Analytical Solution to the Dirac Equation for Few-Electron Ions of Transuranium Elements

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Abstract. The paper presents relativistic generalization of the well-known method of multidimensional angular Coulomb functions. Two-component multidimensional angular functions have been constructed and they are used as a basis for expanding in series the many-electron wave function of the many-particle Dirac equation. A system of ordinary differential equations which factors are expressed in terms of matrix elements of various operators of the Dirac equation has been obtained for the expansion amplitudes. The binding energy of helium-, lithium-, beryllium- and carbon-like ions of transuranium elements has been calculated (Z = 92–101). Wave functions have been constructed for some states of transuranium ions. The developed method allows taking into account the many-particle effects during the calculation of relativistic many-electron systems which are described by the many-particle Dirac equation with Coulomb interactions. The obtained results can be applied to specify the probability of transitions and particle paths in high energy-density processes.

Introduction
The paper is the next step forward in the studies described in [1-5]. The properties of few-electron systems are studied using a specific example of C-like ions of heavy elements by solving the Dirac equation for six electrons in the heavy nucleus field.

The developed relativistic option of the method of multidimensional angle Coulomb functions [6-8] allows finding an exact solution to the Dirac equation, which, in its turn, allows calculating probabilities of various physical processes using the available expressions for two-component wave functions, as well as Breit-Wigner corrections and corrections for radiation.

This paper presents the band 0⁺ spectrum for C-like ions of elements with Z=92 to Z=101. The electron density profile has been obtained using the analytical wave function (WF) and the contribution from the lower WF component has been studied.

1. Hyperradial equations of the relativistic method of multidimensional angle Coulomb functions (MACF)

Moving electrons of a C-like ion in the central-symmetry electrical field of nucleus are described by the Dirac equation.
In the relativistic system of units, the Dirac equation for components of wave function \( \Psi = \begin{pmatrix} \Phi \\ X \end{pmatrix} \) looks like

\[
E + \sum_{i=1}^{6} \frac{Z}{r_i} - \sum_{i=1}^{6} \frac{1}{|r_i - r_j|} \Phi = \sum_{i=1}^{6} c \sigma_i \hat{p}_i X,
\]

(1.1)

\[
E + 12 + \sum_{i=1}^{6} \frac{Z}{r_i} - \sum_{i=1}^{6} \frac{1}{|r_i - r_j|} X = \sum_{i=1}^{6} c \sigma_i \hat{p}_i \Phi.
\]

(1.2)

The system’s binding energy in these equations is \( E = \varepsilon - 6 < 0 \), where \( \varepsilon \) is the system’s total energy \((mc^2)\).

To solve the equation above with MACF method, it is necessary to represent the WF components in terms of a series of multidimensional angle functions (MAF).

With minimum approximation, the wave function of state \( ^0\text{C} \) of C-like ions in the spinor representation corresponding to electron configuration \((1s^22s^21p^2)\) has the form:

\[
\Psi = \begin{pmatrix} \Phi \\ X \end{pmatrix} = \frac{1}{\rho^{3/2}} \begin{pmatrix} MU \\ NW \end{pmatrix},
\]

(1.3)

where \( \rho = \sum |r_i| \) is collective variable, \( M \) and \( N \) are amplitudes of the MAF factorization of the upper and lower WF components, respectively, and MAFs are Slater determinants:

\[
U = \frac{N_k}{(-it\rho)^2} \begin{pmatrix} \psi_1(1) & \psi_1(2) & \ldots & \psi_1(6) \\ \psi_2(1) & \psi_2(2) & \ldots & \psi_2(6) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_6(1) & \psi_6(2) & \ldots & \psi_6(6) \end{pmatrix},
\]

\[
W = \frac{N_k}{(-it\rho)^2} \begin{pmatrix} \xi_1(1) & \xi_1(2) & \ldots & \xi_1(6) \\ \xi_2(1) & \xi_2(2) & \ldots & \xi_2(6) \\ \vdots & \vdots & \ddots & \vdots \\ \xi_6(1) & \xi_6(2) & \ldots & \xi_6(6) \end{pmatrix},
\]

(1.4)

where \( N_k \) is normalization constant and orthonormal basis functions \( \psi \) and \( \xi \), which are associated with an electron on a certain shell with a set of quantum numbers \( \{n,j,l,m\} \) and, in general, have the form:

\[
\psi_{njlm} = \frac{1}{\Gamma(n+1)} \Omega_{njlm} I_n^j(-itr), \quad \xi_{njm} = (-1)^{j-l} \frac{1}{\Gamma(n+1)} \Omega_{njm} I_n^{l'}(-itr).
\]

(1.5)

In the expressions above, the following symbols are used for the basis functions: \( I_n^j \) are Laguerre polynomials; \( \Omega_{njlm} \) are spinor spherical functions, and \( l' = 2j - l \). For the system of interest, the set of basis functions has the form:
2. Matrix elements of the operator of electron-nucleus interaction

For the upper WF component, matrix element (ME) of electron-nucleus interaction has the form

\[
P_{e-n} = \langle U' | \sum_{j} \frac{Z}{r_j} | U \rangle,
\]

(2.1)
and ME for the lower WF component looks like

\[ Q_{e-a} = \left\langle W^* \left| \sum_{i=1}^{6} \frac{Z}{r_i} \right| W \right\rangle. \]  

(2.2)

Matrix elements \( P_{e-a} \) and \( Q_{e-a} \) are calculated in the same way and because of this we demonstrate here the calculation of matrix element \( P_{e-a} \) of the upper WF component.

In view of the fact that the potential energy operator \( \sum_{i=1}^{6} \frac{Z}{r_i} \) is a single-particle operator, we can reduce equation (2.1) to the sum over subshells [9] and, hence, we obtain

\[ P_{e-a}(\rho) = \sum_{i=1}^{6} \left\langle \psi_{\omega}^* \frac{Z}{r} \psi_{\omega} \right\rangle. \]  

(2.3)

With regard to normalization and orthonormalized spin-angle functions the expression for matrix element in equation (2.3) can be represented in its general form (for arbitrary basis functions):

\[ \left\langle \psi_{\omega}^* \left| \frac{1}{r} \right| \psi_{\omega} \right\rangle = \frac{\Gamma(3A+2K)}{A!} \frac{1}{2\pi\rho^3} \frac{1}{\Gamma(3+n_{\omega})} \frac{A!}{\Gamma(3+n_{\omega})} \int_{-\infty}^{\infty} e^{i\rho r} \int_{-\infty}^{\infty} e^{i\rho r} \left[ L_{n_{\omega}}^2 (-itr) \right] rdr. \]  

(2.4)

Hereinafter, \( \omega \) is the basis function’s number denoting the corresponding set of quantum numbers. Thus, the principal quantum number is \( n_{\omega} = 0 \) for basis functions \( \psi_1, \psi_2, \psi_5 \), and \( n_{\omega} = 1 \) for basis functions \( \psi_3 \) and \( \psi_4 \) (see (1.6)).

Laguerre polynomial in equation (2.4) must be represented as a sum of Laguerre polynomials of a lower power [10]:

\[ L_{n_{\omega}}^2 (-itr) = \sum_{m_{\omega}=1}^{n_{\omega}} L_{m_{\omega}}^m (-itr). \]  

(2.5)

Owing to the orthogonal nature of Laguerre polynomials the integral in ME of electron-nucleus interaction can be represented as

\[ \int e^{i\rho r} \left[ L_{n_{\omega}}^2 (-itr) \right] rdr = \frac{1}{(-it)^2} \sum_{m_{\omega}=0}^{n_{\omega}} \frac{\Gamma(2+m_{\omega})}{\Gamma(1+m_{\omega})} = \frac{1}{(-it)^2} \sum_{m_{\omega}=0}^{n_{\omega}} (1+m_{\omega}) = \frac{1}{(-it)^2} \frac{(n_{\omega}+2)(n_{\omega}+1)}{2}. \]  

(2.6)

Thus, for ME of electron-nucleus interaction we obtain

\[ \left\langle \psi_{\omega}^* \left| \frac{1}{r} \right| \psi_{\omega} \right\rangle = \frac{\Gamma(3A+2K)}{A!} \frac{(n_{\omega}+1)(n_{\omega}+2)}{\Gamma(3+A+2K-1)} \frac{1}{\rho} = \frac{(3A+2K-1)}{2\Gamma(3+n_{\omega})} \frac{1}{\rho}. \]  

(2.7)

As a result, for all MEs of electron-nucleus interaction of C-like ions in configuration \( 1s^2 2s^2 1p_{1/2}^2 \) we obtain

\[ \left\langle \psi_{\omega}^* \left| \frac{Ze^2}{r} \right| \psi_{\omega} \right\rangle = \left\langle \xi_{\omega}^* \left| \frac{Ze^2}{r} \right| \xi_{\omega} \right\rangle = \frac{21Ze^2}{2\rho}, \quad \omega = 1, \ldots, 6. \]  

(2.8)
Upon summation over shells one can write
\[ P_{e-a} = Q_{e-a} = \frac{63 Z e^2}{\rho}. \] (2.9)

3. Matrix elements of the kinetic energy operator

To obtain the differential equation system for amplitudes of the two-component WF expansion, it is required to calculate the following MEs of the kinetic energy operator:

\[ B = \langle U | \sum_{i=1}^{\epsilon} \sigma_{\epsilon} \hat{p} | X \rangle, \] (3.1)
\[ H = \langle W | \sum_{i=1}^{\epsilon} \sigma_{\epsilon} \hat{p} | \Phi \rangle. \] (3.2)

With regard to the form of multidimensional angle functions \( U \) and \( W \) it seems easier to calculate MEs of the form

\[ B = \left( U \left| \sum_{i=1}^{\epsilon} \sigma_{\epsilon} \hat{p} \right| N(\rho) \frac{1}{\rho^{1/2}} \left( \rho \hat{W} \right) \right), \] (3.3)
\[ H = \left( W \left| \sum_{i=1}^{\epsilon} \sigma_{\epsilon} \hat{p} \right| M(\rho) \frac{1}{\rho^{1/2}} \left( \rho \hat{U} \right) \right). \] (3.4)

Since operator \( \sigma \hat{p} \) is a single-particle operator, equation (3.3) can be written as a sum over shells [9]:

\[ B = \sum_{\omega} \left( \psi_{\omega} | \sigma_{\omega} N(\rho) \frac{1}{\rho^{1/2}} \xi_{\omega} \right). \] (3.5)

Similarly, equation (3.4) is written in the form:

\[ H = \sum_{\omega} \left( \xi_{\omega} | \sigma_{\omega} M(\rho) \frac{1}{\rho^{1/2}} \psi_{\omega} \right). \] (3.6)

Using the explicit form of momentum operator \( \hat{p} = -i \hbar \frac{\partial}{\partial r} \) and the definition of collective variable \( \rho \), we can write Eqs. (3.5) and (3.6) as

\[ B = \sum_{\omega} \left[ \frac{N(\rho)}{\rho^{1/2}} \left( \psi_{\omega} | \sigma_{\omega} \frac{d}{d\rho} \right) - \frac{i \hbar}{\rho} \left( \frac{d}{d\rho} - \frac{3A+2K-1}{2\rho} \right) N(\rho) \left( \psi_{\omega} | \sigma_{\omega} \frac{r}{\rho} \right) \right], \] (3.7)
\[ H = \sum_{\omega} \left[ \frac{M(\rho)}{\rho^{1/2}} \left( \xi_{\omega} | \sigma_{\omega} \frac{d}{d\rho} \right) - \frac{i \hbar}{\rho} \left( \frac{d}{d\rho} - \frac{3A+2K-1}{2\rho} \right) M(\rho) \left( \xi_{\omega} | \sigma_{\omega} \frac{r}{\rho} \right) \right]. \] (3.8)

To calculate single-particle MEs in the last expressions, it is possible to use the following relation between spinors [11]:
Using the explicit form of the momentum operator the last expression can be reduced to the form:

\[
\vec{\sigma} \vec{p} \varphi_{\lambda} = i^{2l_2-2r+1} \hbar \sqrt{\frac{1}{\Gamma(3+n)}} \left( \frac{1}{\Gamma(3+n)} \left( \nabla_r + r \nabla + \vec{a} \vec{i} \right) \right) \frac{L_n^2(-i\tau r)}{r} \Omega_{j\lambda m} = -\hbar \sqrt{\frac{1}{\Gamma(3+n)}} \left( \frac{3 + r \frac{\partial}{\partial r} + \vec{a} \vec{i} \right) \frac{L_n^2(-i\tau r)}{r} \Omega_{j\lambda m},
\]

where \( \vec{i} = \left[ \vec{r} \vec{p} \right] \) is the orbital momentum operator. The eigenvalues of product \( \vec{a} \vec{i} = 2s \vec{i} \) are

\[2s \vec{i} = (j^2 - l^2 - s^2) = j(j+1) - l(l+1) - \frac{3}{4} = \begin{cases} j - \frac{1}{2}, & l = j - \frac{1}{2}, \\ -j - \frac{3}{2}, & l = j + \frac{1}{2}. \end{cases}\]

Equation (3.11) can be rewritten to obtain

\[
\vec{\sigma} \vec{p} \varphi_{\lambda} = -\hbar \sqrt{\frac{1}{\Gamma(3+n)}} \frac{1 - \kappa_{jl}}{r} \varphi_{j\lambda m},
\]

where

\[
\kappa_{jl} = \begin{cases} -(l+1), & j = l + \frac{1}{2}, \\ l, & j = l - \frac{1}{2}. \end{cases}
\]

It should be noted that in equation (3.12) we omit the term obtained during the Laguerre polynomial differentiation, because this term is proportional to the Laguerre polynomial, which has one unit less power, and it gives zero during integration.

Similar approach allows obtaining

\[
\vec{\sigma} \vec{p} \varphi_{j\lambda m} = \hbar \sqrt{\frac{1}{\Gamma(3+n)}} \frac{1 + \kappa_{jl}}{r} \varphi_{j\lambda m},
\]

matrix elements \( \langle \xi_a | \sigma_r^j \varphi_{\lambda m} \rangle \) and \( \langle \varphi_{\lambda m} | \sigma_r^j \xi_a \rangle \) are trivially calculated using Eq.(3.9). The basis functions and properties of Pauli matrices are defined as

\[
i \langle \xi_a | \sigma_r^j \varphi_{\lambda m} \rangle = -\langle \xi_a | \xi_{a\lambda} \rangle = -1,
\]

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Hence, equations (3.7) and (3.8) can be rewritten to obtain

\[ B = -\frac{\hbar}{\rho^{2+2\ell+1}} \sum_{\omega} \left[ \frac{dN(\rho)}{d\rho} - \frac{3A + 2K - 1}{2\rho} N(\rho) + \left< \frac{1 - \kappa_{\omega}}{r} \right| \psi_{\omega} \right> \left< \frac{1 - \kappa_{\omega}}{r} \right| \psi_{\omega} \right] N(\rho), \]  

(3.17)

\[ H = \frac{\hbar}{\rho^{2+2\ell+1}} \sum_{\omega} \left[ \frac{dM(\rho)}{d\rho} - \frac{3A + 2K - 1}{2\rho} M(\rho) - \left< \frac{1 - \kappa_{\omega}}{r} \right| \xi_{\omega} \right> \left< \frac{1 - \kappa_{\omega}}{r} \right| \xi_{\omega} \right] M(\rho). \]  

(3.18)

With regard to the expression obtained for matrix element in the previous section,

\[ \left< \frac{1}{r} \right| \psi_{\omega} \right> = \left< \frac{1}{r} \right| \xi_{\omega} \right> = \frac{(3A + 2K - 1) 1}{2\Gamma(n_{\omega})}\rho \]  

(3.19)

for equations (3.17) and (3.18) one can write

\[ B = -\frac{\hbar}{\rho^{2+2\ell+1}} \sum_{\omega} \left[ \frac{dN(\rho)}{d\rho} - \kappa_{\omega} \left( \frac{3A + 2K - 1}{2\Gamma(n_{\omega})} \right) \right] N(\rho), \]  

(3.20)

\[ H = \frac{\hbar}{\rho^{2+2\ell+1}} \sum_{\omega} \left[ \frac{dM(\rho)}{d\rho} - 2 + \kappa_{\omega} \left( \frac{3A + 2K - 1}{2\Gamma(n_{\omega})} \right) \right] M(\rho). \]  

(3.21)

Table 1 gives values of coefficient \( \kappa \) for several states.

| \( \omega \) | 1s\(_{1/2} \) | 2s\(_{1/2} \) | 1p\(_{1/2} \) | 1p\(_{3/2} \) |
|----------------|----------------|----------------|----------------|----------------|
| \( \kappa_{\omega} \) | -1 | -1 | 1 | -2 |

For C-like ions with electron configuration \( 1s^2 2s^2 1p\(_{1/2}^2 \) \) the summation over all shells gives us

\[ B = -\frac{2h}{\rho^{2+2\ell+1}} \frac{21}{2\rho} N(\rho) - \frac{6h}{\rho^{2+2\ell+1}} \frac{dN(\rho)}{d\rho}, \]  

(3.22)

\[ H = -\frac{10h}{\rho^{2+2\ell+1}} \frac{21}{2\rho} M(\rho) + \frac{6h}{\rho^{2+2\ell+1}} \frac{dM(\rho)}{d\rho}. \]  

(3.23)
4. Matrix elements of the operator of electron-electron interaction

Direct expansion of determinants shows that MEs of electron-electron interaction for the upper WF component of C-like ions have the form:

\[
\left< U \sum_{\ell=1}^{6} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} U \right> = \sum_{\ell=1}^{6} \left< \psi_\ell^* (1) \psi_\ell^* (2) \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \psi_\ell (1) \psi_\ell (2) - \psi_\ell (2) \psi_\ell (1) \right>.
\]

Thus, it is necessary to consider the summation over six shells.

This paper describes in details the calculation of only the first term in the sum (4.1). The rest of terms are calculated in the same way and here we give only final results of such calculations for these terms.

The orthogonal nature of the basis functions corresponding to electrons of shell 1s is due to the orthogonal nature of spin-functions and, hence, the exchange part of the matrix element of interest equals zero.

With regard to normalization, the direct-interaction part of the first term has the form:

\[
\left< 1s_1 (1) 1s_1 (2) \right> = \frac{\Gamma(22)^*}{2\pi^{3/2}} \frac{\Gamma(22)^*}{2\pi^{3/2}} \int e^{-|\mathbf{r}_i - \mathbf{r}_j|} \psi_\ell^* (1) \psi_\ell (2) \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \psi_\ell (1) \psi_\ell (2) \, d\mathbf{r}_i d\mathbf{r}_j.
\]

If we use multipole expansion

\[
\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} = \sum_{q} \frac{4\pi}{2q + 1} Y_q^{(1)} Y_q^{(2)} \left( \frac{r_j^q}{r_i^{q+1}} \right),
\]

then for the angular part of integral (4.2) one can write

\[
\int \Omega_q^{(1)} (1) \Omega_q^{(2)} (2) \sum_{q} \frac{4\pi}{2q + 1} Y_q^{(1)} (2) \Omega_q^{(2)} (1) \Omega_q^{(2)} (2) d\Omega_1 d\Omega_2.
\]

In view of the orthonormalized nature of spinors it becomes evident that only terms with \( q = 0 \) differ from zero and integral taken over the angular part of (4.2) equals 1.

So, the expression for matrix element of \( \left< 1s_1 (1) 1s_1 (2) \right> \) can be transformed to obtain

\[
\left< 1s_1 (1) 1s_1 (2) \right> = \frac{\Gamma(22)^*}{2\pi^{3/2}} \frac{\Gamma(22)^*}{2\pi^{3/2}} \int e^{-|\mathbf{r}_i - \mathbf{r}_j|} \psi_\ell^* (1) \psi_\ell (2) \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \psi_\ell (1) \psi_\ell (2) \, d\mathbf{r}_i d\mathbf{r}_j.
\]

The integral over coordinates \( \mathbf{r}_i \) and \( \mathbf{r}_j \) has the following value:

\[
\int \frac{r_i^2 dr_i e^{i(n_1 r_i)}}{r_i} + \int \frac{r_j^2 dr_j e^{i(n_1 + n_2) r_j}}{r_j} = \frac{1}{(-it)^5} \frac{5}{4}.
\]
As a result, for (4.5) one can write

\[ \langle 1s, 1 \rangle | 1s, 2 \rangle = \frac{1}{2\pi^2} \frac{\Gamma(22)}{(\Gamma(3))^2} \int \frac{e^{-\alpha r}}{(it)^{3/2}} \, dt \frac{5}{4} \frac{\Gamma(22)}{(\Gamma(3))^2} \frac{5}{4} \frac{105}{16} \frac{1}{\rho}. \quad (4.7) \]

Table 2 gives the values of matrix elements for the operator of electron-electron interaction for the basis MAFs of the upper WF component of C-like ion, which have been calculated by the method shown in this section.

Table 2. Matrix elements of the operator of electron-electron interaction for the basis MAFs of the upper WF component.

| Numbers of shells \( i, j \) | Direct-interaction part | Exchange interaction part | Numbers of shells \( i, j \) | Direct-interaction part | Exchange interaction part |
|------------------------------|------------------------|---------------------------|------------------------------|------------------------|---------------------------|
| 1-2 \( \langle 1s, 1 \rangle 1s, 2 \rangle \) | 105 \( \frac{1}{\rho} \) | 0 | 2-6 \( \langle 1s, 1 \rangle 1p, 2 \rangle \) | 105 \( \frac{1}{\rho} \) | -7 \( \frac{1}{\rho} \) |
| 1-3 \( \langle 1s, 1 \rangle 2s, 2 \rangle \) | 4 \( \frac{1}{\rho} \) | 3-4 | 147 \( \frac{1}{\rho} \) | 0 |
| 1-4 \( \langle 1s, 1 \rangle 2s, 2 \rangle \) | 4 \( \frac{1}{\rho} \) | 3-5 | 21 \( \frac{1}{\rho} \) | -7 \( \frac{1}{\rho} \) |
| 1-5 \( \langle 1s, 1 \rangle 1p, 2 \rangle \) | 105 \( \frac{1}{\rho} \) | 3-6 | 21 \( \frac{1}{\rho} \) | -7 \( \frac{1}{\rho} \) |
| 1-6 \( \langle 1s, 1 \rangle 1p, 2 \rangle \) | 16 \( \frac{1}{\rho} \) | 4-5 | 21 \( \frac{1}{\rho} \) | -7 \( \frac{1}{\rho} \) |
| 2-3 \( \langle 1s, 1 \rangle 2p, 2 \rangle \) | 4 \( \frac{1}{\rho} \) | 4-6 | 21 \( \frac{1}{\rho} \) | -7 \( \frac{1}{\rho} \) |
| 2-4 \( \langle 1s, 1 \rangle 2s, 2 \rangle \) | 4 \( \frac{1}{\rho} \) | 5-6 | 105 \( \frac{1}{\rho} \) | 0 |
| 2-5 \( \langle 1s, 1 \rangle 1p, 2 \rangle \) | 16 \( \frac{1}{\rho} \) | 7 \( \frac{1}{\rho} \) | 2555 \( \frac{1}{\rho} \) | 32 |

MEs of electron-electron interaction for MAF of the upper WF component have the form

\[ \langle W | \sum_{i \neq j} \frac{1}{|\vec{r}_i - \vec{r}_j|} | W \rangle = \sum_{i \neq j} \langle \xi^* (1) \xi^* (2) \left| \frac{1}{|\vec{r}_i - \vec{r}_j|} \right| \xi (1) \xi (2) - \xi (1) \xi (2) \xi (1) \rangle. \quad (4.8) \]

The terms of the sum above for the lower component are integrated similarly to those for MAF of the upper WF component. Table 3 gives the obtained values of MEs.
Table 3. Matrix elements of the operator of electro-electron interaction for the basis MAFs of the lower WF component.

| Numbers of shells $i, j$ | Direct-interaction part | Exchange interaction part | Numbers of shells $i, j$ | Direct-interaction part | Exchange interaction part |
|--------------------------|--------------------------|---------------------------|--------------------------|--------------------------|---------------------------|
| 1-2                      | 105 1                    | 0                         | 2-6                      | 105 1                    | 7 1                       |
| $\{1s, (1)l_{s}, (2)\}$  | $\frac{16}{\rho}$        | $\frac{16}{\rho}$         | $\{1s, (1)l_{p}, (2)\}$  | $\frac{16}{\rho}$        | $\frac{16}{\rho}$         |
| 1-3                      | 21 1                     | 21 1                      | 3-4                      | 147 1                    | 0                         |
| $\{1s, (1)2s, (2)\}$     | $\frac{4}{\rho}$         | $\frac{16}{\rho}$         | $\{2s, (1)2s, (2)\}$     | $\frac{32}{\rho}$        | 0                         |
| 1-4                      | 21 1                     | 3-5                       | 21 1                     | 7 1                       |
| $\{1s, (1)2s, (2)\}$     | $\frac{4}{\rho}$         | 0                         | $\{2s, (1)1p, (2)\}$     | $\frac{4}{\rho}$         | $\frac{48}{\rho}$         |
| 1-5                      | 105 1                    | 7 1                       | 3-6                      | 21 1                     | 7 1                       |
| $\{1s, (1)1p, (2)\}$     | $\frac{16}{\rho}$        | $\frac{16}{\rho}$         | $\{2s, (1)1p, (2)\}$     | $\frac{4}{\rho}$         | $\frac{24}{\rho}$         |
| 1-6                      | 105 1                    | 7 1                       | 4-5                      | 21 1                     | 7 1                       |
| $\{1s, (1)2p, (2)\}$     | $\frac{16}{\rho}$        | $\frac{8}{\rho}$          | $\{2s, (1)1p, (2)\}$     | $\frac{4}{\rho}$         | $\frac{24}{\rho}$         |
| 2-3                      | 21 1                     | 4-6                       | 21 1                     | 7 1                       |
| $\{1s, (1)2p, (2)\}$     | $\frac{4}{\rho}$         | 0                         | $\{2s, (1)1p, (2)\}$     | $\frac{4}{\rho}$         | $\frac{48}{\rho}$         |
| 2-4                      | 21 1                     | $\frac{21}{16}$           | 5-6                      | 105 1                    | 0                         |
| $\{1s, (1)2p, (2)\}$     | $\frac{4}{\rho}$         | $\frac{16}{\rho}$         | $\{1p, (1)1p, (2)\}$     | $\frac{16}{\rho}$        | $\frac{2555}{32}$         |

5. The solution to the Dirac equation for C-like ions

With regard to the obtained ME values, the system of differential equations (1.10) and (1.11) describing C-like ions in state $\{1s^2 2s^2 1p_{1/2}^2\}$ has the form:

$$M' - \frac{35}{2\rho} M - \frac{1}{6} \left( E + 12 + \alpha \frac{(63Z - 2555/32)}{\rho} \right) N = 0,$$

$$N' + \frac{7}{2\rho} N + \frac{1}{6} \left( E + \alpha \frac{(63Z - 2555/32)}{\rho} \right) M = 0. \tag{5.2}$$

The solution to the equation system above is given in [1] and, in general case, it may be written as

$$M(r) = \sqrt{E + 2A \cdot e^{-\alpha r / A}} \left( \frac{2A}{\alpha} \right)^{1/2} \times$$

$$\times \left(A_{1}F\left(-n_{x}, 2\gamma - 1 - (a_{1} - a_{2}), \frac{2\alpha \rho}{A}\right) + B_{1}F\left(-n_{x} + 1, 2\gamma - 1 - (a_{1} - a_{2}), \frac{2\alpha \rho}{A}\right)\right), \tag{5.3}$$
\[
N(r) = -\sqrt{-E}e^{-\rho/r} \left( \frac{2\lambda\rho}{A} \right)^{-\gamma} \times \\
\times \left( A F\left( -n_r, 2\gamma -1, (a_1 - a_2), \frac{2\lambda\rho}{A} \right) - B F\left( -n_r + 1, 2\gamma -1 - (a_1 - a_2), \frac{2\lambda\rho}{A} \right) \right). \tag{5.4}
\]

Normalization constants \(A_1\) and \(B_1\) of degenerated hypergeometric functions can be found from the requirement of WF normalization to 1.

In the expressions above, \(A\) is the number of electrons; \(\lambda = \sqrt{-E(E + 2A)}\); 

\[
\gamma = 1 + \frac{a_1 - a_2}{2} + \frac{(a_1 + a_2)^2}{4} - \frac{(c_1 Z - d_1)(c_2 Z - d_2)\alpha^2}{A^2};
\]

\(a_1, a_2, c_1, c_2, d_1,\) and \(d_2\) are coefficients, which have been obtained in the calculation of MEs of the operators of kinetic energy, electron-nucleus and electron-electron interactions, respectively; \(n_r\) is radial quantum number.

Calculations of MEs of the electron-nucleus and electron-electron interactions demonstrate that

\[
c_1 = c_2 = c, d_1 = d_2 = d
\]

for C-like ions. Owing to the requirement of WF finiteness at infinity (this requirement is met, if \(n_r\) takes integral positive values) we obtain the following expression for binding energy:

\[
E = A \left[ 1 + \frac{\alpha^2(cZ - d)^2}{\left( An_r + \sqrt{A^2(a_1 + a_2)^2/4 - \alpha^2(cZ - d)^2} \right)^2} \right]^{-1/2} - 1. \tag{5.6}
\]

Table 4 gives the binding energy values for C-like ions of heavy elements with various values of quantum number \(n_r\). The first four columns of this table (\(n_r = 0, \ldots, 3\)) show spurious levels occurred because of the Coulomb interaction taken into account. The binding energy of the ground state of C-like ions is given in the fifth column (\(n_r = 4\)). The binding energy of the excited state is in the sixth column (\(n_r = 5\)).

**Table 4.** The binding energy (KeV) of C-like ions in heavy elements.

| \(n_r\) | 0   | 1   | 2   | 3   | 4   | 5   |
|--------|-----|-----|-----|-----|-----|-----|
| \(Z\)  |     |     |     |     |     |     |
| 92     | -768.293 | -652.991 | -559.479 | -483.163 | -420.429 | -368.462 |
| 93     | -788.255 | -670.301 | -574.504 | -496.241 | -431.857 | -378.495 |
| 94     | -808.616 | -687.975 | -589.855 | -509.609 | -443.542 | -388.754 |
| 95     | -829.386 | -706.024 | -605.543 | -523.276 | -455.492 | -399.247 |
| 96     | -850.576 | -724.458 | -621.577 | -537.252 | -467.714 | -409.981 |
| 97     | -872.199 | -743.290 | -637.970 | -551.548 | -480.220 | -420.964 |
| 98     | -894.268 | -762.532 | -654.733 | -566.173 | -493.017 | -432.205 |
| 99     | -916.797 | -782.197 | -671.879 | -581.139 | -506.117 | -443.713 |
| 100    | -939.800 | -802.301 | -689.421 | -596.459 | -519.530 | -455.497 |
| 101    | -963.292 | -822.857 | -707.373 | -612.146 | -533.268 | -467.570 |
If quantum number $n_r$ is defined as a sum of quantum numbers of occupied shells, $n_r = 4$ is obtained for the ground state of C-like ions. Such approach is justified by the agreement achieved between the calculated binding energy values and data from other literary sources (Table 5).

Table 5 gives the binding energy values of uranium ions with ionization degree from 86 (C-like ion) to 90 (He-like ion) calculated using various methods.

| Electron configuration | $U^{90+}$ | $U^{90+}$ | $U^{90+}$ | $U^{88+}$ | $U^{86+}$ |
|------------------------|-----------|-----------|-----------|-----------|-----------|
|                        | (1s$^2$)  | (1s$^1$2s$^1$) | (1s$^2$2s$^1$) | (1s$^2$2s$^2$) | (1s$^2$2s$^2$ 2p$^5_{1/2}$) |
| MACF [12]              | -262.45   | -165.49   | -281.24   | -336.52   | -420.42   |
| ATOM [13]              | -264.14   | -166.15   | -298.22   | -332.29   | -400.31   |
| GRASP [14, 15]         | -256.25   | -159.26   | -288.34   | -319.93   | -380.44   |

Note that there is a satisfactory agreement between the binding energy values obtained with MACF method and some other methods.

6. Electron density

The analytical solutions to the multiple-electron Dirac equation given above are used to calculate the electron density of a C-like uranium ion.

The electron density of A-electron ions is calculated from expression

$$n(r) = \int \Psi^\dagger \sum_{i=1}^{a} \delta(\mathbf{r} - \mathbf{r}_i) \Psi d\mathbf{r}_1 d\mathbf{r}_2 .$$  \hspace{1cm} (6.1)

With zero approximation by the relativistic MACF method the electron density can be represented as a sum density of electrons of the upper and lower components of the bi-spinor wave function:

$$n(r) = \rho_1 (r) + \rho_2 (r) ,$$  \hspace{1cm} (6.2)

where expressions for the terms corresponding to the upper and lower components of the bi-spinor wave function look like

$$\rho_1 (r) = \frac{\Gamma (3A + 2K)}{2\pi} \int \frac{M^2 (\rho)}{\rho^{3A+2K-1}} \int_{-\infty}^{\infty} e^{-i\mathbf{r} \cdot \mathbf{r}} \sum_{\omega} \psi_{\omega}^\dagger (-i\mathbf{r}) d\mathbf{r} d\rho ,$$  \hspace{1cm} (6.3)

$$\rho_2 (r) = \frac{\Gamma (3A + 2K)}{2\pi} \int \frac{N^2 (\rho)}{\rho^{3A+2K-1}} \int_{-\infty}^{\infty} e^{-i\mathbf{r} \cdot \mathbf{r}} \sum_{\omega} \xi_{\omega}(-i\mathbf{r}) d\mathbf{r} d\rho .$$  \hspace{1cm} (6.4)

For C-like ions (A=6, K=4), we obtain with regard to the basis functions that

$$n(r) = \frac{\Gamma (22)}{4\pi (19)} \int \left( M^2 (\rho) + N^2 (\rho) \right) \left( \frac{\rho-r}{\rho^2} \right)^{16} \left[ 5\rho^2 - 46r\rho + 143r^2 \right] d\rho .$$  \hspace{1cm} (6.5)

Figure 1 illustrates results of calculations using MACF method for the electron density of a C-like uranium ion in its ground state.
To check the results obtained for validity, the total electron charge of a C-like ion has been calculated:

\[ 4\pi \int_0^\infty n(r) r^2 \, dr = 6. \]  

(6.6)

**Conclusion**

The closed-form analytic expressions for the wave function and binding energy of state 0+ of C-like ions of elements with Z=92 to Z=101 have been found with minimum approximation by the relativistic MACF method.

The method allows calculating the spectrum and WF levels differing in parity and moments in the form of bands with the given quantum numbers. There are limitations in the calculation of transitions between different levels of photoionization, ionization by an electron collision, etc., because at present time we have the wave functions and binding energies calculated only for several states.
The studied properties of C-like and other type ions of transuranium elements allow specifying the parameters of high-temperature plasma (several KeVs) of transuranium elements. Ions with few electrons prevail in such plasmas.

The matrix elements calculated will be used to carry out calculations for other ions of heavy elements.

The paper illustrates the presence of spurious states for the Dirac operator with Coulomb interaction, which occur owing to its unboundedness.

The developed method opens prospects for studying the effect of mixed configurations on the calculation of transition probabilities and also allows considering the process of exciting a nucleus due to electron transitions.

References

[1] Sadovoy A A and Ulyanov A S 2007 A new method to calculate properties of He-like ions of transuranium elements VANT Ser.: Theor. and Appl. Phys. 2–3 58
[2] Sadovoy A A and Ulyanov A S 2008 The electron density of highly ionized ions of transuranium elements VTSci. and Technol. Conf. «Youth in Science» (Sarov, Russia, 2007).
[3] Neznamov V P, Sadovoy A A and Ulyanov A S Calculation of matrix elements in the Foldy-Wouthuysen representation 2009 VANT Ser.: Theor. and Appl. Phys. 3 18
[4] Sadovoy A A and Ulyanov A S 2010 Studying the properties of He- and C-like ions of heavy elements using the analytical solution to the Dirac equation 15 N Novgorod session of young scientists. Proc. of young scientists in natural-science disciplines (N. Novgorod, Russia, 2010)
[5] Sadovoy A A and Ulyanov A S 2011 Some features of the few-electron Dirac equation and description of ions with high ionization degree. 16 N Novgorod session of young scientists. Proc. of young scientists in natural-science disciplines (N. Novgorod, Russia, 2011)
[6] Sadovoy A A 1994 The Multidimensional Angular Function Methods in Theoretical and Applied Physics (Arzamas-16: VNIEF Publishers)
[7] Sadovoy A A 2000 The Multidimensional Angular Coulomb Function Method in Atomic and Molecular Physics Few-Body Systems Suppl. 12 66
[8] Sadovoy A A and Ulyanov A S 2008 New methods to solve problems of few bodies in atomic, molecular and nuclear physics: A book of scientific papers ed A A Sadovoy (Sarov: FSUE «RFNC-VNIIEF»)
[9] Bete G 1965 Quantum mechanics (Moscow: Physmathgiz)
[10] Gradshtein I S and Ryshik I M 1963 Tables of integrals, sums, series and products (Moscow: Physmathgiz)
[11] Berestetsky V V, Lifshits E M and Pitayevsky A P 1968 Relativistic quantum theory P.1 (Moscow: Science)
[12] Desclaux J P Relativistic 1973 Dirac-Fock Expectation Values for Atoms with Z=1 to Z=120 Atomic Data and Nuclear Data Tables 12 N. 4 311
[13] Philippov A V, Povyshov V M, Sadovoy A A, Shevelko V P, Shirkov G D, Vasina E G and Vatulin V V 2002 Electron-impact ionization cross sections of Ti, Kr, Sn, Ta, U atoms and their ions in the electron energy range from the threshold up to 200 KeV. Part 2. JINR (Preprint E9-2002-5)
[14] Grant I P, McKentzie B J, Norrington P H, Mayers D F and Pyper N C 1980 An atomic multiconfiguration Dirac-Fock package Comp. Phys. Comm. 21 207
[15] Dyall K G, Grant I P, Johnson C T,Parpia F A and Plummer E P 1989 GRASP: A general-purpose relativistic atomic structure program Comp. Phys. Comm. 55 425