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Investigation of Ground State Nuclear Structure Features of ^{238}U Nuclei by Using Skyrme-Hartree-Fock Method

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ABSTRACT

In this study, the ground state properties of the ^{238}U nucleus were investigated using a phenomenological potential Skyrme-force. The nuclear structure properties were calculated using the nuclear calculation code "HAFOMN" and the computer code "HFBRAD", which can calculate with the Hartree-Fock method and the Hartree-Fock-Bogoliubov method. In this investigation, many Skyrme force parameters were used, among which the S6 and SKX parameter sets were successful. Equidistant radial grids named N-grid and R-step in the "HAFOMN" nuclear program code are scanned with 0.05 steps, N-Grid from 50 to 200 and R-step from 0.05 to 1. As a result of this scan, the nuclear charge radius of the ^{238}U nucleus was obtained exactly as the value in the literature (5.8571 fm) when the S6 Skyrme parameter was used. The most suitable value for the total binding energy was obtained experimentally in the SKM parameter set. It has been observed that the calculations of S6 and SKM Skyrme-force parameters obtained with SHF and SHFB provide very successful predictions when compared with the experimentally determined values.

Keywords: *^{238}U, Skyrme Force, Hartree-Fock, RMS radii, Binding Energy*

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Introduction

Uranium is a naturally occurring actinide element with atomic number 92, found in nature primarily as three isotopes: uranium-238 (U-238), uranium-235 (U-235), and uranium-234 (U-234). Among these, U-238 is the most abundant, constituting about 99.3% of natural uranium, while U-235 accounts for roughly 0.7% and U-234 exists only in trace amounts. These isotopes are radioactive and differ in their nuclear stability, with U-238 having a half-life of approximately 4.5 billion years and U-235 about 704 million years. Due to its fissile nature, U-235 plays a crucial role in reactor physics and nuclear energy production, as it can sustain a self-propagating chain reaction. In contrast, U-238 is not fissile with thermal neutrons but is fertile: it can undergo neutron capture to form uranium-239 (^{239}U), which subsequently undergoes β^- decays to produce plutonium-239 (^{239}Pu), a fissile material. Therefore, although U-238 cannot by itself sustain a chain reaction under thermal conditions, it remains strategically important in the nuclear fuel cycle by serving as a fertile precursor for secondary fissile isotopes.

In addition to these isotopic characteristics, the quantitative nuclear structure properties of uranium, such as binding energy, neutron separation energy, and nuclear charge radii provide deeper insight into its role within the nuclear fuel cycle. This extraordinary energy yield underscores the strategic importance of uranium in the pursuit of sustainable and large-scale electricity generation. Considering the rich properties attributed to uranium, nuclear structure calculations related to this nucleus hold great significance. The total binding energy of the ^{238}U nucleus is approximately 1.807 GeV, corresponding to about 7.57 MeV per nucleon, which is characteristic of heavy nuclei with high binding energies. Furthermore, its neutron separation energy of roughly 4.8 MeV reflects its neutron absorption properties and highlights its potential for conversion into new fissile material within the uranium fuel cycle. In this respect, ^{238}U is significant in nuclear energy technologies not primarily as a direct fission source, but rather through its contribution to the production of secondary fissile isotopes.

In this context, the phenomenological Skyrme potential used in nuclear structure calculations is widely preferred for determining ground-state properties of the nucleus, such as total binding energy and charge radius. Skyrme proposed the effective interaction potential, which was constructed for Hartree-Fock (HF) calculations of nuclei [1] Vautherin and Brink designed SI and SIII parameters as the so-called conventional Skyrme potential parameter groups [2]. These parameters have been determined in agreement with experimental data sets. Krivine et. al. developed the SKM parameter for heavy nuclei [3]. Brack et al. proposed modified versions of SKM and SKM*[4]. Chabanat et al. also developed new Skyrme-effective interactions SLy4 for neutron-rich nuclei, supernovae and neutron stars [5]. Skyrme-Hartree-Fock-Bogolyubov (SHFB) theory consist of Hartree-Fock calculations, in connection with the Relativistic Mean Field (RMF) [6]. Tel et al. proposed using the Skyrme potential to calculate the initial exciton number for pre-equilibrium reaction cross-sections [7].

In the present study, root mean square (rms) nuclear charge radii (the radii of proton, neutron and matter), surface thickness, neutron surface thickness, diffraction radii, total binding energy, potential depth of protons and neutrons for the 238U nucleus were calculated using the Skyrme-Hartree-Fock (SHF) and Skyrme-Hartree-Fock-Bogoliubov (SHFB) theories. The best agreement with experimental values for total binding energies and nuclear charge rms radii has been investigated using Skyrme force parameters.

Skyrme forces encompass a large number of parameters in nuclear models, and different parameter sets have varying success in explaining various properties of nuclear structure. Therefore, in this study, the Skyrme parameter sets given in Table 1 were selected and comparatively examined. The SIII and SLy4 parameters are used to calculate fundamental nuclear properties such as binding energies and radii in the region of medium-heavy and heavy nuclei. The Ska, SKb, and SKX parameters are particularly preferred for accurately modeling the structural properties and spin-orbit separations of heavy and deformed nuclei. The Rσ and S6 parameters sets are prominent in calculating surface energy and nuclear compressibility [8].

Table 1. Skyrme Force Parameters

	SIII	S6	SKa	SKb	SKX	R σ	SLy4
$t_0\,(MeV\,.\,fm^3)$	-1128.75	-1101.81	-1602.78	-1602.78	-1445.3	-1798	-2488.9
$t_1(MeV\,.\,fm^5)$	395	271.67	570.88	570.88	246.9	335.97	486.82
$t_2\,(MeV\,.\,fm^5)$	-95	-138.33	-67.7	-67.7	-131.8	-84.81	-546.39
$t_3\,(MeV\,.\,fm^3)$	14000	17000	8000	8000	12103.9	11083.9	13777
$t_4\,(MeV\,.\,fm^5)$	120	115	125	125	148.6	121.59	123
x_0	0.45	0.583	-0.02	-0.165	0.34	-0.4036	0.834
x_1	0	0	0	0	0.58	0	-0.344
x_2	0	0	0	0	0.127	0	-1
x_3	1	1	-0.286	-0.286	0.03	-0.8705	1.354
α	1	1	1/3	1/3	1/2	3/10	1/6

Using the effective Skyrme force with S6 and SKX parameters, the behaviors of charge, neutron, proton, mass density distributions, as well as the potential depths of protons and neutrons, have been calculated. The calculated ground-state features have been compared with available experimental data and results. In addition, we calculated total binding energy using the Semiempirical Binding Energy formula (SBE). The results obtained were compared with experimental values and with the calculations of Tel. et al. reported in the literature[9].

Theoretical Calculations and Methods

Skyrme proposed the Conventional Skyrme (CS) force. The Conventional Skyrme force describes two-body terms, which and three-body terms, are given by,

$$V_{CS} = \sum_{i<j} V_{ij}^{(2)} + \sum_{i<j<k} V_{ijk}^{(3)} \tag{1}$$

$$V_{ij}^{(2)} = t_0(1+x_0P_\sigma)\delta(\vec{r}) + \frac{1}{2}t_1\left[\delta(\vec{r})\vec{k}^2 + \vec{k}'^2\delta(\vec{r})\right] + t_2\vec{k}'\delta(\vec{r})\vec{k} + iW_0(\vec{\sigma}_i - \vec{\sigma}_j)\cdot\vec{k}\times\delta(\vec{r})\vec{k} \tag{2}$$

$$V_{ijk}^{(3)} = t_3\delta(\vec{r}_i - \vec{r}_j)\delta(\vec{r}_j - \vec{r}_k) \tag{3}$$

Vautherin and Brink proposed that the three-body term can be replaced by a density-dependent two-body term, and this term is given by:

$$V_{ijk}^{(3)} \cong V_{ij}^{(2)} = \frac{1}{6}t_3\rho(\vec{R})\delta(\vec{r}) \tag{4}$$

where $\vec{R} = \frac{1}{2}(\vec{r}_i + \vec{r}_j)$ and $\vec{r} = (\vec{r}_i - \vec{r}_j)$, and also the relative momentum operators are given by; $\vec{k} = \frac{\nabla_i - \nabla_j}{2i}$, acting on the right, and $\vec{k}'^2 = -\frac{\nabla_i - \nabla_j}{2i}$, acting on the left . Ge L.X. et al. proposed the extended Skyrme force as follows:

$$V_{Skyrme} = t_0(1+x_0p_\sigma)\delta(\vec{r}) + \frac{1}{2}t_1(1+x_1P_\sigma)\{\delta(\vec{r})\vec{k}^2 + \vec{k}'^2\delta(\vec{r})\} + t_2(1+x_2P_\sigma)\vec{k}'\cdot\delta(\vec{r})\vec{k} + \frac{1}{6}t_3(1+x_3P_\sigma)\rho^\alpha(\vec{R})\delta(\vec{r}) + it_4\vec{k}'\cdot\delta(\vec{r})(\vec{\sigma}_i - \vec{\sigma}_j)\times\vec{k} \tag{5}$$

Here, t_0, t_1, t_2, t_3, t_4 and x_0, x_1, x_2, x_3, α are the Skyrme force parameters, and $\delta(\vec{r})$ is the delta function. P_σ is the space-exchange operator. $\vec{k}$ is the relative momentum. $\vec{\sigma}$ is the vector of Pauli spin matrices [10]. The Hartree-Fock equations are derived from the total Hamiltonian energy functional of the nucleus and given by:

$$E = E_{Skyrme} + E_{Coulomb} + E_{Pair} - E_{cm} \quad (6)$$

Here, the total energy E of the nucleus comprises several components: E_{Skyrme}, representing the energy from the Skyrme interaction; $E_{Coulomb}$, accounting for the Coulomb energy between protons; E_{Pair}, which arises from nucleon pairing correlations; E_{cm}, a correction term to eliminate the spurious contribution from the center-of-mass motion in the mean-field approximation. When this potential operates on the wave function, it takes the following form:

$$E_{Skyrme} = \langle \varphi | (T + V_{Skyrme} | \varphi \rangle = \sum_i \left\langle i \left| \frac{p^2}{2m} \right| i \right\rangle + \frac{1}{2}\sum_{ij}\langle ij | V_{ij} | ij \rangle + \frac{1}{6}\sum_{ijk}\langle ijk | V_{ijk} | ijk \rangle = \int H_{Skyrme}(\rho_q, \tau_q, J_q) d^3r \quad (7)$$

The single-particle wave functions φ_i of nucleons can be expressed in the form of a Slater determinant:

$$\Phi(x_1, x_2 \ldots\ldots x_j) = \frac{1}{\sqrt{A!}} det|\varphi_i(x_j)| \quad (8)$$

Here, A is the number of nucleons of the nucleus. The ground state energy E, is written as follows:

$$E = \langle \varphi | (T + V) | \varphi \rangle = \int H(\vec{r})\, d\vec{r} \quad (9)$$

Here, $H(\vec{r})$ is a function of the nucleon densities ρ_n, ρ_p, the kinetic energy densities τ_n, τ_p and spin-orbit densities $\vec{J}_n$, $\vec{J}_p$. The dependence of energy density in the case of extended Skyrme forces is given as follows:

$$H(\rho, \tau, \vec{J}) = \frac{\hbar^2}{2m}\tau + \frac{1}{2}t_0\left[\left(1 + \frac{1}{2}x_0\right)\rho^2 - \left(x_0 + \frac{1}{2}\right)(\rho_n^2 + \rho_p^2)\right] + \frac{1}{4}(t_1 + t_2)\rho\tau + \frac{1}{8}(t_2 - t_1)(\rho_n\tau_n + \rho_p\tau_p) + \frac{1}{16}(t_2 - 3t_1)\rho\nabla^2\rho + \frac{1}{32}(3t_1 + t_2)(\rho_n\nabla^2\rho_n + \rho_p\nabla^2\rho_p) + \frac{1}{4}t_3\rho_n\rho_p\rho - \frac{1}{2}W_0(\rho\vec{\nabla}\cdot\vec{J} + \rho_n\vec{\nabla}\cdot\vec{J_n} + \rho_p\vec{\nabla}\cdot\vec{J_p}) \quad (10)$$

where $H_C(\vec{r})$ is the direct part of the Coulomb interaction. Densities are dependent on nucleon wave functions

$$\rho_q(\vec{r}) = \sum_{i,\sigma}|\varphi_i(\vec{r}, \sigma, q)|^2$$

$$\tau_q(\vec{r}) = \sum_{i,\sigma}\left|\vec{\nabla}\varphi_i(\vec{r}, \sigma, q)\right|^2 \quad (11)$$

$$\vec{J}_q(\vec{r}) = -i\sum_{i,\sigma,\sigma'}\varphi_i^*(\vec{r}, \sigma, q)[\vec{\nabla}\varphi_i(\vec{r}, \sigma, q)x\langle\sigma|\vec{\sigma}|\sigma'\rangle]$$

The variation of this ground states energy E with respect to the single particle wave function φ_i leads to an HF equation as follows,

$$[-\vec{\nabla}\cdot\frac{\hbar^2}{2m_q^*}\vec{\nabla} + U_q(\vec{r}) + W_q(\vec{r})(-i)(\vec{\nabla}\times\vec{\sigma})]\varphi_i = \rho_i\varphi_i \quad (12)$$

Where, U_q represents the mean-field potential and W_q denotes the spin-orbit potential. As can be observed from Equation (12), since the effective mass m_q^* does not vary with the radial coordinate r, the Hartree-Fock (HF) equation simplifies to a conventional radial Schrödinger equation. However, in the context of Skyrme-type interactions, this nonlocality is effectively incorporated through the radial dependence of the nucleons effective mass. Consequently, the HF equation takes the form of a differential equation, which is more suitable for numerical treatment [11]. Nucleon density functions can be written as follows:

$$\rho_q(\vec{r}) = \sum_{\beta\in q} w_\beta\phi_\beta(\vec{r})^+\phi_\beta(\vec{r}) \quad (13)$$

where ϕ_β is the single-particle wave function of state β, and isospin label q runs over $q \in \{pr, ne\}$ (pr=proton and ne=neutron). The occupation probability of the state β is denoted by ω_β. The single-particle wave functions can be divided by:

$$\phi_\beta(\vec{r}) = \frac{R_\beta(r)}{r}Y_{j_\beta l_\beta m_\beta}(\theta, \varphi) \quad (14)$$

functions $Y_{j_\beta l_\beta m_\beta}$ are spinor spherical harmonics and the nucleon densities are given as:

$$\rho_q(r) = \sum_{n_\beta j_\beta l_\beta} w_\beta\frac{2j_\beta + 1}{4\pi}\left(\frac{R_\beta}{r}\right)^2 \quad (15)$$

Protons and neutrons rms radii are described as:

$$\langle r_q^2 \rangle = \int_0^{R_{box}} r^2\rho_q^2(r)d^3r \quad (16)$$

The rms radii of the neutron, proton and charge distributions can be evaluated from $\rho_n(\vec{r})$ and $\rho_p(\vec{r})$ densities:

$$r_q = \langle r_q^2 \rangle^{1/2} = \left[\frac{\int r^2\rho_q(r)dr}{\int \rho_q(r)dr}\right]^{1/2}, \quad q = n, p, c \quad (17)$$

The neutron skin thickness ***t***, can be defined as the difference between the neutron and proton rms radius:

$$t = r_n - r_p \quad (18)$$

Results and Discussions

Skyrme force interactions have central, zero range, only dependence of radial and there is no dependence of angular. In this study, firstly we calculated harmonic oscillator potential wave-function with HAFOMN code [12]. We have given schematic flow card of code in Figure 1.

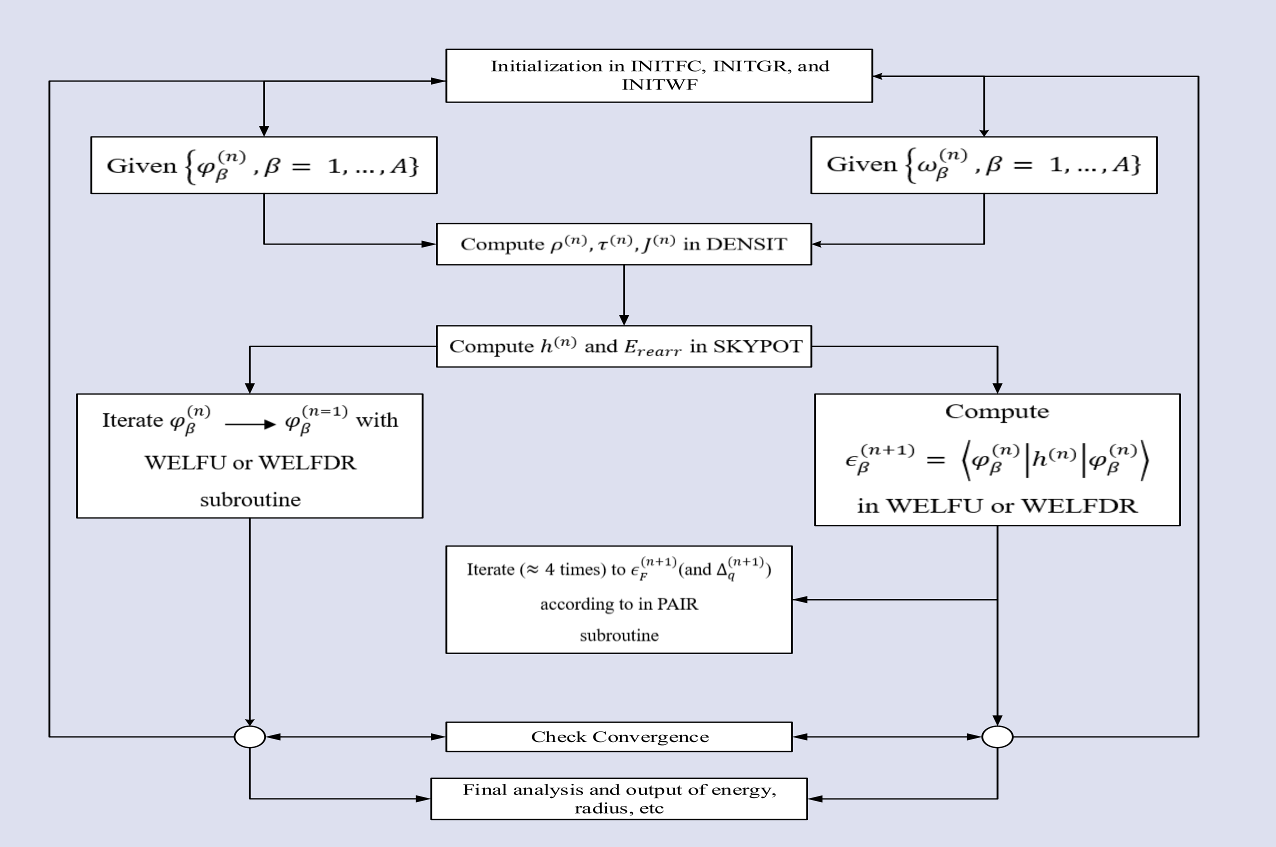

Figure 1. Schematic flow card of HAFOMN code

In the calculations, we used the approximation constant-force for pairing effects with BCS formalism. The pairing energy is given by:

$$E_{pair} = \sum_q G_q \left[\sum \sqrt{w_\beta(1 - w_\beta)}\right]^2 \qquad (19)$$

where G_q are the pairing matrix elements and $\frac{\Delta_q}{G_q} = \sum_{\beta\varepsilon q} \sqrt{w_\beta(1 - w_\beta)}$,. The pairing effects in the BCS (Bardeen-Cooper-Schrieffer) formalism in the approximation constant-force with $G_{pr} = \frac{22MeV}{A}$, $G_{ne} = \frac{29MeV}{A}$, and pairing gap is $\nabla_q = 11.2MeV/\sqrt{A}$, and where A is the total number of the nucleon. We used the Skyrme interaction parameters in Table 1 and for calculations with the program HAFOMN and using HFBRAD (v1.00) code combined with SLy4 forces [13]. In the calculations of SHF method, Ψ_β represents the single-particle wave function of the state β. But in the calculations of SHFB method, Ψ_β represents the quasiparticle wave function of the quasiparticle state β. The results obtained with experimental data experimental rms nuclear charge radii in Table 2. HAFOMN code represents them on an equidistant radial grid. HAFOMN code have used the fact that all integrands that occur in spherical calculations vanish at the origin ($i = 1$) and are negligible at the boundary ($i = N_r$). In this study, we investigated for $i = N_r$, from 57 to 192, and r-step from 0.1 to 0.3. We have found out that S6 (for N_r = 106 and r-step = 0.15) and SKX (for N_r = 125 and r-step = 0.2) parameter are the best agreement with the experimental binding energy and charge rms radii values. And we calculated total binding energy by using the Semiempirical Binding Energy formula (SBE) in Table 2. SBE formula is given by:

$$SBE(A, Z) = a_v A - a_s A^{\frac{2}{3}} - a_c \frac{Z(Z-1)}{A^{\frac{1}{3}}} - a_{sym} \frac{(A-2Z)^2}{A} \pm a_p A^{\frac{-3}{4}} \qquad (20)$$

Where the adjusted constants (to give the best agreement with the experimental); a_v= 15.5 MeV (Volume term), a_s= 16.8 MeV (Surface term), a_c = 0.72 MeV (Coulomb term), a_{sym}= 23 MeV (Symmetry term), a_p = 34 MeV (Pairing term) [14]. We have found out that S6 and SKX parameters are well agreement with the experimental total binding energy and charge rms radii values in Table 2.

Table 2. Skyrme Force Calculations and Experimental values.

Force	***S3***	***S6***	***SKa***	***SKb***	***SKX***	***R_σ***	
E_{tot} *(MeV)*	-1778.3	-1775.8	-1774.1	-1842.7	-1802.9	-1803.2	-1801.689 [16] - 1787.934 [16] -1806.910 (SBE)
E_{pair}*(MeV)*	-11.384	-13.472	-9.7282	-9.5805	-10.332	-12.07	
$R_{rms,charge}$ *(fm)*	5.8571	5.8571	5.8571	5.8571	5.8562	5.8579	5.8587∓ 0.037 [1] 5.8571∓0.0033 [15] 5.81594 (SHFB-SLy4) 5.8562 [9] 5.8674 [9]
$R_{rms,proton}$ *(fm)*	5.81	5.783	5.825	5.77	5.761	5.882	
$R_{rms,neutron}$ *(fm)*	5.941	5.903	6.092	6.25	6.771	5.952	
$R_{rms,mass}$*(fm)*	5.8906	5.8573	5.9903	6.0692	6.3993	5.9251	
Charge Surface Thick (fm)	0.7235	1.125	0.7939	0.7958	0.7625	0.6859	
Proton Surface Thick (fm)	0.5687	1.007	0.6528	0.6564	0.6218	0.522	
Neutron Surface Thick (fm)	0.8286	1.136	0.9273	0.9197	0.9026	0.81	
Mass Surface Thick (fm)	0.7368	1.103	0.8324	0.8222	0.8029	0.7084	
Diffraction Radii ΔR^{charge} *(fm)*	7.361	7.955	7.264	7.286	7.255	7.265	
Diffraction Radii ΔR^{proton} *(fm)*	7.361	7.879	7.263	7.29	7.261	7.267	
Diffraction Radii $\Delta R^{neutron}$ *(fm)*	7.407	7.815	7.411	7.35	7.331	7.455	
Diffraction Radii ΔR^{mass} *(fm)*	7.39	7.889	7.356	7.314	7.304	7.338	
Neutron Skin Thick *t* (fm)	0.131	0.120	0.267	0.480	1.010	0.070	

The distributions of charge, proton, neutron, and mass radii obtained from S6 and SKX calculations are displayed in Figure 2 for comparison.

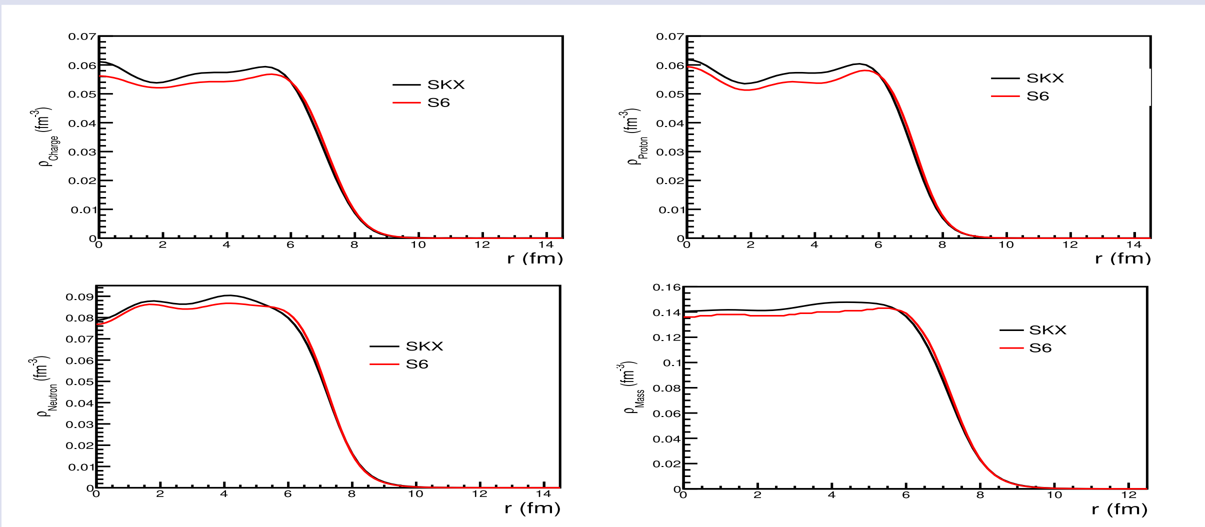

Figure 2. Density distributions of charge, proton, neutron, and mass densities of the 238U nucleus calculated using the Skyrme interactions SKX and S6

Table 3 summarizes the comparison between experimental data and the theoretical predictions obtained with the S6 and SKX Skyrme parametrization. The results indicate that while both parameter sets reproduce the total binding energy and charge radius reasonably well, the SKX interaction provides slightly better agreement with the experimental values, particularly for the charge radius. Figure 3 presents the charge, proton, neutron, and mass density distributions calculated with the S6 and SKX parameter sets, allowing a direct comparison of the nuclear structure predicted by both interactions. In addition, Figure 4 illustrates the potential depths for protons and neutrons, providing further insight into single-particle properties associated with each parameterization.

Table 3. Comparison of Experimental Observables and Skyrme-HF Predictions (S6 and SKX)

Quantity	***Experimental***	***S6 (calc)***	***% error (S6)***	***SKX (calc)***	***% error (SKX)***
E_{tot} (MeV)	-1801.689	-1775.800	1.437	-1802.900	0.0672
$R_{rms,charge}$ (fm)	5.8571 ± 0.0033	5.8571	0.000	5.8562	0.0154

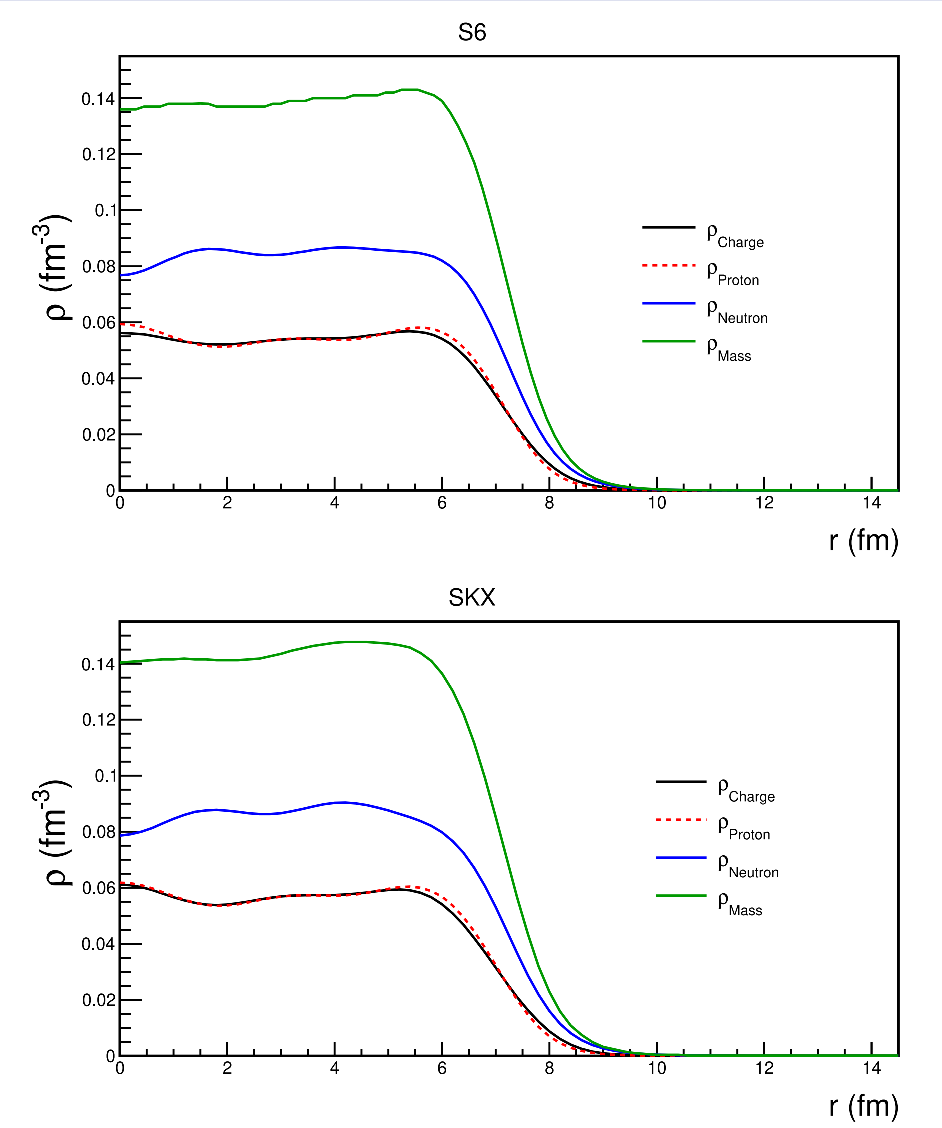

Figure 3. Density distributions of the ^{238}U nucleus calculated using S6 and SKX Skyrme-force parameter sets

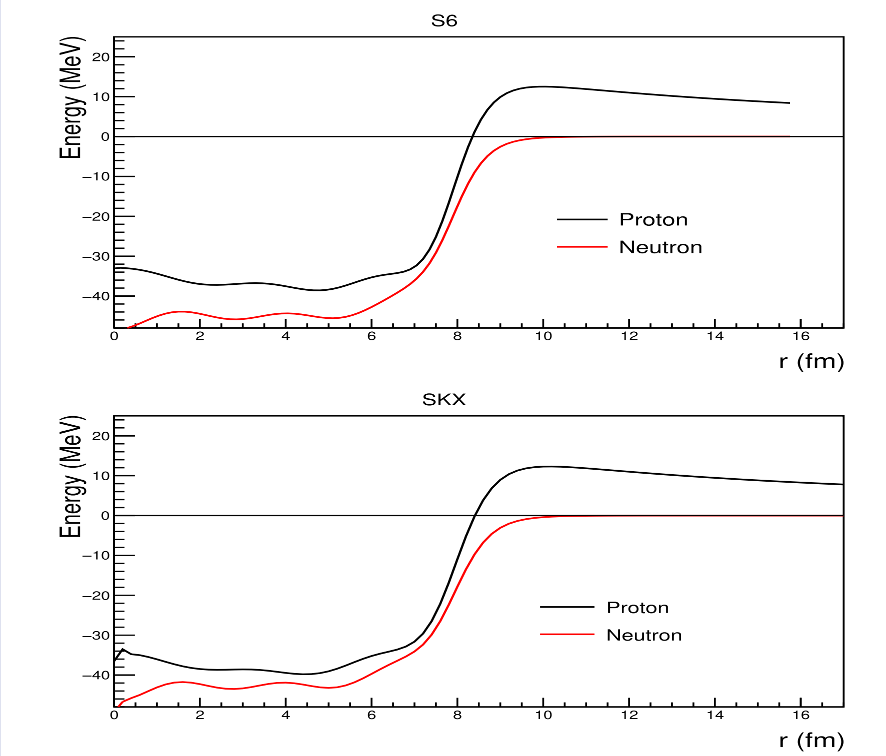

Figure 4. Single-particle energy potential depths of neutrons and protons for the ^{238}U nucleus calculated using S6 and SKX Skyrme-force parameter sets

Conclusions

In this work, firstly root mean square (rms) values nuclear charge, proton, neutron and mass radii; surface thickness and neutron surface thickness; diffraction radii; total binding energy, potential depth of protons and neutrons for the 238U nuclei were calculated by using Skyrme-Hartree-Fock (SHF) and Skyrme-Hartree-Fock-Bogoliubov (SHFB) theory. SHF and SHFB methods have been very successful in explaining the ground state features of 238U nuclei. We can obtain that, equidistant radial grid parameters ($i = N_r$, and r-step) are quite important parameters for Skyrme force calculations. In this study, we have found out that S6 (for N_r = 106 and r-step = 0.15) and SKX (for N_r = 125 and r-step = 0.2) parameters are the best agreement with the experimental binding energy and charge rms radii values. To quantify the agreement between calculated and experimental values, we report absolute deviations and percentage errors. For energies the absolute value of the experimental reference is used in the denominator. Table 1 lists the absolute and relative deviations for the S6 and SKX parameter sets. Where experimental uncertainties are available (e.g. Rrms,ch = 5.8571 ± 0.0033 fm) we also compare the calculated deviation to the quoted uncertainty (expressed in standard-deviation units). Error Table 3 shows that SKX reproduces the total binding energy most accurately (0.067% deviation), while S6 provides better agreement for neutron and mass rms radii. These obtained results can be used for better understanding the nuclear structure of uranium isotopes, transuranium elements and for the initial exciton numbers of calculations for pre-compound reactions cross-sections.

Conflicts of interest

There are no conflicts of interest in this work

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