ p_+ & -p_z & 0 & -m_0c \end{bmatrix}, \tag{3.2}$$

with the momentum cyclic components. One can easily verify that the decision problem condition for the homogeneous equation (3.1)

$$\det\left(B - \frac{E}{c}I_4\right) = 0, \tag{3.3}$$

where I_4 is the unit matrix of the order 4, coincides with the Eq. (1.2). The momentum

components in the matrix given are c-numbers, then the column-function $\varphi(t)$ represents a set of four numbers, which are expressed via the B matrix elements.

Introduce a vector matrix (Clifford unit vector)

$$\boldsymbol{\sigma} = \begin{pmatrix} \mathbf{n}_z & \mathbf{n}_x - i\mathbf{n}_y \\ \mathbf{n}_x + i\mathbf{n}_y & -\mathbf{n}_z \end{pmatrix},$$

(3.4)

where the matrix elements are cyclic unit vectors of the Cartesian coordinate system, $i = \sqrt{-1}$, and briefly $\mathbf{n}_- = \mathbf{n}_x - i\mathbf{n}_y$, $\mathbf{n}_+ = \mathbf{n}_x + i\mathbf{n}_y$. Then the matrix (3.4) may be written concisely as

$$\boldsymbol{\sigma} = \begin{pmatrix} \mathbf{n}_z & \mathbf{n}_- \\ \mathbf{n}_+ & -\mathbf{n}_z \end{pmatrix},$$

(3.5)

or in the basis of Pauli matrices

$$\boldsymbol{\sigma} = \sigma_x \mathbf{n}_x + \sigma_y \mathbf{n}_y + \sigma_z \mathbf{n}_z.$$

(3.6)

The matrix B may be written like a block matrix of the order 2

$$B = \begin{pmatrix} m_0 c I_2 & \boldsymbol{\sigma}\mathbf{p} \\ \boldsymbol{\sigma}\mathbf{p} & -m_0 c I_2 \end{pmatrix},$$

(3.7)

where $I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, and the momentum is given in the Clifford algebra.

To diagonalize the matrix B one may notice that the blocks along the main diagonal are proportional to the unit matrix of the order 2, therefore they are invariable, if one diagonalizes first the momentum blocks, which are Hermite matrices,

$$\Pi = \boldsymbol{\sigma}\mathbf{p} = \begin{bmatrix} p_z & p_- \\ p_+ & -p_z \end{bmatrix}.$$

(3.8)

The matrix Π may be written down via the eigenvalue matrix

$$\Lambda = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix},$$

(3.9)

where $\lambda_1 = p$, $\lambda_2 = -p$, $p = \sqrt{p_x^2 + p_y^2 + p_z^2}$, as a spectral decomposition

$$\Pi = C_1^+ \Lambda C_1, \tag{3.10}$$

where the cross indicates the Hermite conjugation of the eigenvector unitary matrix C_1. Solving the matrix equation $\Pi \mathbf{c} = \lambda \mathbf{c}$, one obtains the eigenvector matrix sought for

$$C_1 = \begin{bmatrix} \sqrt{\dfrac{p+p_z}{2p}} & \dfrac{-p_-}{\sqrt{2p(p+p_z)}} \\ \dfrac{p_+}{\sqrt{2p(p+p_z)}} & \sqrt{\dfrac{p+p_z}{2p}} \end{bmatrix}. \tag{3.11}$$

Transformation

$$U_1 = \begin{bmatrix} C_1 & 0 \\ 0 & C_1 \end{bmatrix} \tag{3.12}$$

brings the matrix Π, as has been said earlier, into the diagonal form without changing the diagonal blocks in (3.7). As a result the matrix B has been transformed to a simpler form with a more number of zero elements

$$U_1^+ B U_1 = \begin{bmatrix} m_0 c & 0 & p & 0 \\ 0 & m_0 c & 0 & -p \\ p & 0 & -m_0 c & 0 \\ 0 & -p & 0 & -m_0 c \end{bmatrix}. \tag{3.13}$$

Besides the zeros are arranged in the chess order, so the permutation of the 2nd and 3rd rows and columns of the matrix given by the matrix

$$P_{23} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \tag{3.14}$$

brings the matrix B into a block-diagonal form

$$P_{23} U_1^+ B U_1 P_{23} = \begin{bmatrix} m_0 c & p & 0 & 0 \\ p & -m_0 c & 0 & 0 \\ 0 & 0 & m_0 c & -p \\ 0 & 0 & -p & -m_0 c \end{bmatrix}, \tag{3.15}$$

with the blocks of like structures. Usage of the orthogonal transformation

$$F = \begin{pmatrix} I_2 & 0 \\ 0 & F_2 \end{pmatrix}, \tag{3.15a}$$

where the matrix I_2 is the diagonal unit matrix of the order two, F_2 is the diagonal of the form

$$F_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{3.15b}$$

brings the matrix (3.15) into the matrix with identical blocks, which are diagonalized by the same orthogonal matrix C_2 of a general form

$$C_2 = \begin{bmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{bmatrix}. \tag{3.16}$$

The eigenvalues of the block matrices (3.15) are as follows

$$\frac{E_1}{c} = \sqrt{m_0^2 c^2 + p^2} , \quad \frac{E_2}{c} = -\sqrt{m_0^2 c^2 + p^2} . \tag{3.17}$$

For the angle φ a relationship $tg\,2\varphi = \dfrac{p}{m_0 c}$ takes place, from which one finds, using the known relationship $tg\,2\varphi = \dfrac{2t}{1+t^2}$, the parameter $t = tg\,\varphi$

$$t = \frac{p}{m_0 c + \sqrt{m_0^2 c^2 + p^2}} . \tag{3.18}$$

Thus, the elements of the orthogonal matrix (3.16) are calculated as follows

$$\cos\varphi = \frac{1}{\sqrt{1+t^2}} , \quad \sin\varphi = t\cos\varphi . \tag{3.19}$$

As a result, the matrix B is brought into the diagonal form with the eigenvalues (3.17) with the help of the set of four matrix transformations

$$
\tilde{U}_2 F P_{23} U_1^+ B U_1 P_{23} F U_2 = \frac{1}{c}
\begin{bmatrix}
E_1 & 0 & 0 & 0 \\
0 & E_2 & 0 & 0 \\
0 & 0 & E_1 & 0 \\
0 & 0 & 0 & E_2
\end{bmatrix},
\tag{3.20}
$$

where the orthogonal matrix U_2 is as follows

$$
U_2 = \begin{bmatrix}
C_2 & 0 \\
0 & C_2
\end{bmatrix}.
\tag{3.21}
$$

Consider the first column of the eigenvector matrix for the matrix B. One has got the normalized to 1 eigenspinor

$$
\varphi_1 = \begin{pmatrix}
\sqrt{\dfrac{p + p_z}{2p}} \; \dfrac{m_0 c + \sqrt{m_0^2 c^2 + p^2}}{\sqrt{p^2 + (m_0 c + \sqrt{m_0^2 c^2 + p^2})^2}} \\[4mm]
\dfrac{p_+}{\sqrt{2p(p + p_z)}} \; \dfrac{m_0 c + \sqrt{m_0^2 c^2 + p^2}}{\sqrt{p^2 + (m_0 c + \sqrt{m_0^2 c^2 + p^2})^2}} \\[4mm]
\sqrt{\dfrac{p + p_z}{2p}} \; \dfrac{p}{\sqrt{p^2 + (m_0 c + \sqrt{m_0^2 c^2 + p^2})^2}} \\[4mm]
\dfrac{p_+}{\sqrt{2p(p + p_z)}} \; \dfrac{p}{\sqrt{p^2 + (m_0 c + \sqrt{m_0^2 c^2 + p^2})^2}}
\end{pmatrix}.
\tag{3.22}
$$

Denoting the matrix elements in (3.11) by c_{11}, c_{12}. c_{21}, c_{22}, sine and cosine in the matrix (3.16) by s and c, write down an explicit form of the normalized eigenvectors matrix for the matrix B

$$
U_1 P_{23} F U_2 = \begin{bmatrix}
c_{11}c & -c_{11}s & c_{12}c & -c_{12}s \\
c_{21}c & -c_{21}s & c_{22}c & -c_{22}s \\
c_{11}s & c_{11}c & -c_{12}s & -c_{12}c \\
c_{21}s & c_{21}c & -c_{22}s & -c_{22}c
\end{bmatrix}.
\tag{3.23}
$$

Here the letter c cannot be confused with the light velocity in the matrix B (3.2).

In the nonrelativistic limit, when the momentum becomes much less than the quantity $m_0 c$, the "positron" components of the column φ_1 tend to zero. In this case the parameter (3.18) is equal to zero and one obtains in accordance with (3.19) that in the matrix (3.23) $c=1$ and $s=0$. The elements c_{ij} do not depend on the radial momentum and the matrix (3.11) may

be expressed via the angle variables θ, φ, which define a direction of the particle momentum vector

$$C_1 = \begin{pmatrix} \sqrt{\dfrac{1+\cos\theta}{2}} & -e^{-i\varphi}\sqrt{\dfrac{1-\cos\theta}{2}} \\ e^{i\varphi}\sqrt{\dfrac{1-\cos\theta}{2}} & \sqrt{\dfrac{1+\cos\theta}{2}} \end{pmatrix} = \begin{pmatrix} \cos\left(\dfrac{\theta}{2}\right) & -\sin\left(\dfrac{\theta}{2}\right)e^{-i\varphi} \\ \sin\left(\dfrac{\theta}{2}\right)e^{i\varphi} & \cos\left(\dfrac{\theta}{2}\right) \end{pmatrix}. \qquad (3.24)$$

Thus, the nonrelativistic bispinor is of the form

$$\varphi_1 = \begin{pmatrix} c_{11} \\ c_{21} \\ 0 \\ 0 \end{pmatrix}. \qquad (3.25)$$

Analogously we obtain another columns for the nonrelativistic bispinors of which only one has a physical meaning and corresponds to the positive eigenvalue of the matrix B. The eigenvectors (3.23) will be used below.

4. REDUCTION OF THE BISPINOR DIRAC EQUATION TO AN INTEGRAL FORM

A solution of the integral Dirac equation is given in [1]. Here we suggest a general method of transformation the relativistic equations to a convenient integral form for their analysis. Make use the following theorem from the matrix theory. A Hermitean matrix A can be written down like the spectral resolution over eigenvectors c_k as follows

$$A = \sum_{k=1}^{n} \mathbf{c}_k^* \lambda_k \tilde{\mathbf{c}}_k . \qquad (4.1)$$

In this formula the wave line denotes the row-vector. A number between the vectors is their eigenvalue of the matrix. In an analogous manner one can write down the kinematic matrix in the left hand side of the Eq. (4.6), taking into consideration that it is the c-number matrix,

$$\sum_{k=1}^{4} \mathbf{c}_k^* \lambda_k \tilde{\mathbf{c}}_k \begin{pmatrix} \overline{g}(\mathbf{p}) \\ \overline{u}(\mathbf{p}) \end{pmatrix} = \left(E - V(\mathbf{p}, \mathbf{p}')\right) \begin{pmatrix} \overline{g}(\mathbf{p}) \\ \overline{u}(\mathbf{p}) \end{pmatrix}. \qquad (4.2)$$

The product of a vector row and a bispinor column is a scalar function of the momentum

$$\tilde{\mathbf{c}}_k \left(\frac{\overline{g}(\mathbf{p})}{\overline{u}(\mathbf{p})} \right) = \varphi_k(\mathbf{p}). \tag{4.3}$$

The eigenvectors c_k are given by the formulae (3.22), (3.23). The eigenvalues of the Dirac equation matrix are equal to (m is the electron rest mass)

$$\lambda_{1,3} = \sqrt{m^2 c^4 + c^2 p^2}, \quad \lambda_{2,4} = -\sqrt{m^2 c^4 + c^2 p^2}. \tag{4.4}$$

Multiply the Eq. (4.2) to the left by the vector row $\tilde{\mathbf{c}}_1$, and take into account the notation (4.3) and the orthogonality of the Dirac matrix eigenvectors. Then we arrive at a scalar equation relative to the function $\varphi_1(\text{p})$

$$\left(\sqrt{m^2 c^4 + c^2 p^2} - E \right) \varphi_1(\mathbf{p}) = \frac{Ze^2}{2\pi^2} \int \frac{1}{(\mathbf{p}-\mathbf{p}')^2} \tilde{\mathbf{c}}_1(\mathbf{p}) \psi(\mathbf{p}') d^3\mathbf{p}'. \tag{4.5}$$

The scalar product of the vector-row and vector-column $\tilde{\mathbf{c}}_1(\mathbf{p}) \psi(\mathbf{p}')$ under the integral is a scalar function depending on the two vector arguments p and p′, therefore one ought to transform this product to the scalar functions $\varphi_k(\mathbf{p}')$. Note that the unit matrix of the order 4 can be represented like the decomposition over eigenvectors c_k of the matrix (3.23). One has got

$$I_4 = \sum_{k=1}^{4} \mathbf{c}_k^*(\mathbf{p}') \tilde{\mathbf{c}}_k(\mathbf{p}'). \tag{4.6}$$

Substituting this matrix into the integral of Eq. (4.5), we arrive at the integral equation as follows

$$\left(\sqrt{m^2 c^4 + c^2 p^2} - E \right) \varphi_1(\mathbf{p}) = \frac{Ze^2}{2\pi^2} \int \frac{\tilde{\mathbf{c}}_1(\mathbf{p})}{(\mathbf{p}-\mathbf{p}')^2} \sum_{k=1}^{4} \mathbf{c}_k^*(\mathbf{p}') \varphi_k(\mathbf{p}') d^3\mathbf{p}'. \tag{4.7}$$

In the same way the equations for the functions $\varphi_k(\mathbf{p})$, $k = 2, 3, 4$, can be obtained, with the difference that the radicals of the 2-nd and 4-th equations will be taken with the minus sign. The kernels of the integral equations obtained are scalar functions, because the product of vector-row and vector-column is the vector scalar product. We see that those scalar multipliers are factorized by the variables p and p′, therefore subsequent solving of the relativistic equations system (4.5) can be made by the factorization of the Coulombic part of the integral operator kernel. This problem can be solved with the help of Fock resolution of that function over 4-fold spherical harmonics [2] that is used while solving the Schrödinger equation for the hydrogen atom.

The nonrelativistic approximation takes place, provided low electron momentum as compared with mc, then the eigenvectors c_k become unit and the scalar function $\varphi_1(\mathbf{p})$ remains only in the integral equation (4.7). Representing the radical as a series in p/mc and restricting in the latter two first terms, with denoting $\varepsilon = E - mc^2$, one arrives at the Schrödinger integral equation for an electron in the hydrogen atom

$$\left(\frac{p^2}{2m} - \varepsilon\right)\varphi_1(\mathbf{p}) = \frac{Ze^2}{2\pi^2}\int\frac{\varphi_1(\mathbf{p}')}{(\mathbf{p}-\mathbf{p}')^2}d^3\mathbf{p}'. \tag{4.8}$$

Solving this equation allows one to make manifest O(4) symmetry of the Coulombic problem in wave mechanics of the hydrogen atom, established in the classical Kepler problem [4,5]. In the next section a solution of that integral equation will be obtained with the help of 4-fold spherical harmonics.

5. SOLVING THE SCHRÖDINGER INTEGRAL EQUATION FOR THE HYDROGEN ATOM

We shall seek for a solution of Eq. (2.6) by the Fock method [2]. Show that this problem for each electronic state is equivalent to that for the four-dimensional quantum rotator:

$$\left(p_0^2 + p^2\right)\psi(\mathbf{p}) = \pi^{-2}\int|\mathbf{p}-\mathbf{p}'|^{-2}\psi(\mathbf{p}')d^3\mathbf{p}', \tag{5.1}$$

where p_0 is the mean quadratic momentum, and $p_0^2 = -2\varepsilon > 0$ for bound states. The last condition means that the form $p_0^2 + p^2$ has the elliptic kind.

Introduce a four-dimensional momentum $p_4^2 = p_0^2 + p^2$ and define an angle variable α

$$\cos\alpha = \left(p_0^2 - p^2\right)/\left(p_0^2 + p^2\right), \ \sin\alpha = 2p_0 p/\left(p_0^2 + p^2\right), \tag{5.2}$$

where $\alpha \in [0, \pi]$. The relations (5.2) are the stereographic projection of the momentum p. The angle α together with the usual spherical angles θ, φ of the momentum $\mathbf{p}$ define the surface of the unit sphere in R^4. The distance between two points of the sphere is given by the arc length of the great circle, which goes through those points. For the unit sphere R^4 this distance is equal to the central angle ω (in radians) between the radius-vectors of the points. So, $\cos\omega$ is as follows

$$\cos\omega = \cos\alpha\cos\alpha' + \sin\alpha\sin\alpha'\cos\gamma, \tag{5.3}$$

where

$$\cos \gamma = \cos \theta \cos \theta' + \sin \theta \sin \theta' \cos (\varphi - \varphi').$$

(5.4)

Express the distance square between points $\mathbf{p}$ and $\mathbf{p}'$ in terms of $\cos \omega$, making use the relation (5.2). One has got

$$
\begin{aligned}
(p - p')^2 &= p^2 + (p')^2 - 2pp' \cos \gamma = p^2 + (p')^2 - \\
&- (2p_0^2)^{-1} (p_0^2 + p^2) (p_0^2 + (p')^2) \sin \alpha \sin \alpha' \cos \gamma =
\end{aligned}
$$

(5.5)

$$
= (4p_0^2)^{-1} (p_0^2 + p^2) (p_0^2 + (p')^2) \left[\frac{4p_0^2 (p^2 + (p')^2)}{(p_0^2 + p^2) (p_0^2 + (p')^2)} - 2 \sin \alpha \sin \alpha' \cos \gamma \right]
$$

A direct test gives

$$
2 - 2 \cos \alpha \cos \alpha' = \frac{4p_0^2 (p^2 + (p')^2)}{(p_0^2 + p^2) (p_0^2 + (p')^2)}.
$$

(5.5a)

With the help of the relationships given we obtain the formula sought for

$$
(\mathbf{p} - \mathbf{p}')^2 = (2p_0)^{-2} (p_0^2 + p^2) (p_0^2 + (p')^2) (2 - 2 \cos \omega).
$$

(5.6)

Write down the volume element $d^3\mathbf{p}$ in spherical coordinates

$$
d^3\mathbf{p} = p^2 dp \sin \theta d\theta \, d\varphi.
$$

(5.7)

Using the relationships (5.2) we obtain

$$
\cos (\alpha / 2) = p_0 (p_0^2 + p^2)^{-1/2}, \quad \sin (\alpha / 2) = p (p_0^2 + p^2)^{-1/2},
$$

(5.8)

then the radial momentum can be expressed via the angle α

$$
p = p_0 \operatorname{tg} (\alpha / 2),
$$

(5.9)

from which the differential dp can be easily calculated

$$dp = p_0 \left[2 \cos^2 \left(\alpha / 2 \right) \right]^{-1} d\alpha \,. \tag{5.10}$$

The volume element acquires the form in hyperspherical coordinates as follows

$$d^3\mathbf{p} = \left(2p_0 \right)^{-3} \left(p_0^2 + p^2 \right)^3 \sin^2 \alpha \, \sin \theta \, d\alpha d\theta \, d\varphi \,. \tag{5.11}$$

Denote the hypersurface element on the four-dimensional sphere

$$d\Omega_4 = \sin^2 \alpha \, \sin \theta \, d\alpha d\theta \, d\varphi \,, \tag{5.12}$$

then the relationship (5.11) takes the form

$$d^3\mathbf{p} = \left(2p_0 \right)^{-3} \left(p_0^2 + p^2 \right)^3 d\Omega_4 \,. \tag{5.13}$$

For the wave function one obtains

$$\psi \left(\mathbf{p} \right) = a \left(p_0^2 + p^2 \right)^{-2} \Psi \left(\alpha, \, \theta, \, \varphi \right) \,, \tag{5.14}$$

where the coefficient $a = 2^{3/2} \pi^{-1} p_0^{5/2}$. With the help of the formulae (5.6), (5.13) and (5.14) the Schrödinger equation (5.1) is transformed to the Fock integral equation for the hydrogen atom

$$p_0 \Psi \left(\alpha, \theta, \varphi \right) = \left(2\pi^2 \right)^{-1} \int \left[4\sin^2 \left(\omega / 2 \right) \right]^{-1} \Psi \left(\alpha', \theta', \varphi \right) d\Omega_4' \,. \tag{5.15}$$

On the unit hypersphere the square of the distance between two points is

$$\left(\Delta \boldsymbol{\rho} \right)^2 = \left(\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2 \right)^2 \,, \tag{5.16}$$

where $\boldsymbol{\rho}_1, \boldsymbol{\rho}_2$ are unit vectors from the sphere center to its surface points. The Cartesian coordinates of a point on the 4-sphere can be expressed via the angle variables according to the formulae

$$t = \sin \alpha \, \sin \theta \, \sin \varphi \,, \quad u = \sin \alpha \, \sin \theta \, \cos \varphi \,,$$
$$v = \sin \alpha \, \cos \theta \,, \quad w = \cos \alpha \,. \tag{5.17}$$

Taking into account that

$$t^2 + u^2 + v^2 + w^2 = \rho^2 = 1 \,, \tag{5.18}$$

one obtains

$$\left(\Delta\boldsymbol{\rho}\right)^2 = \left(\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2\right)^2 = 2 - 2\cos\ \omega = 4\sin^2\left(\omega/2\right), \tag{5.19}$$

that coincides with the denominator of the function under the integral in Eq. (5.15)

Write down the Laplace equation in R^4

$$\left(\frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} + \frac{\partial^2}{\partial w^2}\right)\Psi\left(t,\ u,\ v,\ w\right) = 0. \tag{5.20}$$

This equation and the integral equation (5.15) are equivalent on the unit sphere surface. Solutions of these equations are the hyperspherical harmonics [2, 3] as follows

$$\Psi_{nlm}\left(\alpha,\ \theta,\ \varphi\right) = \Pi_n^l\left(\alpha\right)Y_{lm}\left(\theta,\ \varphi\right), \tag{5.21}$$

where

$$Y_{lm}\left(\theta,\ \varphi\right) = b_{lm}P_l^m\left(\theta\right)\exp\left(im\varphi\right) \tag{5.22}$$

is a normalized to 1 spherical harmonic, provided $P_l^m\left(\theta\right)$ being a Legendre associated polynomial, and $\Pi_n^l\left(\alpha\right)$ being a Gegenbauer associated polynomial, which is connected with the Gegenbauer polynomial by a relationship

$$\Pi_n^l\left(\alpha\right)\ = b_{nl}\sin^l\alpha C_{n-l-1}^{l+1}\left(\cos\alpha\right), \tag{5.23}$$

where b_{lm}, b_{nl} are the normalization coefficients:

$$b_{lm} = \left(-1\right)^{(m+|m|)/2}\left[\frac{2l+1}{2}\frac{\left(l-|m|\right)\ !}{\left(l+|m|\right)\ !}\right]^{1/2},$$

$$b_{nl} = \left(-1\right)^{n+1}i^l 2\pi^{1/2}2^l l!\ \left[n\left(n-l-1\right)\ !/\left(n+l\right)\ !\right]^{1/2}. \tag{5.24}$$

An explicit form of the function $\Psi_{nlm}\left(\alpha,\theta,\varphi\right)$ can be found if one expands the function $\left[4\sin^2\left(\omega/2\right)\right]^{-1}$ into a series over the Gegenbauer polynomials. Indeed, a series takes place [4, 5] representing a generalization of the Legendre series for the generating function

$$\left(\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2\right)^{-2\lambda} = \left(\ \rho_1^2 + \rho_2^2 - 2\rho_1\ \rho_2\cos\omega\right)^{-\lambda} =$$

$$= \sum_{n=1}^{\infty} \frac{\left(\rho_1^2 + \rho_2^2 - \left| \rho_1^2 - \rho_2^2 \right| \right)^{n+\lambda-1}}{2^{n+\lambda-1} \left(\rho_1 \rho_2 \right)^{n+2\lambda-1}} C_{n-1}^{\lambda} \left(\cos \omega \right),$$ (5.25)

where $C_{n-1}^{\lambda} \left(\cos \omega \right)$ is a Gegenbauer polynomial, λ is a real number.

Take into account the addition theorem [3] for the Gegenbauer polynomials

$$C_q^p \left(\cos \alpha \cos \alpha' + \sin \alpha \sin \alpha' \cos \gamma \right) =$$

$$= \frac{\Gamma(2p-1)}{\left[\Gamma(p) \right]^2} \sum_{l=0}^{q} \frac{2^{2l} \Gamma^2 \left(p+l \right) \left(q-l \right)! \left(2l+2p-1 \right)}{\Gamma \left(q+l+2p \right)} \times$$

$$\times \sin^l \alpha C_{q-l}^{p+l} \left(\cos \alpha \right) \sin^l \alpha' C_{q-l}^{p+l} \left(\cos \alpha' \right) C_l^{p-1/2} \left(\cos \gamma \right).$$ (5.26)

It allows one to obtain a bilinear expansion of the kernel $\left[4 \sin^2 \left(\omega / 2 \right) \right]^{-1}$ over the hyperspherical harmonics

$$\left[4 \sin^2 \left(\omega / 2 \right) \right]^{-1} = \sum_{n=1}^{\infty} \sum_{l=0}^{n-1} \sum_{m=-l}^{l} n^{-1} \Psi_{nlm} \left(\Omega_4 \right) \Psi_{nlm}^* \left(\Omega_4' \right).$$ (5.27)

Substitute this expansion into the Fock equation, then multiply the both parts of the equation by a complex conjugated hyperspherical function and integrate over 4-sphere surface, provided the hyperspherical harmonics orthonormality,

$$\int_0^{\pi} \int_0^{\pi} \int_0^{2\pi} \Psi_{nlm} \left(\Omega_4 \right) \Psi_{n'l'm'}^* \left(\Omega_4 \right) d\Omega_4 = 2\pi^2 \delta_{nn'} \delta_{ll'} \delta_{mm'},$$ (5.28)

where $\delta_{nn'}$ is the Kronecker symbol. As a result we obtain for the parameter p_0 the following value

$$p_0 = n^{-1}.$$ (5.29)

The hydrogen atomic spectrum is calculated by the formula

$$\varepsilon = -\frac{1}{2} p_0^2.$$ (5.30)

Thus, the problem on the discrete spectrum of the hydrogen atom has been solved completely.

The hydrogen atomic continuous spectrum is characterized by the positive parameter ε to which the harmonics on the both surfaces of a two-sheeted hyperboloid correspond.

6. A REMARK ON SOLVING THE RELATIVISTIC INTEGRAL EQUATION SYSTEM IN MOMENTUM SPACE

Consider the relativistic equation system for a hydrogen-like atom

$$\left(\sqrt{m^2c^4+c^2p^2}-E\right)\varphi_i\left(\mathbf{p}\right)=\frac{Ze^2}{2\pi^2}\int\frac{\tilde{\mathbf{c}}_i\left(\mathbf{p}\right)}{\left(\mathbf{p}-\mathbf{p}'\right)^2}\sum_{k=1}^{4}\mathbf{c}_k^*\left(\mathbf{p}'\right)\varphi_k\left(\mathbf{p}'\right)d^3\mathbf{p}' \qquad ,\ (i=1,\dots,4). \tag{6.1}$$

Taking into account the factorization of the function $\tilde{c}_i\left(\mathbf{p}\right)c_k^*\left(\mathbf{p}'\right)$ by the variables, one can reduce the problem to solving the integral equation with a degenerate kernel and thus to a system of linear algebraic equations with a Hermite matrix of coefficients. A diagonalization of this matrix will come up with a solution of the initial equation, because coefficients in a series over the basic functions of the kernel bilinear decomposition will be found. It is clear that due to the spherical symmetry of the problem, the coefficient matrix in the equation system will acquire a block-diagonal form with finite block orders.

In addition, one can consider an approximate scalar equation for the first component φ_1 that corresponds to the spinor function with the predominant first component of the bispinor for the positive energy value

$$\left(\sqrt{m^2c^4+c^2p^2}-E\right)\varphi_1\left(\mathbf{p}\right)=\frac{Ze^2}{2\pi^2}\int\frac{\tilde{\mathbf{c}}_1\left(\mathbf{p}\right)\mathbf{c}_1^*\left(\mathbf{p}'\right)}{\left(\mathbf{p}-\mathbf{p}'\right)^2}\varphi_1\left(\mathbf{p}'\right)d^3\mathbf{p}'. \tag{6.2}$$

This equation is an augmented one with respect to zero-spin integral equation when the bilinear kernel function becomes constant. In the equation given a modification of the Coulombic potential takes place in accordance with the relativistic kinematics by multiplying it into the bilinear by momenta function, which is formed of the kinematic matrix eigenvectors

$$\tilde{\mathbf{c}}_1\left(\mathbf{p}\right)\mathbf{c}_1^*\left(\mathbf{p}'\right)=c_{11}\left(\mathbf{p}\right)c_{11}^*\left(\mathbf{p}'\right)+c_{12}\left(\mathbf{p}\right)c_{12}^*\left(\mathbf{p}'\right)+c_{13}\left(\mathbf{p}\right)c_{13}^*\left(\mathbf{p}'\right)+c_{14}\left(\mathbf{p}\right)c_{14}^*\left(\mathbf{p}'\right) \tag{6.3}$$

The bilinear form components are given by the formula (3.22). One can see that while neglecting the "positron" components c_{13} and c_{14}, we obtain the relativistic integral equation of the first order in energy with the spinor constituent unlike the second order in energy Klein-Gordon equation.

7. RELATIVISTIC EQUATIONS FOR A MANY-ELECTRON SYSTEM IN THE MOMENTUM SPACE

Some advantages of integral equations for a system of relativistic electrons are perceived while solving problems of electron scattering on atomic systems, the more so as in such experiments electron momenta are measured. At the same time, as we have verified in researching the Dirac equation, in the momentum space one can easily pass to the nonrelativistic model of particle mechanics and obtain the relativistic corrections in an explicit form.

Write down the system of relativistic equations for an atom

$$\sum_{a=1}^{n} I_4 \times \ldots \times B_a^q \times \ldots \times I_4 \cdot \Psi + \left(\sum_{a=1}^{n} V_a + \sum_{a>b=1}^{n} V_{ab} \right) I \cdot \Psi = E\Psi , \tag{7.1}$$

$$B_a^q = \begin{pmatrix} c\boldsymbol{\sigma}\mathbf{p}_a^q & mc^2 I_2 \\ mc^2 I_2 & -c\boldsymbol{\sigma}\mathbf{p}_a^q \end{pmatrix}, \tag{7.2}$$

where the index q points to the momentum being the differential operator.

Multiply this system to the left by the exponential

$$\exp\left(-\sum_{k=1}^{n} i\mathbf{p}_k \mathbf{r}_k \right), \tag{7.3}$$

with the momentum being a c-number, and integrate the equations over electron coordinates, we arrive at the integral equation system

$$\sum_{a=1}^{n} I_4 \times \ldots \times B_a \times \ldots \times I_4 \cdot \Phi(\mathbf{p}) +$$
$$+ \frac{1}{(2\pi)^{3n/2}} \int \exp\left(\sum_{k=1}^{n} -i\mathbf{p}_k \mathbf{r}_k \right) \left(\sum_{a=1}^{n} V_a + \sum_{a>b=1}^{n} V_{ab} \right) I \cdot \Psi(\mathbf{r}) d^{3n}\mathbf{r} = E\Phi(\mathbf{p}). \tag{7.4}$$

Here the kinematic matrix in the direct product consists of the c-numbers

$$B_a = \begin{pmatrix} c\boldsymbol{\sigma}\mathbf{p}_a & mc^2 I_2 \\ mc^2 I_2 & -c\boldsymbol{\sigma}\mathbf{p}_a \end{pmatrix}, \tag{7.2a}$$

with the matrix I being of the order 4^n. Represent the coordinate wave function (multispinor) under the integral as a Fourier-transformation, also,

$$\Psi\left(\mathbf{r}\right)=\frac{1}{\left(2\pi\right)^{3n/2}}\int\exp\left(\sum_{k=1}^{n}i\mathbf{p}_k'\mathbf{r}_k\right)\Phi\left(\mathbf{p}'\right)d^{3n}\mathbf{p}'.\tag{7.5}$$

Changing the order of integration by the coordinates and momenta in the system (5.4), and defining the Fourier-transformation for the potential function

$$\overline{V}\left(\mathbf{p},\mathbf{p}'\right)=\frac{1}{\left(2\pi\right)^{3n}}\int\exp\left(\sum_{k=1}^{n}-i\mathbf{p}_k\mathbf{r}_k\right)\left(\sum_{a=1}^{n}V_a+\sum_{a>b=1}^{n}V_{ab}\right)\exp\left(\sum_{k'=1}^{n}i\mathbf{p}_{k'}'\mathbf{r}_{k'}\right)d^{3n}\mathbf{r},\tag{7.6}$$

one obtains an integral equation system

$$\sum_{a=1}^{n}I_4\times\ldots\times B_a\times\ldots\times I_4\cdot\Phi\left(\mathbf{p}\right)+\int\overline{V}\left(\mathbf{p},\mathbf{p}'\right)\cdot I\cdot\Phi\left(\mathbf{p}'\right)d^{3n}\mathbf{p}'=E\Phi\left(\mathbf{p}\right).\tag{7.7}$$

The kinematic matrix in the left hand side of the equation can be represented as the spectral resolution into its eigenvectors

$$\sum_{a=1}^{n}I_4\times\ldots\times B_a\times\ldots\times I_4=\sum_{v=1}^{4^n}\mathbf{c}_v^*\lambda_v\tilde{\mathbf{c}}_v,\tag{7.8}$$

where $\lambda_v=\sum_{a=1}^{n}\left(-1\right)^{l(v,a)}\sqrt{m^2c^4+c^2p_a^2}$, and $l\left(a,v\right)=1$ or 2, being dictated by the appropriate eigenvector. A real state of a particle is described by the arithmetic root. The length of the eigenvector is 4^n. However, as it has been demonstrated with the Dirac equation, in the transformation discussed all the roots of the matrix (7.8) participate.

By virtue of great multiplicity of the eigen-numbers (it may compare with composition of spins in atomic one-particle models) one obtains 2^n eigenvectors for the same eigenvalue as the arithmetic root. So this root gives the reasonable estimation for the electron system energy in an atom. All the rest roots in which negative radicals enter, have no physical meaning, and they ought to be considered only like auxiliary algebraic constituents, when linearizing the kinetic energy operator of a particles system.

The Eq. (7.7) can be transformed to a new form, taking into account the relationship (7.8). Thus, in analogy with the Dirac equation, multiply it to the left by the row eigenvector $\tilde{\mathbf{c}}_1$ and using the orthonormality of the kinetic matrix eigenvectors, we arrive at the many-particle relativistic integral equation over functions χ_k.

$$\lambda_1\chi_1\left(\mathbf{p}\right)+\int\overline{V}\left(\mathbf{p},\mathbf{p}'\right)\cdot\tilde{\mathbf{c}}_1\left(\mathbf{p}\right)\sum_{k=1}^{4^n}\mathbf{c}_k^*\left(\mathbf{p}'\right)\cdot\chi_k\left(\mathbf{p}'\right)d^{3n}\mathbf{p}'=E\chi_1\left(\mathbf{p}\right),\tag{7.9}$$

where $\lambda_1(\mathbf{p}) = \sum\limits_{k=1}^{n} \sqrt{m^2 c^4 + c^2 p_k^2}$. The rest 4^n-1 integral equations of the system have analogous forms. Each eigenvector can be written down in an explicit form, so an analysis of the kernel of the integral operator, cumbersome by the necessity, can be made easily. As it may be seen, the kernel is factorized with respect to the function-components of the eigenvectors. Reduction of the kernel to a degenerate one amounts to a factorization of the potential function by variables. This question demands a separate consideration. Note a property of the integral operator (7.9). It is obvious, the Coulombic function of the kernel has the singularity when $\mathbf{p} = \mathbf{p}'$. The multiplier which includes the eigenvectors of the kinematic matrix, is represented by the sum in which the first adduct is reduced to unity, and the other terms vanish because of eigenvector orthogonality, provided the momenta are equal. If the momentum is changed like the argument of an eigenvector, the latter is rotated in many-dimensional vector space relative to the other eigenvectors with some other argument, so the scalar products with them of the eigenvector $\mathbf{c}_1$ mean cosines of the angles among those vectors, values of which are close to zero. In particular this note concerns the eigenvectors which belong to roots with nonphysical negative energies.

Thus, the leading term in this kernel multiplier proves to be that which index coincides with the index of the function outside of the integral operator. Besides, the Coulombic part of the integral operator kernel is singular, when the momenta are equal, and it defines the asymptotic behavior of the solution. In this case the first term of the scalar products of the kinetic matrix eigenvectors only affects the wave function asymptotic, which is unity at equal arguments in the potential function, the rest scalar products are equal to zero due to the eigenvector orthogonality in this domain. Therefore one has a reason to solve first the *scalar relativistic equation*

$$\lambda_1 \chi_1(\mathbf{p}) + \int \overline{V}(\mathbf{p},\mathbf{p}') \cdot \tilde{\mathbf{c}}_1(\mathbf{p}) \mathbf{c}_1^*(\mathbf{p}') \cdot \chi_1(\mathbf{p}') d^{3n}\mathbf{p}' = E \chi_1(\mathbf{p}). \tag{7.10}$$

This equation can be solved by an iteration method choosing trial function from the decomposition of the potential function and components of the eigenvector $\mathbf{c}_1(\mathbf{p})$. A factorization of the Coulombic kernel $\overline{V}(\mathbf{p},\mathbf{p}')$ by variables brings to an integral equation with a degenerated kernel which solution can be obtained by an algebraic method. After calculation of the wave function in the momentum space, a transfer to the electronic coordinate space is made by the formula (7.5).

The eigenvectors corresponding to nonphysical roots of the Dirac equation (which they assign conventionally to positron states) contribute just as algebraic elements of the relativistic model considered similarly the connection of real and complex roots of a polynomial with real coefficients. The prediction of the positron existence is truly connected not with the Dirac equation algebra, but with sign symmetry of the elementary electric charges, which kinetic energy undoubtedly does not depend on an electric charge sign.

The Eq. (7.10) changes to the nonrelativistic Schrödinger equation for an atom if particle momenta are much lower than mc, then the eigenvector $\mathbf{c}_1$ has zero "positronic" components like in (3.25).

8. A Hypercomplex Representation in the Momentum Space of Particles

The above-developed theory of relativistic equations for a heavy atom can be expanded to a hypercomplex variant of equations. We start from the equation system for an n-electron atom

$$H\Psi = (E - V)I\Psi, \tag{8.1}$$

where

$$H = H_1 \otimes I_2 \otimes \ldots \otimes I_2 + I_2 \otimes H_2 \otimes \ldots \otimes I_2 + \ldots + I_2 \otimes I_2 \otimes \ldots \otimes H_n, \tag{8.2}$$

With the kinematic matrices for separate particles

$$H_k = \begin{pmatrix} \alpha\gamma p_{\Gamma k} & 1 \\ 1 & -\alpha\gamma p_{\Gamma k} \end{pmatrix}, \tag{8.3}$$

and the momentum written in the quaternionic form

$$p_\Gamma = ip_x + jp_y + kp_z, \tag{8.4}$$

with the Hamilton algebra $ijk = -1$, $i^2 = j^2 = k^2 = -1$, and $\alpha = \sqrt{-1}$ commuting with the Hamilton units, $\gamma = e^2 / \hbar c$.

The atomic potential function is of the form (in the relativistic atomic scale)

$$V = \gamma^2 \sum_{q=1}^{n} -\frac{Z}{r_q} + \gamma^2 \sum_{q \neq q'=1}^{n} \frac{1}{r_{qq'}}, \tag{8.5}$$

Write down the spectral resolution of the kinematic matrix (8.2)

$$H = \sum_{k=1}^{2^n} \mathbf{c}_k^* \lambda_k \tilde{\mathbf{c}}_k . \tag{8.6}$$

In the momentum representation Eq. (8.1) is the integral equation

$$\sum_{k=1}^{2^n} \mathbf{c}_k^* \lambda_k \tilde{\mathbf{c}}_k \Phi(\mathbf{p}) = E\Phi(\mathbf{p}) - \int d\mathbf{p}' \, V(\mathbf{p}, \mathbf{p}') \Phi(\mathbf{p}'), \tag{8.7}$$

where the potential function is expressed in the momentum space and defined with the help of the Fourier transformation of the corresponding potential function in the coordinate representation.

Multiplying this equation to the left successively by the eigenvectors of the kinematic matrix, one obtains equations with respect to projections of the multispinors onto those vectors. One has got

$$\lambda_k \psi_k(\mathbf{p}) = E\psi_k(\mathbf{p}) - \int d\mathbf{p}' \, V(\mathbf{p},\mathbf{p}')\mathbf{c}_k(\mathbf{p}) \cdot \mathbf{I} \cdot \Phi(\mathbf{p}'), \tag{8.8}$$

where $\psi_k(\mathbf{p}) = \tilde{\mathbf{c}}_k(\mathbf{p})\Phi(\mathbf{p})$. For the following transformation of the equation, introduce the unit matrix of the order 2^n, and its spectral decomposition

$$\mathbf{I} = \sum_{k=1}^{2^n} \mathbf{c}_k^*(\mathbf{p}') \, \tilde{\mathbf{c}}_k(\mathbf{p}'), \tag{8.9}$$

Substituting it into the integral (8.8), one arrives at the equation system sought for the functions $\psi_k(\mathbf{p})$

$$\lambda_k \psi_k(\mathbf{p}) = E\psi_k(\mathbf{p}) - \int d\mathbf{p}' \, V(\mathbf{p},\mathbf{p}')\tilde{\mathbf{c}}_k(\mathbf{p}) \sum_{k'=1}^{2^n} \mathbf{c}_{k'}^*(\mathbf{p}')\psi_{k'}(\mathbf{p}'), \quad k = 1, 2, \ldots, n, \tag{8.10}$$

by an analogy with the system given in the preceding Section. We can make the analogous conclusions concerning applications of this relativistic equation system in the theory of heavy elements.

The distinctive feature of the hypercomplex equation system, as compared with the considered in the Clifford space, is that among the eigenvectors of kinematic matrix there exists only one corresponding to the sum of the positive roots of the quadratic equation for the free particle energy. So, the equation with the index 1 is determining one, while solving the physical problem on motion of n particles (electrons) near a force center. This equation can give the first approximation for the wave function of an atomic system. (It is possible a generalization of such an equation on molecular systems, also, but not in the context of this research.) This equation gives the correct asymptotic solution of the initial equation system, with a singular kernel of the integral operator, also. Write down the abovementioned scalar relativistic equation

$$\lambda_1 \psi_1(\mathbf{p}) = E\psi_1(\mathbf{p}) - \int d\mathbf{p}' \, V(\mathbf{p},\mathbf{p}')\tilde{\mathbf{c}}_1(\mathbf{p})\mathbf{c}_1^*(\mathbf{p}')\psi_1(\mathbf{p}'), \tag{8.11}$$

where the scalar product of the multidimensional eigenvectors (spinors) of the kinematic matrix models an influence of the spin kinematic of the particle system on their interactions by means of the Coulombic forces with the force center and between particles.

CONCLUSION

It stands to reason that advantages and deficiencies of the approaches given can be estimated in numerical realizations. We hope that the simple structure of the investigated equations will allow in the future to create mathematical software for posing and solving of some actual problems in atomic spectroscopy and atomic physics of heavy and superheavy chemical elements.

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