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Investigation of Nuclear Ground State Properties of Fuel Materials of ^{232}Th and ^{238}U Using *Skyrme-Extended-Thomas-Fermi* Approach Method

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Abstract. It has been performed the nuclear ground state properties investigation of ^{232}Th and ^{238}U using Skyrme interaction. The local density, the kinetic energy density, and the spin-orbit density for proton and neutron have been calculated using Extended-Thomas-Fermi approach method. Then the calculation results have been compared with Skyrme-Hartree-Fock results (using HAFOMN and HFBRAD codes). Total energy calculations obtained from this research are -1792.973947 MeV (for ^{232}Th) deviated 0.29244% from experiment energy and -1761.519459 MeV (for ^{238}U) deviated 0.48369% from experiment energy. The distribution profiles of local density and local potential for ^{232}Th and ^{238}U are quite similar with Skyrme-Hartree-Fock results. It is indicated that Skyrme-Extended-Thomas-Fermi method can be used to study the nuclear ground state properties, especially even nuclei.

1. Introduction

In a nuclear reactor, one of the most important components is fuel. Some of common nuclear fuels which are used in nuclear reactor are thorium oxide, uranium oxide, or combination of uranium oxide and thorium oxide. Some of the elements contained in nuclear fuel are ^{232}Th and ^{238}U. In this research, it is performed an investigation of the nuclear ground state properties of ^{232}Th and ^{238}U by using Skyrme-Extended-Thomas-Fermi (SETF) method.

In this research, SETF method is chosen to be used because this method is quite good in explaining the nuclear ground state properties. In addition, the used formula of this method is semi-classical and it uses statistical approach. However, the result of the calculation is quite able to explain the experimental results and the results obtained by Skyrme-Hartree-Fock (SHF) method [1, 2].

The purposes of this research are to calculate numerically the ground state energy of ^{232}Th and ^{238}U by using SETF method with SLy4 set parameters and to simulate the local density and the local potential distributions for both proton and neutron of ^{232}Th and ^{238}U. The advantage of this research is to get information of the ground state properties of ^{232}Th and ^{238}U, which can be used in scattering research to calculate the microscopic cross section of ^{232}Th and ^{238}U. Such data is needed in nuclear reactor analysis.

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2. Theory

2.1. Skyrme Interaction

Studying about nuclear properties, especially for neutron-rich nuclei, needs a special method because many-body problem in nuclear is more complicated than in atomic. One approach that is widely used to describe the nucleon interaction phenomena is Skyrme interaction, proposed by T.H.R. Skyrme. First, it is commenced from the Hamiltonian for the nuclear with the formulation:

$$\hat{H} = \sum_{i=1}^{A} -\frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}\sum_{i,j=1}^{A}\hat{v}_{ij}^{(2)Nucl} + \frac{1}{6}\sum_{i,j,k=1}^{A}\hat{v}_{ijk}^{(3)Nucl} + \frac{1}{2}\sum_{i,j=1}^{Z}\hat{v}_{ij}^{(2)Coul} \tag{1}$$

where the first term is the kinetic term, the second and third parts are the term of nucleons interactions within nuclear, and the fourth term is the Coulomb interaction term between protons within nuclear [3]. Furthermore, it is focused to the second and third terms. On this issue, it is applied the Skyrme interaction, where nucleon potential can be represented by

$$\begin{aligned}\hat{v}_{cs} = \sum_{i<j}\hat{v}_{ij}^{(2)} + \sum_{i<j<k}\hat{v}_{ijk}^{(3)} &= t_0(1+x_0P_\sigma)\delta(\vec{r}_{ij}) + \tfrac{1}{2}t_1(1+x_1P_\sigma)\{\vec{p}_{12}^{\,2}\delta(\vec{r}_{ij}) + \delta(\vec{r}_{ij})\vec{p}_{12}^{\,2}\} \\ &+ t_2(1+x_1P_\sigma)\vec{p}_{12}\cdot\delta(\vec{r}_{ij})\vec{p}_{12} + it_4\vec{p}_{12}\cdot\delta(\vec{r}_{ij})(\vec{\sigma}_i+\vec{\sigma}_j)\times\vec{p}_{12} + \tfrac{1}{6}t_3(1+x_3P_\sigma)\rho^\alpha(\vec{\bar{r}})\delta(\vec{r}_{ij})\end{aligned} \tag{2}$$

with $\hat{v}_{ij}$ represents the two-body interaction and $\hat{v}_{ijk}$ represents the three-body interaction [4, 5]. The constants of t_0, t_1, t_2, t_3, x_0, x_1, x_2, x_3, α, and W_0 are the Skyrme set parameters, P_σ is the space exchange operator, ρ represents the density, $\vec{k}'$ and $\vec{k}$ are the relative momentum acting on left and right, $\delta(\vec{r})$ is delta function, and σ is the vector of Pauli spin matrices [5]. In this research, it is utilized the SLy4 set parameter because this set parameter is powerful to investigate neutron-rich nuclei.

Table 1. The *SLy4* set parameters for *Skyrme* interaction [6].

Parameter	*SLy4*	Parameter	*SLy4*	Parameter	*SLy4*	Parameter	*SLy4*
t_0 (MeV fm^3)	-2488	x_0	0.834	t_1 (MeV fm^5)	486.82	x_1	-0.344
t_2 (MeV fm^5)	-546.3	x_2	-1	t_3 (MeV fm^4)	13777	x_3	1.354
W_0 (MeV fm^5)	123	α	0.167				

From eq. (1), it can be obtained the formula of total energy which is expressed as

$$\varepsilon_{total} = \varepsilon_{kinetic} + \varepsilon_{Skyrme} + \varepsilon_{Coul} \tag{3}$$

The kinetic energy density can be approached as:

$$\varepsilon_{kinetic} = \frac{\hbar^2}{2m}\left(1-\frac{1}{A}\right)\tau \tag{4}$$

where τ is the total kinetic energy density of nucleons (the sum of the kinetic energy densities of protons and neutrons) and the term in parentheses is the center of mass correction [7]. The Skyrme energy density can be approximated by [5, 6]:

$$\begin{aligned}\varepsilon_{Skyrme} =& \tfrac{1}{2}t_0[(1+\tfrac{x_0}{2})\rho^2 - (x_0+\tfrac{1}{2})(\rho_n^2+\rho_p^2)] + \tfrac{t_3}{12}(1+\tfrac{x_3}{2})\rho^{2+\alpha} - \tfrac{t_3}{12}(x_3+\tfrac{1}{2})\rho^\alpha(\rho_n^2+\rho_p^2) \\ &+ \tfrac{1}{4}[t_1(1+\tfrac{x_1}{2}) + t_2(1+\tfrac{x_2}{2})]\rho\tau - \tfrac{1}{4}[t_1(x_1+\tfrac{1}{2}) - t_2(x_2+\tfrac{1}{2})](\rho_p\tau_p+\rho_n\tau_n) \\ &+ \tfrac{1}{16}[3t_1(1+\tfrac{x_1}{2}) - t_2(1+\tfrac{x_2}{2})](\vec{\nabla}\rho)^2 - \tfrac{1}{16}[3t_1(x_1+\tfrac{1}{2}) + t_2(x_2+\tfrac{1}{2})][(\vec{\nabla}\rho_p)^2 + (\vec{\nabla}\rho_n)^2] \\ &- \tfrac{1}{16}(t_1x_1 - t_2x_2)\vec{J}^2 + \tfrac{1}{16}(t_1-t_2)(\vec{J}_p^2+\vec{J}_n^2) - \tfrac{W_0}{2}(\rho\vec{\nabla}\cdot\vec{J} + \rho_p\vec{\nabla}\cdot\vec{J}_p + \rho_n\vec{\nabla}\cdot\vec{J}_n)\end{aligned} \tag{5}$$

where $\hbar$ is the reduced Planck constant, m is the mass of the nucleon, $\tau_{p(n)}$ is the kinetic energy density of proton (p) or neutron (n), and $\vec{J}_{p(n)}$ is the spin-orbit density of proton or neutron. Coulomb term is expressed as [8]:

$$\varepsilon_{Coul}(\vec{r}) = \frac{e^2}{2}\int \frac{\rho_p(\vec{r'})\rho_p(\vec{r})}{\left|\vec{r}-\vec{r'}\right|}d^3r' - \frac{3}{4}e^2\left(\frac{3}{\pi}\right)^{1/3}\rho_p^{4/3}(\vec{r'}) \tag{6}$$

The total energy can be formulated as:

$$E = \int (\varepsilon_{kin} + \varepsilon_{Skyrme} + \varepsilon_{Coul})d^3\vec{r} = \int [\varepsilon_{total}(\rho, \tau, \vec{J})]d^3\vec{r} \tag{7}$$

From the formulation of the energy density in eq. (3), it can be derived the formula for the central potential of nucleon as [9]:

$$\begin{aligned} V_q(\vec{r}) =& t_0[(1+\tfrac{x_0}{2})\rho - (x_0+\tfrac{1}{2})\rho_q] + \tfrac{1}{4}[t_1(1+\tfrac{x_1}{2}) + t_2(1+\tfrac{x_2}{2})]\tau - \tfrac{1}{4}[t_1(x_1+\tfrac{1}{2}) - t_2(x_2+\tfrac{1}{2})]\tau_q \\ & - \tfrac{1}{8}[3t_1(1+\tfrac{x_1}{2}) - t_2(1+\tfrac{x_2}{2})](\nabla^2\rho) + \tfrac{1}{8}[3t_1(x_1+\tfrac{1}{2}) + t_2(x_2+\tfrac{1}{2})](\nabla^2\rho_q) + V_{Coul}(\vec{r})\delta_{pq} \\ & + (2+\alpha)\tfrac{t_3}{12}(1+\tfrac{x_3}{2})\rho^{\alpha+1} - \tfrac{t_3}{12}(x_3+\tfrac{1}{2})[\alpha\rho^{\alpha-1}(\rho_p^2+\rho_n^2) + 2\rho^\alpha\rho_q] - \tfrac{1}{2}W_0[\vec{\nabla}\cdot\vec{J} + \vec{\nabla}\cdot\vec{J}_q] \end{aligned} \tag{8}$$

where [8]

$$V_{Coul}(\vec{r}) = e^2\int \frac{\rho_p(\vec{r'})}{\left|\vec{r}-\vec{r'}\right|}d^3\vec{r'} - e^2\left(\frac{1}{\pi}\right)^{1/3}\rho_p^{1/3}(\vec{r'}) \tag{9}$$

2.2. Extended-Thomas-Fermi Approach Method

In this research, it is used SETF approach method to solve the quantities of the nucleon local density $\rho_q(\vec{r})$, the kinetic energy density $\tau_q(\vec{r})$, and the spin-orbit density $\vec{J}_q(\vec{r})$. Those formulas have been derived from quantum mechanics calculation, but those quantities are approached using semi-classical and statistical approximations [3, 9]. In SETF method, the kinetic energy density is expressed as:

$$\tau_q^{(ETF)}[\rho_q] = \tau_q^{(TF)}[\rho_q] + \tau_q^{(2)}[\rho_q] + \tau_q^{(4)}[\rho_q] + \tau_q^{(4)so}[\rho_q] \tag{10}$$

The formulation of the spin-orbit density is expressed as:

$$\vec{J}_q(\rho_q) = \vec{J}_q^{[2]}(\rho_q) + \vec{J}_q^{[4]}(\rho_q) \tag{11}$$

where the complete formula of eq. (10) and (11) can be found in Bartel and Bencheikh journal [9]. In this research, it is concerned to the spherical symmetry case, where the divergence of a vector field involves only the radial component. After the entire quantities of kinetic energy density and spin-orbit density are expressed as a function of the local density, it can be calculated the eq. (7) by applying the variational methods using the local density as a varied quantity, which follows:

$$\delta E = \delta\int \varepsilon(\rho_p, \rho_n)d^3r = 0 \tag{12}$$

The ground state nucleon density can be approximated by adopting the Fermi-Dirac distribution formula and it can be formulated as [9, 10]:

$$\rho_p(\vec{r}) = \rho_{0q}\left[1 + exp\left(\frac{r-R_{0q}}{a_q}\right)\right]^{-\gamma_q} \tag{13}$$

The nucleon density parameter ρ_{0q} can be determined by the terms of normalized

$$\int \rho_q(\vec{r}) d^3r = Z(N) \tag{14}$$

because it is known that the number of protons (Z) and neutrons (N) are conservative. The rms (*root-mean-square*) radii for proton and neutron are defined as [7]:

$$r_q^{rms} = \sqrt{(r_q^2)} = \sqrt{\frac{\int r^2 \rho_q d^3r}{\int \rho_q d^3r}} \tag{15}$$

3. Research/Calculation Method

For calculation process, the integral of eq. (7) can be calculated with assistances of eq. (5), (6), (10), and (11), in which the proton and neutron densities are calculated by using eq. (13) and (14). To perform the energy function optimization process, eq. (5) is amended so that it becomes a formula that depends only on the nucleon local density. For divergence calculation, the vector component is taken only on the radial component, not on the angular components, as the assumption that the analyzed nuclear is spherical symmetry. From eq. (5) and eq. (7), it is appeared that after optimization process, as the eq. (12), it is obtained six parameters, i.e. R_{0p}, R_{0n}, a_{0p}, a_{0n}, γ_p, and γ_n then those parameters are utilized to calculate the local densities of proton and neutron. By knowing the local density, the kinetic energy density and the spin-orbit density can be calculated.

In this research, it is cosntructed a code named SETFA to calculate binding energy of ^{232}Th and ^{238}U, where optimization of eq. (13) is performed in order to obtain the optimal total energy values of ^{232}Th and ^{238}U. The numerical differentiation calculation is performed using finite-difference method and the numerical integration calculation is performed using Riemann sum. To optimize the value of the total energy density, it is used Nelder-Mead method. For comparison, it is used the calculation results of HFBRAD code (using Skyrme-Hartree-Fock-Bogolyubov method) [7] and HAFOMN code (using Skyrme-Hartree-Fock method) [4].

4. Result and Discussion

4.1. Calculation Results

In this research, it is calculated numerically the total energy, kinetic energy, spin-orbit density, and local potential of ^{232}Th and ^{238}U. The calculation results of this research are showed in Tabel 3. The calculation results of this research are also compared with the result of another

Table 2. Nucleon rms radius calculation results of proton and neutron in ^{232}Th and ^{238}U using Skyrme interaction with SLy4 set parameters.

Nucleus	Parameter	SETFA	HFBRAD	HAFOMN
^{232}Th	Proton rms radius (fm)	5.658	5.697	5.707
	Neutron rms radius (fm)	5.839	5.864	5.873
^{238}U	Proton rms radius (fm)	5.673	5.763	5.764
	Neutron rms radius (fm)	5.892	5.926	5.928

method/code, i.e. the results of HAFOMN and HFBRAD codes. From Tabel 2, it can be seen that the proton and neutron rms radii resulted from this research are lower than resulted from HAFOMN and HFBRAD codes.

Table 3. The Calculation Results.

Parameters	^{232}Th	^{238}U
Proton density distribution radius R_{0p} (fm)	7.28705	7.30705
Neutron density distribution radius R_{0n} (fm)	7.55385	7.63385
Proton density diffusivity a_{0p} (fm)	0.55826	0.55826
Neutron density diffusivity a_{0n} (fm)	0.63034	0.63034
Proton density exponent γ_p	1.5161	1.5161
Neutron density exponent γ_n	1.6191	1.6291
Proton density parameter ρ_{0p} (fm^3)	0.0613780817	0.062218973
Neutron density parameter ρ_{0p} (fm^3)	0.0895403289	0.089330927
Kinetic Energy (MeV)	4332.751898	4461.935743
Skyrme Energy (MeV)	-7021.04675	-7221.30697
Spin-Orbit Energy (MeV)	-85.21482	-87.51060
Direct Coulomb Energy (MeV)	961.03051	1001.58281
Exchange Coulomb Energy (MeV)	-34.25512	-35.18553
Coulomb Total Energy (MeV)	926.77539	966.39728
Total Energy (MeV)	-1761.51940	-1792.97395
Experiment Energy (MeV)	-1766.68603	-1801.68856
Deviation (%)	0.29244	0.48369

4.2. Distribution Model

It is also simulated the calculation results to describe the distribution model of local density and local potential for proton and neutron of ^{232}Th and ^{238}U and this research results are compared with the results of HAFOMN code and Tel et al. [11], where Tel et al. used the Skyrme-Hartree-Fock with T3 Skyrme set parameters. From those displayed figures, it can be seen that the obtained results of this research, HAFOMN code, and Tel et al. are similar especially for the slope and the surface region. In local potential distribution, in near center region, the result of

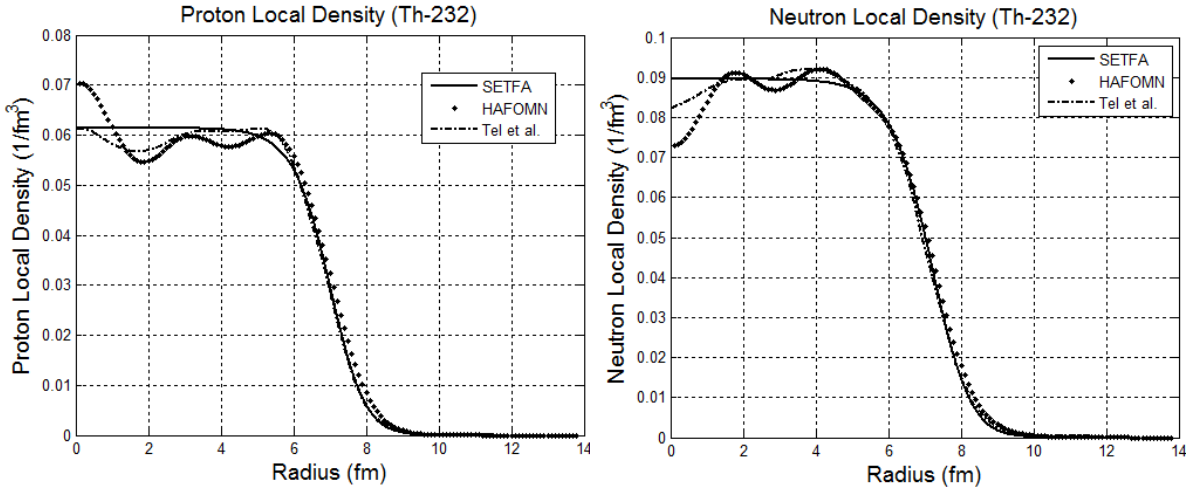

Figure 1. The distribution model of the local potential of proton (left) and neutron (right) of ^{232}Th. The dotted line represents HAFOMN result, the dash-dotted line represents calculation result of Tel et al [11], and the solid line represents SETFA result (this research result).

this research shows constant value but the others show the curvatures model. The difference is only found near the center. It is because of the difference approach used in each method. In SETFA code, it is utilized statistical approach to determine local density of nucleons, and in HAFOMN code or HFBRAD code, it is utilized the nucleon wave function to determine local density of nucleons. In local potential, HAFOMN and this research results have similar results especially for the slope and the surface region. For near center region, it is not significantly different in potential depth. It is indicated that SETF method can be used to study the nuclear ground state properties, especially for even nuclei.

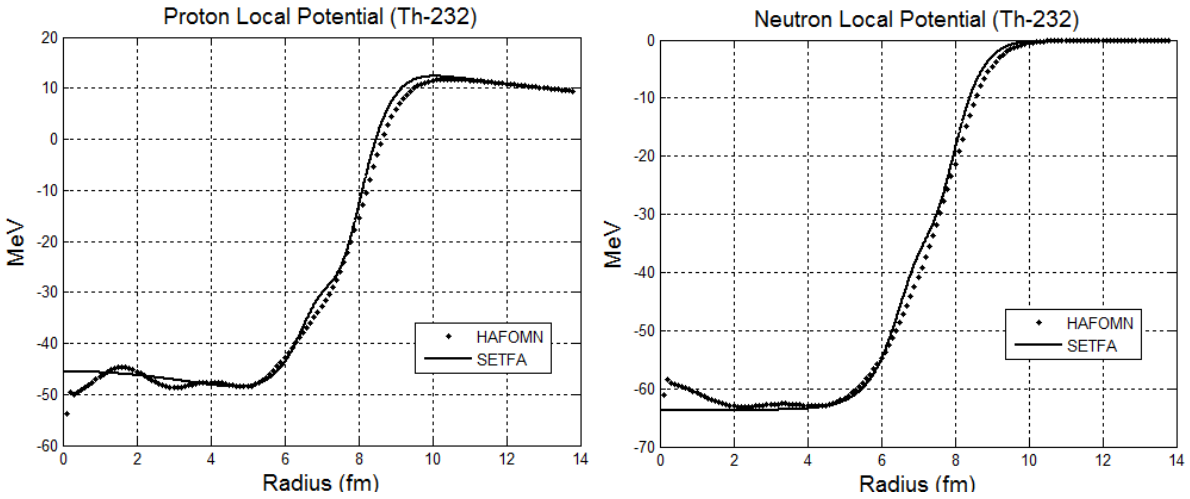

Figure 2. The distribution model of the local potential of proton (left) and neutron (right) of ^{232}Th. The dotted line represents HAFOMN result and the solid line represents SETFA result (this research result).

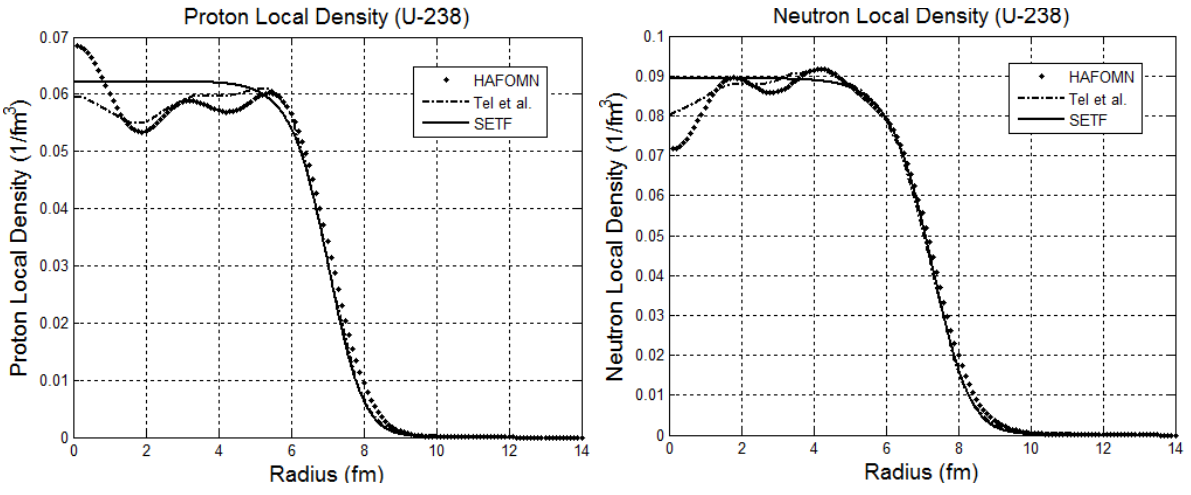

Figure 3. The distribution model of the local potential of proton (left) and neutron (right) of ^{238}U. The dotted line represents HAFOMN result, the dash-dotted line represents calculation result of Tel et al [11], and the solid line represents SETFA result (this research result).

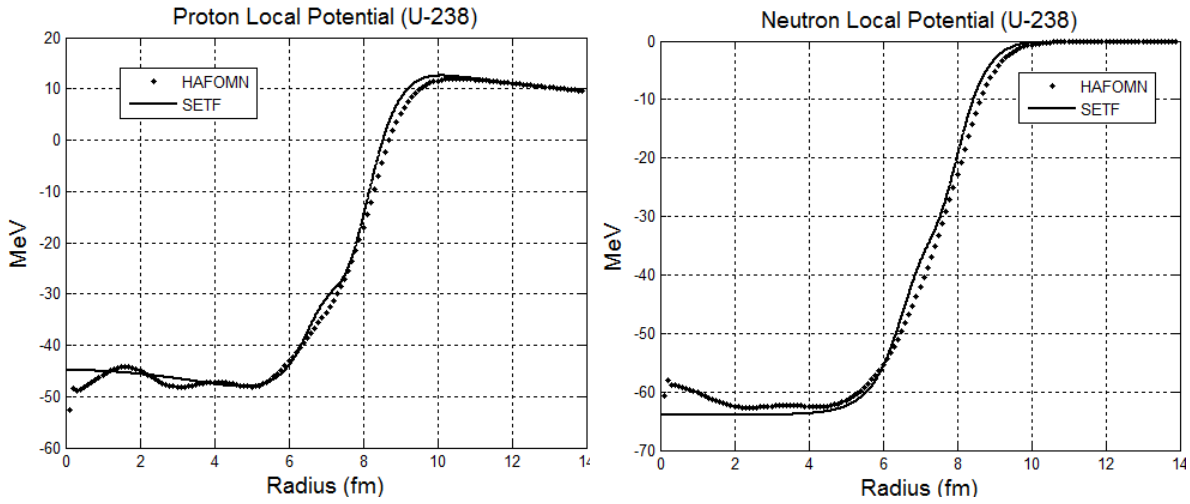

Figure 4. The distribution model of the local potential of proton (left) and neutron (right) of ^{238}U. The dotted line represents HAFOMN result and the solid line represents SETFA result (this research result).

5. Summary

In this research, it is performed the total energy calculations of ^{232}Th and ^{238}U using Skyrme-Extended-Thomas-Fermi (SETF) approach method with SLy4 set parameters. The total energy calculation resulted from this research are -1792.973947 MeV (for ^{232}Th) deviated 0.29244% from experiment energy and -1761.519459 MeV (for ^{238}U) deviated 0.48369% from experiment energy. It is also simulated the distribution of local density and local potential for proton and neutron in ^{232}Th and ^{238}U and compared with HAFOMN and Tel et al. models. The results of this research are similar with the results of other methods, especially for the slope and the surface region. It is indicated that the Skyrme-Extended-Thomas-Fermi method can be used to study the ground state properties of nuclear, especially for even nuclei.

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References

[1] Aymard F, Gulminelli F, and Margueron J 2014 *Phys. Rev.* C **89** 065807.
[2] Baran A, Pomorski K, and Bartel J 2002 *Ann. Univ. Marie Curie* V **57** 2 p 23-67.
[3] Ring P and Shuck P 1980 *The Nuclear Many Body Problem* (Berlin: Springer).
[4] P G Reinhard 1991 *Skyrme-Hartree-Fock Model of the Nuclear Ground State* (Computational Nuclear Physics 1 - Nuclear Structure) ed. S E Koonin, (Springer-Verlag Berlin Heidelberg) chapter 2 pp 28-50.
[5] Vautherin D and Brink D M 1972 *Phys. Rev.* C **5** p 626-647.
[6] Chabanat E, Bonce P, Haensel P, Meyer J, and Schaefer R 1997 *Nucl. Phys.* A **627** 710.
[7] Bennaceur K and Dobaczewski J 2005 *Computer Physics Communications* **168** p 96-122.
[8] Gu H Q, Liang H, Long W H , Giai N V, and Meng J 2013 *Phys. Rev.* C **87** 041301.
[9] Bartel J and Bencheikh K 2002 *Eur. Phys. J.* A **14** p 179-190.
[10] Denisov V and Nesterov V 2006 *Ukr. J. Phys.* V **51** N **5** p 440-448.
[11] Tel E, Sahin H M, Yalcin S, Altinok T, Kaplan A, and Aydin A 2008 *Annals of Nuclear Energy* **35** p 220-227.