INTEGRAL–DIFFERENTIAL EQUATIONS FOR SEMI-RELATIVISTIC NUCLEAR SHELL MODEL

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In previous papers the relativistic corrections for the mass and potential energy to one-nucleon levels and the significant terms of the relativistic corrections for the mass of nucleons were obtained. In this paper the mathematical problems of semi-relativistic model are considered. The semi-relativistic single-particle equation is a differential equation of the fourth-order and it can be reduced to the integral–differential equations. The general solution of this equation must be expressed by the superposition of the four linearly independent solutions. Developing the modified method of Lagrange's and the multiplicative perturbation theory we obtained the integral–differential equations for the wave functions with usual asymptotic at the origin r^{L+1} and unusual r^{L+3}, r^{-L+2}. The wave functions with asymptotic at the origin r^{L+3} must be used when the singular realistic nuclear potentials are included.

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1. Introduction

Usually we consider the nuclei as the non-relativistic systems. We must take into consideration [1] that the nuclear force has a repulsive core (-0.4 fm) and a great spin–orbit interaction, which has the relativistic descent. The repulsive core is generating the wave functions with high momentum [1] and we cannot solve the task of the energy-spectra for nucleus without including relativistic corrections for mass of nucleons and potential [2]. The aim of our paper is to obtain the integral equations for the solutions of semi-relativistic equation.

We begin from the consideration of the semi-relativistic Hamiltonian for one-particle wave equation

$$H_r = H_m + \frac{\vec{p}^{\,2}}{2m} + H_\nu + V(r) + V_{sl}(r)\,. \tag{1.1}$$

The first term of Hamiltonian

$$H_m = -\frac{\vec{p}^{\,4}}{8m^3c^2} \tag{1.2}$$

and the third term of it

$$H_\nu = \frac{\hbar^2}{4m^2c^2}\left(\frac{d}{dr}V(r)\right)\frac{d}{dr} \tag{1.3}$$

include the relativistic corrections to the mass of nucleons and the potential of their interaction. The following term

$$V_{sl}(r) = -\kappa\frac{1}{r}\left(\frac{d}{dr}V(r)\right)\cdot(\vec{\sigma}\cdot\vec{l}\,) \tag{1.4}$$

is the spin–orbit potential which has also the relativistic origin. The semi-relativistic equation for the eigenfunction

$$R_\alpha = \frac{U_\alpha}{r} \tag{1.5}$$

can be obtained [2] from Hamiltonian (1.1) for the central potential $V(r)$, spin–orbit potential $V_{sl}(r)$ and model potential $V_1(r)$ in the form

$$\frac{d^2}{dr^2}U_\alpha - \frac{L(L+1)}{r^2}U_\alpha + C(E_\alpha - V_D - V_1(r))U_\alpha = 0\,, \tag{1.6}$$

$$V_D = V(r) + V_{sl}(r) - V_1(r) + \frac{C_1}{C}D(r) + C_1 r\left(\frac{d}{dr}V(r)\right)\frac{d}{dr}\frac{1}{r}\,, \tag{1.7}$$

$$\begin{aligned}
&C = \frac{2m}{\hbar^2}, \quad C_1 = \left(\frac{\hbar}{2mc}\right)^2, \qquad CC_1 = \frac{1}{2mc^2}\,,\\
&D(r) = \frac{d^4}{dr^4} - \frac{2L_0}{r^2}\frac{d^2}{dr^2} + \frac{4L_0}{r^3}\frac{d}{dr} + \frac{(L_0)^2 - 6L_0}{r^4}\,,\\
&L_0 = L(L+1)\,.
\end{aligned} \tag{1.8}$$

The fourth and the fifth terms in (1.7) represent the relativistic corrections for the mass of nucleons and potential. Substituting the asymptotic expression of the eigenfunction $U_\beta \cong r^\beta$ as $r \to 0$ in (1.6) we get four partial independent asymptotic solutions

$$U_{\beta 1} = r^{L+1}\,, \qquad U_{\beta 2} = r^{-L}\,, \qquad U_{\beta 3} = r^{L+3}\,, \quad U_{\beta 4} = r^{-L+2}\,. \tag{1.9}$$

Then a general solution of the fourth order linear differential equation can be expressed as a linear combination of these linear independent solutions

$$\begin{aligned} U_\alpha(r) \;=\; & \varphi_{\alpha 1}(r)U_{\beta 1}(r) + \varphi_{\alpha 2}(r)U_{\beta 2}(r) \\ & + \varphi_{\alpha 3}(r)U_{\beta 3}(r) + \varphi_{\alpha 4}(r)U_{\beta 4}(r)\,. \end{aligned} \tag{1.10}$$

The wave functions $U_{\alpha i} = \varphi_{\alpha i} U_{\beta i}$ with asymptotic $U_{\alpha 1} \cong r^{L+1}$ and singular solutions $U_{\alpha 2} \cong r^{-L}$ have different behavior at the origin for $r \to 0$ and are named as physical and nonphysical solutions [3] of radial Schrödinger equation. For the semi-relativistic equation (1.6) we obtained the complementary physical solutions $U_{\alpha 3} \cong R^{L+3}$ for $L = 0, 1, 2, \ldots$. For the quantum numbers $L = 0$ and $L = 1$ of the orbital angular momentum we have regular physical solution $U_{\alpha 4} \cong r^{-L+2}$ at the origin.

Assuming that the potential energies $V(r)$ and $V_{sl}(r)$ vanish at great distances, we can find the asymptotic expression of differential equation (1.6)

$$C_1 \frac{d^4}{dr^4} U_\alpha(r) + \frac{d^2}{dr^2} U_\alpha(r) + C E_\alpha U_\alpha(r) = 0 \tag{1.11}$$

and the following four asymptotic solutions of (1.6) in the exponential form $U_\alpha \cong \mathrm{e}^{k_\alpha r}$. In this case we get

$$\begin{aligned} & k_{\alpha 1} = -k_\alpha,\; k_{\alpha 2} = k_\alpha,\; k_\alpha = \frac{1}{\sqrt{2C_1}}\big(-1 + \sqrt{1 - 4C_1 C E_\alpha}\big)^{1/2}, \\ & k_{\alpha 3} = i k_{\alpha m},\; k_{\alpha 4} = k_{\alpha m},\; k_{\alpha m} = \frac{1}{\sqrt{2C_1}}\big(1 + \sqrt{1 - 4C_1 C E_\alpha}\big)^{1/2}\,. \end{aligned} \tag{1.12}$$

Usually $4C_1 C E_\alpha < 1$ and we can use for bound states the approximate expression $k_\alpha \approx \sqrt{-CE_\alpha}$. Taking into account (1.12) we see that the energies for the semi-relativistic k_α represent the more tightly bounded nucleons. The semi-relativistic bound energies of the nucleons are larger than the bound energies in the non-relativistic case [2]. The partial solutions of (1.6) can be expressed in the following form:

$$U_{\alpha i} = \varphi_{\alpha i} r^{\beta(i)}\,, \qquad i = 1, 2, 3, 4. \tag{1.13}$$

2. The solutions of the integral–differential semi-relativistic equation for the singular potentials

The integral–differential semi-relativistic equation (1.6) was considered in [2] like some perturbation of the Schrödinger equation. The semi-relativistic solutions represent more tightly bounded nucleons and are decreasing at infinity more fast than the solutions of the Schrödinger equation. This fact is important in consideration of stability of nucleons shells for the super-heavy nuclei. For the semi-relativistic equation at the origin we have three kinds of different physical solutions $U_{\alpha 1}$, $U_{\alpha 3}$, $U_{\alpha 4}$ when for the Schrödinger equation we have only one — $U_{\alpha 1}$.

The semi-relativistic solutions $U_{\alpha 1}$ can be used for non-singular or for singular potentials which behave at the origin like $r^{-\gamma}$ where $0 < \gamma < 2$. The solutions $U_{\alpha 1}$ of the first kind of equation (1.6) can be used for Coulomb, Yukawa, Woods–Saxon and spin–orbit potentials [1] for average field of nucleus. These potentials have the asymptotic r^{-1} at the origin and semi-relativistic solutions with asymptotic r^{L+1} are similar to the wave functions of the Schrödinger equation. Also in the semi-relativistic approach [2] we have the non-physical solutions $U_{\alpha 2}$ with the behavior at the origin like r^{-L}. We can use the second physical semi-relativistic solution $U_{\alpha 3}$ where the singular potentials [1] with the singularity r^{-3} can be included because the last term in (1.8) of semi-relativistic equation (1.6) has the asymptotic r^{-4} at the origin. Using solutions $U_{\alpha 1}$, $U_{\alpha 3}$ we can find the expectation values for all terms of the realistic Hamada–Johnston potential [1], which has singularity r^{-6}. Introducing a dimensionless parameter $\rho = r/F$ in the radial semi-relativistic equation (1.6) with (1.7), (1.8) we obtain [2]

$$\begin{aligned} & C_F D(\rho) U_\alpha + C_F C \rho \Big(\frac{d}{dr} V\Big) \frac{d}{d\rho} \frac{U_\alpha}{\rho} + \frac{d^2}{d\rho^2} U_\alpha \\ & - \frac{L_0}{\rho^2} U_\alpha + C F^2 (E_\alpha - V) U_\alpha = 0, \\ D(\rho) &= \frac{d^4}{d\rho^4} - \frac{2L_0}{\rho^2} \frac{d^2}{d\rho^2} + \frac{4L_0}{\rho^3} \frac{d}{d\rho} + \frac{(L_0)^2 - 6L_0}{\rho^4}, \\ L_0 &= L(L+1), \qquad C_F = \frac{C_1}{F^2}, \qquad C_2 = C_1 C. \end{aligned} \tag{2.1}$$

Now we can see that for large F the semi-relativistic equation (2.1) reduces into the Schrodinger equation. For the nucleons localized around the center of force about 1 fm we have $C_F = 0.011$. In the region of repulsive core (0.4 fm) $C_F = 0.07$. For the electrons in the first Bohr orbit $C_F = 1.3 \times 10^{-5}$. These results show that in the theory of atomic spectroscopy we can calculate the relativistic corrections with the sufficient accuracy in the first approximation of the perturbation theory [2]. But for calculations of the nuclear energy levels or consideration of the bound quark–antiquark systems we must include the higher order perturbations and all solutions $U_{\alpha 1}$, $U_{\alpha 3}$ and $U_{\alpha 4}$ of semi-relativistic equation (1.6) must be used.

3. The system of integral semi-relativistic equations

General solutions of the Schrödinger equation in the potential representation can be presented in the form of integral equations [3]. In this representation the one-particle wave functions are expressed as a product of the unperturbed solution and the function, which depends on the perturbation potential. This method was used [2] in semi-relativistic equation for the one-particle case for calculations of relativistic corrections in the average field of neutron and proton shells. Now we can generalize this method for the differential equation (2.1) of the fourth order

$$p_0 U_\alpha^{(4)} + p_2 U_\alpha^{(2)} + p_3 U_\alpha^{(1)} + p_4 U_\alpha = q_\alpha(\rho), \quad U_\alpha^{(n)} = \frac{d^n U_\alpha(\rho)}{d\rho^n}, \tag{3.1}$$

where comparing the last equation with (1.6), (2.1) we have

$$\begin{aligned} p_0 &= C_F\,, \qquad\qquad p_2 = -C_F \frac{2L_0}{r^2}\,, \\ p_3 &= C_F \frac{4L_0}{r^3}\,, \qquad p_4 = C_F \frac{(L_0)^2 - 6L_0}{r^4}\,, \end{aligned} \tag{3.2}$$

$$\begin{aligned} q_\alpha(\rho) &= -C_F C\rho(\frac{d}{d\rho}V)\frac{d}{d\rho}\frac{U_\alpha}{\rho} - \frac{d^2}{d\rho^2}U_\alpha \\ &+ \frac{L_0}{\rho^2}U_\alpha - CF^2(E_\alpha - V)U_\alpha\,. \end{aligned} \tag{3.3}$$

Without the right-hand side of the equation (3.1) it becomes the homogeneous equation, which solutions coincide with (1.9). Using the multiplicative perturbation theory considered in papers [3–5] and taking into the care that zero approximation or unperturbed solutions (1.9) coincide with exact partial solutions (1.9) of the inhomogeneous equation (2.1) only at the origin when $\rho \to 0$ it will be better if the first approximation of the perturbed solution (1.13) will be close to the exact solution of the inhomogeneous equation (2.1) in all interval $0 \le \rho \le \infty$. In order to get the single-nucleon levels the model harmonic oscillator potential can be used [2]

$$V_1(r) = \frac{m\omega^2 r^2}{2} \tag{3.4}$$

for average field of the nucleus. The radial wave functions and singular nonphysical solutions [2] for the model potential (3.4)

$$U_{nL,i} = \mathrm{e}^{-0.5\rho^2}\rho^{\beta(i)}\sum_{k=0}^{n-1} a_k\rho^{2k} \quad \text{and} \quad F_{nL,i} = \mathrm{e}^{-0.5\rho^2}\rho^{\gamma(i)}\sum_{k=0}^{\infty} b_k\rho^{2k}, \quad (3.5)$$

where

$$\begin{aligned}
\rho^2 &= \frac{r^2}{F^2}, \quad F = \sqrt{\frac{\hbar}{m\omega}}, \; n = 1,2,3,\dots, \\
\beta(i) &= -L+2, \quad L \le 1, \quad \beta(i) = L+1, L+3, \; L = 0,1,2,\dots, \\
\gamma(i) &= -L, \quad L = 0,1,2,\dots, \quad \gamma(i) = -L+2, \quad L \ge 2, \quad i = 1,3,4, \\
a_0 &= 1, \quad a_{k+1} = \frac{k - 0.5(\varepsilon_{nL,i} - \beta(i) - 0.5)}{(k+1)(k+\beta(i)+0.5)} a_k, \\
b_0 &= 1, \quad b_{k+1} = \frac{k - 0.5(\varepsilon_{nL,i} - \gamma(i) - 0.5)}{(k+1)(k+\gamma(i)+0.5)} b_k,
\end{aligned}$$

of Schrödinger equation

$$\frac{d^2}{d\rho^2}U_\alpha - \frac{L(L+1)}{\rho^2}U_\alpha - CF^2(E_{nL,i} - V_1)U_\alpha = 0. \quad (3.6)$$

These wave functions have the following eigenvalues

$$E_{nL,i} = \varepsilon_{nL,i}\hbar\omega, \quad \varepsilon_{nL,i} = 2n + \beta(i) - \frac{3}{2}, \quad n = 1,2,3,\dots \quad (3.7)$$

for $\beta(1) = L+1$, $\beta(3) = L+3$, $L = 0,1,2,3,\dots$, $\beta(4) = -L+2$, $L = 0,1$.

Requiring that partial solutions (1.10) must satisfy the following boundary conditions at the origin

$$\begin{aligned}
&\lim_{\rho\to 0} U_{\alpha 1}\cdot\rho^{-L-1} = 1, \qquad \lim_{\rho\to 0} U_{\alpha 2}\cdot\rho^{L} = 1, \\
&\lim_{\rho\to 0} U_{\alpha 3}\cdot\rho^{-L-3} = 1, \qquad \lim_{\rho\to 0} U_{\alpha 4}\cdot\rho^{L-2} = 1,
\end{aligned} \quad (3.8)$$

and at infinity

$$\begin{aligned}
&\lim_{\rho\to\infty} \varphi_{\alpha 1}\cdot\rho^{L+1} = 0, \qquad \lim_{\rho\to\infty} \varphi_{\alpha 2}\cdot\rho^{-L} = \infty, \\
&\lim_{\rho\to\infty} \varphi_{\alpha 3}\cdot\rho^{L+3} = 0, \qquad \lim_{\rho\to\infty} \varphi_{\alpha 4}\cdot\rho^{-L+2} = 0.
\end{aligned} \quad (3.9)$$

Using the method of undefinited coefficients [6] the following integral equations for the partial physical solutions, we obtained of the linearly independent solutions (3.8) with Wronskian

$$W = -64L^4 - 128L^3 - 32L^2 + 32L + 12.$$

Taking into account this fact and denoting

$$d_1 = \frac{8L^2+16L+6}{W}\,, \quad d_2 = \frac{8L^2-2}{W}\,, \quad d_3 = -d_2\,, \quad d_4 = -d_1\,,$$

$$I_{1,\infty} = \int\limits_{\rho}^{\infty} \rho^{-L+2} q_\alpha d\rho\,, \quad I_{2,0} = \int\limits_{0}^{\rho} \rho^{L+3} q_\alpha d\rho\,, \quad I_{2,\infty} = \int\limits_{\rho}^{\infty} \rho^{L+3} q_\alpha d\rho\,,$$

$$I_{3,0} = \int\limits_{0}^{r} \rho^{-L} q_\alpha d\rho, \quad I_{3,\infty} = \int\limits_{\rho}^{\infty} \rho^{-L} q_\alpha d\rho\,,$$

$$I_{4,0} = \int\limits_{0}^{\rho} \rho^{L+1} q_\alpha d\rho\,, \quad I_{4,\infty}(L=0,1) = \int\limits_{\rho}^{\infty} \rho^{L+1} q_\alpha d\rho\,,$$

$$I_{1,0,\infty} = \int\limits_{0}^{\infty} \rho^{-L+2} q_\alpha d\rho\,, \quad I_{3,0,\infty} = \int\limits_{0}^{\infty} \rho^{-L} q_\alpha d\rho\,, \quad I_{4,0,\infty} = \int\limits_{0}^{\infty} \rho^{L+1} q_\alpha d\rho\,,$$

we obtained for $L = 0, 1, 2, 3, \ldots$

$$\begin{aligned} \varphi_{\alpha 1}\rho^{L+1} &= \rho^{L+1}\frac{I_{1,\infty}}{I_{1,0,\infty}} + \rho^{-L}\frac{d_2 I_{2,0}}{d_1 I_{1,0,\infty}} \\ &\quad + \rho^{L+3}\frac{d_3 I_{3,\infty}}{d_1 I_{1,0,\infty}} + \rho^{-L+2}\frac{d_4 I_{4,\infty}}{d_1 I_{1,0,\infty}}\,,\ (L=0,1)\,, \qquad (3.10) \\ &\quad I_{4,\infty} \to I_{4,0} \quad \text{when} \quad L = 2, 3, \ldots; \\ \varphi_{\alpha 2}\rho^{-L} &= \rho^{-L} + d_2\rho^{-L} I_{2,\infty} + d_1\rho^{L+1} I_{1,\infty} \\ &\quad + d_3\rho^{L+3} I_{3,0} + d_4\rho^{-L+2} I_{4,0}\,; \qquad (3.11) \\ \varphi_{\alpha 3}\rho^{L+3} &= \rho^{L+3}\frac{I_{3,\infty}}{I_{3,0,\infty}} + \rho^{L+1}\frac{d_1 I_{1,\infty}}{d_3 I_{3,0,\infty}} \\ &\quad + \rho^{-L}\frac{d_2 I_{2,0}}{d_3 I_{3,0,\infty}} + \rho^{-L+2}\frac{d_4 I_{4,\infty}}{d_3 I_{3,0,\infty}}\,,\ (L=0,1)\,, \qquad (3.12) \\ &\quad I_{4,\infty} \to I_{4,0} \quad \text{when} \quad L = 2, 3, \ldots; \\ \varphi_{\alpha 4}\rho^{-L+2} &= \rho^{-L+2}\cdot\delta + d_4\rho^{-L+2} I_{4,\infty} + d_1\rho^{L+1} I_{1,\infty} \\ &\quad + d_2\rho^{-L} I_{2,0} + d_3\rho^{L+3} I_{3,\infty}\,, \quad \delta = 0, L \le 1\,, \qquad (3.13) \end{aligned}$$

$\delta = 1,\ L \ge 2$, then

$$I_{4,\infty} \to \frac{I_{4,\infty}}{d_4 I_{4,0,\infty}}\,, \qquad I_{1,\infty} \to \frac{I_{1,\infty}}{d_4 I_{4,0,\infty}}\,,$$
$$I_{2,0} \to \frac{I_{2,0}}{d_4 I_{4,0,\infty}}\,, \qquad I_{3,\infty} \to \frac{I_{3,\infty}}{d_4 I_{4,0,\infty}}\,.$$

When $L = 2, 3, 4, \ldots$ in equations (3.10), (3.12) instead $I_{4,\infty}$ we use $I_{4,0}$ (denoting $I_{4,\infty} \to I_{4,0}$) and in this case only two physical solutions $U_{\alpha 1} = \varphi_{\alpha 1}\rho^{L+1}$ and $U_{\alpha 3} = \varphi_{\alpha 3}\rho^{L+3}$ remain.

The nonphysical singular at the origin solutions $\varphi_{\alpha 2}\rho^{-L}$ have the eigenvalues, which coincide with the eigenvalues for the wave functions $\varphi_{\alpha 1}\rho^{L+1}$. The first approximation of $\varphi_{\alpha 2}\rho^{-L}$ must coincide with F_{nL} in (3.6).

From the boundary conditions at infinity (3.9) and integral–differential equations (3.10), (3.12), (3.13) we can obtain three different sets of eigenvalues of semi-relativistic equation for different physical solutions with $L = 0, 1$ and $i = 1, 3, 4$

$$\begin{aligned} \triangle E_{nLj,i} &= \frac{\int_0^\infty \rho^{L+3}(q_{\alpha i} - (V - V_1))U_{\alpha i} d\rho}{\int_0^\infty \rho^{L+3} U_{\alpha i} d\rho}, \\ E_{nLj,i} &= E_{nL,i} + \triangle E_{nL,i}, \quad j = L \pm \frac{1}{2}. \end{aligned} \tag{3.14}$$

For $L = 2, 3, 4, \ldots$ and $i = 1, 3$ we have only two sets of physical solutions and two sets of the eigenvalues

$$\triangle E_{nLj,i} = \frac{\int_0^\infty \rho^{L+1}(q_{\alpha i} - (V - V_1))U_{\alpha i} d\rho}{\int_0^\infty \rho^{L+1} U_{\alpha i} d\rho}. \tag{3.15}$$

We must solve simultaneously equations (3.10), (3.12), (3.13) and (3.14), (3.15) taking for the first iteration $E_\alpha = E_{nL,i}$ and $U_{\alpha i} = U_{nL,i}$ from (3.7) and (3.5). This approach was successfully used in [2] for the Woods–Saxon potential and the results of high accuracy were obtained using the small number of iterations.

4. Conclusions

In this paper we presented three different sets of physical solutions of semi-relativistic equation with different asymptotic at the origin. The semi-relativistic model in the single-particle approach was considered and the integral equations for the singular realistic nucleon–nucleon potentials were obtained. The important relativistic corrections for mass of nucleons in the obtained integral equations are exactly included. Using results presented in [7], where relativistic corrections in the modified Hartree–Fock terms were included only approximately, the obtained integral equations can be similarly transformed including the exact Hartree–Fock terms for the consideration of energy levels of nucleus and bound quark–antiquark systems [1]. The obtained integral equations can be used for the consideration of stability of protons and neutrons shells of super heavy nucleus where relativistic effects also are important [8].

REFERENCES

[1] K.L.G. Heyde, *The Nuclear Shell Model*, Springer-Verlag, Berlin 1994, p. 438.

[2] A.J. Janavičius, *Acta Phys. Pol. B* **27**, 2195 (1996).

[3] A.J. Janavičius, *Lith. J. Phys.* **38**, 431 (1998).

[4] A.J. Janavičius, D. Jurgaitis, *Lithuanian Phys. Collection*, **25**, 33, (1985), in Russian.

[5] A.J. Janawiczius, R. Planeta, Comon solution of Schrodinger equation in potential representation, Krakow, Raport No 1018/PL, 1978, p. 13, in Russian.

[6] R.S. Guter, A.R. Janploski, Differential equations, High School, Moscow, 1976, p. 304, in Russian.

[7] A.J. Janavičius, R. Bagdonaitė, *Lith. J. Phys.* **41**, No 3, 150 (2001).

[8] A.J. Janavičius, *Lith. J. Phys.* **41**, No. 3, 232 (2001).