RELATIVISTIC CORRECTIONS TO THE ONE-NUCLEON ENERGY LEVELS OF ^{208}Pb

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We have calculated relativistic corrections to one-nucleon levels of ^{208}Pb in the first approximation of the perturbation theory for the mass and potential energy in the Woods–Saxon potential case. We have obtained corrections for the mass increase for the large principal or orbital quantum numbers. The corrections for the mass in the state $1s_{1/2}$ are -0.0087 MeV for neutrons and -0.0097 MeV for protons. Corrections -0.6788 MeV for neutrons and -0.5884 MeV for protons for the excited states $1j_{15/2}$ and $1i_{13/2}$ are comparable with the energy of these levels. Corrections for the potential stay small for all states. Including the relativistic corrections for mass we have obtained a better correlation between theoretical and experimental levels of energy for the excited states.

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1. Introduction

For calculation of the energy levels of nuclei, the nonrelativistic Hartree-Fock equations with spin-orbit potential and effective interaction are used. According to [1], Vautherin and Brink introduced effective mass and Skyrme's forces that have improved this method. The same result was obtained from Dirac equation [1] taking into account that the binding energy E of one-particle states of nuclei is less than the rest energy M. From that premise for central potential case $U(r)$ they have obtained equations

$$\chi = \frac{1}{2M(r)}\vec{\sigma}\vec{p}\varphi\,, \tag{1.1}$$

$$E\varphi = \left[\vec{p}\frac{1}{2M(r)}\vec{p} + U(r) + \frac{1}{r}\frac{d}{dr}\left(\frac{1}{2M(r)}\right)\vec{l}\vec{\sigma}\right]\varphi\,, \tag{1.2}$$

for large φ and small χ components of the bispinor. Here $M(r)$ is the effective mass. It was obtained that inside a nucleus $M(r)/M = 0.6$. One usually assumes that in the shell-model $M(r) = M$ but this is not exact, because mass of the nucleons depends on the state.

Binding energy composes of only one per cent of the rest energy. If we calculate one per cent from the expectation value of the kinetic energy we will get a significant value. The relativistic energy corrections for mass to the harmonic oscillator potential of the nucleus ^{197}Au [2] reach −0.4 MeV. In this paper the relativistic corrections for Woods–Saxon potential were obtained for all bound neutrons and protons states of the nucleus ^{208}Pb.

2. Semi-relativistic equation

According to [3] the semi-relativistic Hamiltonian can be written in the form

$$\hat{H}_r = \hat{H}_m + \frac{\hat{p}^2}{2m} + \hat{H}_V + V(r) + V_{sl}(r)\,. \tag{2.1}$$

The first term of the Hamiltonian

$$\hat{H}_m = -\frac{\hat{p}^4}{8m^3c^2} \tag{2.2}$$

and the third term

$$\hat{H}_V = -\frac{\hbar^2}{4m^2c^2}\frac{dV(r)}{dr}\frac{d}{dr} \tag{2.3}$$

include relativistic corrections for the mass and the potential. The term $V_{sl}(r)$ is the spin-orbital potential

$$V_{sl}(r) = -\kappa\frac{1}{r}\frac{dV(r)}{dr}\left(\vec{s}\,\vec{l}\right)\,. \tag{2.4}$$

The magnitude of this potential κ is found by comparison with the experiments. In the paper [2] as in this paper the magnitude of the relativistic corrections for mass depends on the principal and orbital quantum numbers. These corrections were obtained of the same order as the spin-orbit interactions. Consequently, the determination of κ without taking into account the relativistic corrections for mass will be inexact. According to the operator identity $\hat{p}^2 = 2m\hat{T}$, where $\hat{T}$ is the kinetic energy operator from (2.2), we obtain

$$\hat{H}_m = -\frac{\hbar^4}{8m^3c^2}\left[\frac{d^4}{dr^4} + \frac{4}{r}\frac{d^3}{dr^3} - \frac{\hat{L}^2}{\hbar^2}\left(\frac{2}{r^2}\frac{d^2}{dr^2} + \frac{2}{r^4}\right) + \frac{\hat{L}^4}{\hbar^4}\frac{1}{r^2}\right]\,. \tag{2.5}$$

We take the semi-relativistic equation for the Hamiltonian (2.1) and for the eigenfunction $R_\alpha = U_\alpha/r$ in the central forces case we obtain the equation

$$c_1\left[\frac{d^4U_\alpha}{dr^4}+\left(\frac{1}{c_1}-\frac{2l(l+1)}{r^2}\right)\frac{d^2U_\alpha}{dr^2}+\frac{4l(l+1)}{r^3}\frac{dU_\alpha}{dr}\right.$$
$$\left.+\left(\frac{l^2(l+1)^2-6l(l+1)}{r^4}-\frac{l(l+1)}{c_1r^2}\right)U_\alpha\right]+c_2r\frac{dV(r)}{dr}\frac{d}{dr}\frac{U_\alpha}{r}$$
$$-c_0V(r)U_\alpha-c_0V_{sl}(r)U_\alpha-c_0E_\alpha U_\alpha=0\,,$$
$$c_0=\frac{2m}{\hbar^2}\,,\qquad c_1=\left(\frac{\hbar}{2mc}\right)^2\,,\qquad c_2=\frac{1}{2mc^2}\,. \tag{2.6}$$

Substituting asymptotic expression of the eigenfunction $U_\alpha \simeq r^{\beta_\alpha}$ as $r \to 0$ in (2.6) we get

$$\beta_1=l+1\,,\qquad \beta_2=-l\,,\qquad \beta_3=l+3\,,\qquad \beta_4=-l+2\,. \tag{2.7}$$

In this way we obtain the usual behaviour $U_\alpha \sim r^{l+1}$ and unusual one $U_U \sim r^{l+3}$ at the origin. In this case the relativistic corrections may be calculated in the first approximation

$$E_m=\int_0^\infty U_\alpha \hat{H}_m U_\alpha dr\,, \tag{2.8}$$

$$E_V=\int_0^\infty U_\alpha \hat{H}_V U_\alpha dr\,. \tag{2.9}$$

The matrix element for relativistic corrections of mass may be expressed as [4]:

$$E_m=-\frac{\hbar^4}{8m^3c^2}\left\{\int_0^\infty\left(\frac{d^2U_{nlj}(r)}{dr^2}\right)^2dr+2l(l+1)\int_0^\infty r^{-2}\left(\frac{dU_{nlj}(r)}{dr}\right)^2dr\right.$$
$$\left.+\,l(l+1)(l^2+l-6)\int_0^\infty r^{-4}U_{nlj}^2(r)dr\right\}\,. \tag{2.10}$$

3. The method of calculation and results

Schrödinger's equation may be solved by the discretization method [5]:

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + \rho(r_i)u_i = \lambda u_i \,, \tag{3.1}$$

$$\lambda = -bE, \qquad i = 0, 1, \ldots, n, \qquad h = \frac{C}{n},$$

with the boundary conditions $u(0) = u(C) = 0$. We get eigenfunctions and eigenvalues solving the system of this equations with the programme EIGEN [6].

The programme of numerical differentiation was formed according to the scheme of six points [7]

$$\left.\frac{d^k f}{dx^k}\right|_{x=\xi} = \sum_{i=0}^{5} C_i f(x_i) + 0\left(h^6 f^{(6)}\right), \quad 1 \le k \le 5 \,. \tag{3.2}$$

The proposed method allows one to calculate the derivatives up to the fifth order.

The doubly magic ^{208}Pb nucleus is one of the best cases for studying the matrix elements for the residual two body interactions in the nuclear shell-model calculations and the simple one-nucleon energy level schemes in ^{209}Pb, ^{207}Pb, ^{207}Tl, ^{209}Bi [8].

The energies of the neutrons and protons levels E_{nlj}, expectation values of potential energies V_{nlj}, relativistic corrections for mass E_m and for potential E_V of ^{208}Pb were calculated for the Woods-Saxon potential

$$V_{\mathrm{S}}(r) = -V_0^{N,Z}\left[1 + \exp\{\alpha^{N,Z}(r - R)\}\right]^{-1} \tag{3.3}$$

and spin-orbit potential (2.4) with parameters [8, 9] $V_0^N = 44$ MeV, $V_0^Z = 60.3$ MeV, $\alpha^N = \alpha^Z = 1.5124\ \mathrm{fm}^{-1}$, $R = 1.27\ \mathrm{A}^{1/3}$ fm, $\kappa = 0.353\ \mathrm{fm}^2$. The Coulomb potential was introduced in the usual form [8]

$$V_{\mathrm{C}}(r) = \frac{(Z-1)e^2}{4\pi\varepsilon_0 r}\begin{cases} \frac{3}{2}\frac{r}{R} - \frac{1}{2}\left(\frac{r}{R}\right)^3, & r \le R, \\ 1, & r > R. \end{cases} \tag{3.4}$$

The obtained results for neutrons and for protons are presented in Table I and Table II. Instead of V_{nlj} the kinetic energy $E_k = E_{nlj} - V_{nlj}$ is presented.

TABLE I

The neutrons levels and relativistic corrections for ^{208}Pb

nlj	E_{nlj} MeV	E_k MeV	E_m MeV	$E_{nlj}+E_m$ MeV	E_{ex} MeV	E_V MeV
$3d_{3/2}$	−0.6957	21.01	−0.48340	−1.179	−1.34	−0.008
$2g_{7/2}$	−0.7670	25.62	−0.56160	−1.329	−1.39	0.004
$4s_{1/2}$	−1.4250	20.57	−0.39470	−1.820	−1.83	−0.010
$3d_{5/2}$	−1.9730	24.75	−0.53100	−2.504	−2.30	−0.007
$1j_{15/2}$	−1.9110	38.14	−0.67880	−2.681	−2.45	0.024
$1i_{11/2}$	−3.1590	30.46	−0.48420	−3.643	−3.09	0.032
$2g_{9/2}$	−3.8030	29.76	−0.56430	−4.367	−3.86	0.003
$3p_{1/2}$	−7.4710	24.18	−0.02950	−7.501	−7.36	0.004
$2f_{5/2}$	−8.1320	24.56	−0.22810	−8.360	−7.93	0.012
$3p_{3/2}$	−8.3700	25.18	−0.03600	−8.405	−8.25	0.003
$1i_{13/2}$	−8.6170	32.20	−0.56630	−9.183	−9.00	0.025
$2f_{7/2}$	−10.4200	26.27	−0.43890	−10.860	−10.30	0.010
$1h_{9/2}$	−10.9300	24.12	−0.41280	−11.340	−10.80	0.023
$1h_{11/2}$	−14.9300	25.58	−0.34690	−15.280	–	0.024
$3s_{1/2}$	−15.3800	21.66	−0.29430	−15.670	–	0.012
$2d_{3/2}$	−15.5600	20.94	−0.33670	−15.900	–	0.015
$2d_{5/2}$	−17.0100	21.68	−0.31290	−17.320	–	0.014
$1g_{7/2}$	−18.2100	19.37	−0.26530	−18.470	–	0.020
$1g_{9/2}$	−20.9400	20.17	−0.22560	−21.160	–	0.022
$2p_{1/2}$	−22.7000	16.48	0.00180	−22.700	–	0.015
$2p_{3/2}$	−23.4200	16.74	−0.00200	−23.420	–	0.015
$1f_{5/2}$	−24.8400	14.74	−0.15510	−24.990	–	0.017
$1f_{7/2}$	−26.5300	15.14	−0.13490	−26.660	–	0.019
$2s_{1/2}$	−29.5600	11.78	−0.08510	−29.650	–	0.014
$1d_{3/2}$	−30.7200	10.43	−0.08090	−30.800	–	0.013
$1d_{5/2}$	−31.6100	10.62	−0.07225	−31.680	–	0.015
$1p_{1/2}$	−35.7700	6.59	0.00250	−35.770	–	0.009
$1p_{3/2}$	−36.1300	6.66	0.00120	−36.130	–	0.010
$1s_{1/2}$	−39.9700	3.35	−0.00860	−39.980	–	0.005

TABLE II

The protons levels and relativistic corrections for ^{208}Pb

nlj	E_{nlj} MeV	E_k MeV	E_m MeV	$E_{nlj}+E_m$ MeV	E_{ex} MeV	E_V MeV
$3p_{3/2}$	−0.2865	28.37	−0.0595	−0.346	−0.62	0.017
$2f_{5/2}$	−0.0475	27.12	−0.5744	−0.622	−0.92	0.028
$1i_{13/2}$	−2.7190	34.64	−0.5884	−3.307	−2.15	0.050
$2f_{7/2}$	−3.2200	34.64	−0.5227	−3.743	−2.86	0.026
$1h_{9/2}$	−3.7810	25.91	−0.4940	−4.275	−3.76	0.040
$3s_{1/2}$	−7.8550	23.72	−0.3474	−8.202	−8.97	0.024
$2d_{3/2}$	−8.1620	22.69	−0.3965	−8.558	−9.32	0.029
$1h_{11/2}$	−9.3620	28.06	−0.4014	−9.763	−10.31	0.047
$2d_{5/2}$	−10.1500	23.65	−0.3618	−10.510	−10.64	0.028
$1g_{7/2}$	−11.6900	20.56	−0.3104	−12.000	−12.45	0.034
$1g_{9/2}$	−15.5500	21.90	−0.2967	−15.810	–	0.041
$2p_{1/2}$	−15.8300	17.62	−0.0097	−15.840	–	0.026
$2p_{3/2}$	−16.8200	17.99	−0.0157	−16.830	–	0.027
$1f_{5/2}$	−18.7900	15.45	−0.1773	−18.970	–	0.028
$1f_{7/2}$	−21.2400	16.24	−0.1300	−21.380	–	0.024
$2s_{1/2}$	−23.1300	12.49	−0.0952	−23.220	–	0.021
$1d_{3/2}$	−24.9700	10.77	−0.0898	−25.060	–	0.021
$1d_{5/2}$	−26.3200	11.20	−0.0787	−26.400	–	0.025
$1p_{1/2}$	−30.1100	6.66	−0.0045	−30.110	–	0.014
$1p_{3/2}$	−30.6900	6.85	−0.0061	−30.700	–	0.017
$1s_{1/2}$	−34.1500	3.32	−0.0097	−34.160	–	0.008

The calculated energy levels E_{nlj} for neutrons coincide with the results in [8]. We have obtained better coincidence with experimental levels for protons with $V_0^Z = 60.3$ MeV [9]. The inclusion of the relativistic corrections for the mass improves the results for all excited states of neutrons and $3p_{3/2}$, $2f_{5/2}$, $3s_{1/2}$, $2d_{3/2}$, $1h_{11/2}$, $2d_{5/2}$, $1g_{7/2}$ states of protons for ^{208}Pb. The energy for excited levels are the sum of the expectation values of the kinetic and potential energies. The magnitudes of them can achieve up to 40 MeV and have opposite signs. In that case the small variation of expectation values of the kinetic energies give relative significant exchange of the energy for excited levels.

In our case the insignificant relativistic corrections for potential energy of neutrons do not exceed 0.03 MeV and for protons are less than 0.05 MeV for all states.

4. Conclusions

The corrections for the mass increase when expectation values of the kinetic energies of neutrons and protons are increasing. The biggest corrections for mass for neutrons in the state $1j_{15/2}$ are -0.6788 MeV and for protons in the state $1i_{13/2}$ -0.5884 MeV. These are for greatest expectation value of kinetic energies 38.14 MeV and 34.64 MeV. But there is no clear bond between these physical quantities. For example, the relativistic corrections for mass of neutrons for upper filled state $3p_{1/2}$ is -0.0295 MeV and for state $1h_{9/2}$ is -0.4128 MeV, but the expectation value of kinetic energy is almost the same — 24.1 MeV. Consequently the relativistic corrections for mass depend not only on expectation value of kinetic energy but also on the potential. In the case of states $1s_{1/2}$, $1p_{3/2}$, $1p_{1/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$ the magnitudes of corrections for mass are insignificant for neutrons and protons.

The obtained results show that it is impossible to calculate the energies of the single-particle states without taking into account the relativistic corrections for mass. But we must solve the equation (2.6) if we want to get the exact values of energy levels.

This paper used the programme of high numerical accuracy for differentiation not only in the middle interval but also on the boundary. Without this programme it is impossible to calculate relativistic corrections for mass (2.10) with sufficient accuracy.

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