Numerical Study of Nuclear Ground State Properties of Fuel Elements of Nuclear Reactor by Using 
Skyrme-Hartree-Fock-Bogoliubov Method

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Abstract. In this study, it is investigated the total energy, nuclear radii, and neutron skin thickness of nuclear reactor fuel elements by using Skyrme interaction collaborated with Hartree-Fock-Bogoliubov method. Both proton and neutron densities were calculated by using SIII set parameters. The calculation results of this study are in good agreement with the related experimental results.

1. Introduction
The increase of human population in the world causes the increase of energy demand. Because the sources of non-renewable energies tend to be decreased, it is needed to develop the new alternative energy sources to provide the world energy demands. One of the new alternative energy sources is nuclear power plant, which utilizes the controlled nuclear reaction. In nuclear reactor design, nuclear reaction models are required to provide the estimation of particle-induced reaction cross-section, especially for unavailable experiment data or the difficult cross-section measurement by experiment. In development of reaction systematic, it is useful to understand the nuclear properties, especially the used nuclei on the nuclear reactor.

Nuclear density is one of the basic quantities to describe nuclear structure, which can provide detail information about nuclei internal structure, related to the wave functions of proton and neutron. In addition, nuclear charge radius is also the basic quantity, which represents the most useful observables information in nuclear structure analysis. Nuclear charge radius can provide information about nuclear shape. A method that can be used to study about nuclear structure, especially nuclei far from stability, is Skyrme-Hartree-Fock-Bogoliubov (SHFB) method, which has been used in spherical nuclei treatment extensively [1].

The SHFB method has been performed by Oberacker et al. to investigate the ground-state properties of several neutron-rich nuclei which are close to neutron drip-line [2]. Bassem et al. have used the SHFB method to study the ground-state properties of Mo and Ru [3] isotopes. Even, the SHFB method has been also used by Teran to study about the nuclei far from...
stability [4]. In this study, it is investigated the ground state properties of some common fuel materials, especially $^{232,233}$Th, $^{233,235,238}$U, $^{238-241}$Pu, and $^{241}$Am. The total energies of those materials have been calculated by using SHFB method with SIII set parameters. It is also calculated the nuclear root-mean-square (rms) radii of charge, neutron, and proton. This study aims are to calculate numerically the ground-state energy of some common fuel materials (especially $^{232,233}$Th, $^{233,235,238}$U, $^{238-241}$Pu, and $^{241}$Am) by using the SHFB method with SIII set parameters and to simulate the local densities as well as the local potentials of those nuclei.

2. Theory

2.1. The Skyrme-Hartree-Fock-Bogoliubov Method

In this study, interactions among the nucleons in the nucleus are represented by using Skyrme interaction. In Skyrme interaction, it is possible to work in coordinate space. It is very useful for nuclei close to the neutron drip-line. Skyrme interaction was first proposed by T.H.R. Skyrme in 1959 [5] and has been applied to many nuclei with great achievement in nuclear structure investigations [6, 7, 8]. To calculate the total energy of nucleus, it can be performed by using the following formula:

$$E = \int d^3\vec{r} \left[ \frac{n^2}{2m} \left( 1 - \frac{1}{3} \right) \tau + \varepsilon_{\text{Skyrme}} + \varepsilon_{\text{pair}} + \varepsilon_{\text{Coul}} \right]$$

(1)

where $\tau$ is the total kinetic energy density (the factor in parentheses represents the one-body part of the center-of-mass correction), $\varepsilon_{\text{Skyrme}}$ is the Skyrme energy density, $\varepsilon_{\text{pair}}$ is the pairing energy density, and $\varepsilon_{\text{Coul}}$ is the Coulomb energy density. The detail explanation of the energy derivation can be found in several articles [1, 8, 9]. Next, the Skyrme energy density can be approached as:

$$\varepsilon_{\text{Skyrme}} = \frac{1}{4}t_0 \left( 1 + \frac{1}{2} x_0 \right) \rho^2 - \frac{1}{4}t_0 \left( x_0 + \frac{1}{2} \right) \sum_q \rho_q^2 + \frac{1}{4}t_1 \left( 1 + \frac{1}{2} x_1 \right) \left[ \rho \tau + 3 \left( \nabla \rho \right)^2 \right]$$

$$- \frac{1}{4}t_1 \left( x_1 + \frac{1}{2} \right) \sum_q \left[ \rho_q \tau_q + \frac{3}{4} \left( \nabla \rho_q \right)^2 \right] + \frac{1}{4}t_2 \left( 1 + \frac{1}{2} x_2 \right) \left[ \rho \tau + \frac{1}{4} \left( \nabla \rho \right)^2 \right]$$

$$- \frac{1}{4}t_2 \left( x_2 + \frac{1}{2} \right) \sum_q \left[ \rho_q \tau_q + \frac{3}{4} \left( \nabla \rho_q \right)^2 \right] - \frac{1}{16} \left( t_1 x_1 + t_2 x_2 \right) J^2 + \frac{1}{16} \left( t_1 - t_2 \right) \sum_q J_q^2$$

$$+ \frac{1}{12} t_3 \rho \gamma^2 \left[ \left( 1 + \frac{1}{2} x_3 \right) \rho^2 - \left( x_3 + \frac{1}{2} \right) \sum_q \rho_q^2 \right] + \frac{1}{2} W_0 \left[ J \nabla \rho + \sum_q J_q \nabla \rho_q \right]$$

(2)

where $t_0$, $t_1$, $t_2$, $x_0$, $x_1$, $x_2$, $x_3$, $W_0$, and $\gamma$ are Skyrme set parameters, $\rho$ represents the density, and $J$ is the spin-orbit density. The isospin label $q$ represents proton or neutron, where the densities, without an isospin label in all equations, represent total densities.

| Parameter | SIII | Parameter | SIII | Parameter | SIII | Parameter | SIII |
|-----------|------|-----------|------|-----------|------|-----------|------|
| $t_0$     | -1128.75 | $x_0$     | 0.45 | $t_3$     | 14000 | $W_0$     | 120  |
| $t_1$     | 395   | $x_1$     | 0    | $x_3$     | 1    | $\gamma$  | 1    |
| $t_2$     | -95   | $x_2$     | 0    |           |      |           |      |
The pairing energy density can be approached by using:

$$\varepsilon_{\text{pair}} = \sum_q \frac{1}{4} t_0' (1 - x_q') \rho_q^2 + \frac{1}{4} t_1' (1 - x_q') \left[ \hat{\rho}_q \bar{\rho}_q + \frac{1}{4} \left( \nabla \rho_q \right)^2 \right] + \frac{1}{8} t_2' (1 + x_q') W_0' \left[ \bar{J}^2_q + \frac{1}{2\pi} t_3' (1 - x_q') \rho^\prime \bar{\rho}_q^2 \right]$$  \hspace{1cm} (3)

For Coulomb energy density, the direct and the exchange parts can be respectively expressed as [10]:

$$\varepsilon_{\text{Coul}} = \frac{1}{2} e^2 \int d^3 r' \rho_p(r) \rho_p(r') \frac{1}{|r - r'|} - \frac{2}{3} e^2 \left( \frac{3}{2} \right)^{1/3} \rho_p^{4/3} (r')$$  \hspace{1cm} (4)

The observed nuclei in this study have been treated as spherical nucleus, which means that the treatments were performed only for radial part. In the SHFB framework, for spherical symmetry, the densities, the kinetic energy densities, and the spin-orbit densities of nucleons (normal and pairing) can be respectively approached by using:

$$\rho(r) = \frac{1}{4\pi r^2} \sum_{n \ell j} (2j + 1) u_2^2 (n \ell j, r)$$  \hspace{1cm} (5)

$$\tilde{\rho}(r) = -\frac{1}{4\pi r^2} \sum_{n \ell j} (2j + 1) u_1 (n \ell j, r) u_2 (n \ell j, r)$$  \hspace{1cm} (6)

$$\tau(r) = \sum_{n \ell j} \frac{(2j + 1)}{4\pi r^2} \left[ \left( u_2 (n \ell j, r) - \frac{u_2 (n \ell j, r)}{r} \right)^2 + \left( \frac{\ell (\ell + 1)}{r^2} \right) u_2^2 (n \ell j, r) \right]$$  \hspace{1cm} (7)

$$\tilde{\tau}(r) = -\sum_{n \ell j} \frac{(2j + 1)}{4\pi r^2} \left[ \left( u_1 (n \ell j, r) - \frac{u_1 (n \ell j, r)}{r} \right) \left( u_2 (n \ell j, r) - \frac{u_2 (n \ell j, r)}{r} \right) + \frac{\ell (\ell + 1)}{r^2} u_1 (n \ell j, r) u_2 (n \ell j, r) \right]$$  \hspace{1cm} (8)

$$J(r) = \frac{1}{4\pi r^3} \sum_{n \ell j} (2j + 1) \left[ j (j + 1) - \ell (\ell + 1) - \frac{3}{4} \right] u_2^2 (n \ell j, r)$$  \hspace{1cm} (9)

$$\tilde{J}(r) = -\frac{1}{4\pi r^3} \sum_{n \ell j} (2j + 1) \left[ j (j + 1) - \ell (\ell + 1) - \frac{3}{4} \right] u_1 (n \ell j, r) u_2 (n \ell j, r)$$  \hspace{1cm} (10)

where $u$ is the radial wave function, $n$ is principal quantum number, $\ell$ is the orbital angular momentum, and $j$ is the total angular momentum. From Eq. (5), it can be calculated the rms (root-mean-square) radii of proton and neutron by using

$$\langle r_2^2 \rangle = \int_0^{R_{\text{box}}} r^2 \rho_q(r) d^3 r$$  \hspace{1cm} (11)

The difference between neutron radius and proton radius, well-known as the neutron skin thickness, can be calculated by using [11]

$$t = r_n - r_p$$  \hspace{1cm} (12)

The effective mass (normal and abnormal) due to the dependence of energy density $\varepsilon$ on the kinetic densities can be approached by using

$$M_\varepsilon = \frac{\hbar^2}{2m_q} = \frac{\hbar^2}{2m} + \frac{1}{4} \left[ (1 + \frac{2q}{J}) \rho - \left( x_1 + \frac{1}{2} \right) \rho_q \right] + \frac{1}{4} t_2 \left[ (1 + \frac{2q}{J}) \rho + \left( x_1 + \frac{1}{2} \right) \rho_q \right]$$  \hspace{1cm} (13)
2.2. The Numerov method in HFB equation

The Numerov method in HFB equation of Skyrme force parameters implemented in the HFBRAD code [9].

\[ \tilde{M}_q = \frac{1}{2} t'_1 (1 - x'_1) \rho_q \]  

For particle-hole (Hartree-Fock) field, it is given by

\[ U_q = t_0 \left( 1 + \frac{1}{2} x_0 \right) \rho - t_0 \left( x_0 + \frac{1}{2} \right) \rho_q + \frac{1}{2} t_1 \left( 1 + \frac{1}{2} x_1 \right) \left( \tau - \frac{3}{2} \Delta \rho \right) - \frac{1}{2} W_0 [\nabla J + \nabla J_q] \]

\[ - \frac{3}{4} t_1 \left( x_1 + \frac{1}{2} \right) \left( \tau - \frac{3}{2} \Delta \rho \right) + \frac{1}{4} t_2 \left( 1 + \frac{1}{2} x_2 \right) \left( \tau - \frac{1}{2} \Delta \rho \right) \]

\[ + \frac{3}{4} t_2 \left( x_2 + \frac{1}{2} \right) \left( \tau + \frac{1}{2} \Delta \rho \right) + \frac{1}{12} t_3 \left( 1 + \frac{1}{2} x_3 \right) (2 + \gamma) \rho^{\gamma+1} \]

\[ - \frac{1}{12} t_3 \left( x_3 + \frac{1}{2} \right) \left[ \rho^{\gamma-1} \sum_{q'} \rho^2_{q'} + 2 \rho^2 \rho_q \right] + \frac{1}{12} t'_3 (1 - x'_3) \rho' \rho_q \]

where the pairing field (particle-particle) is given by

\[ \tilde{U}_q = \frac{1}{2} t'_0 (1 - x'_0) \rho^2_q + \frac{1}{4} t'_1 (1 - x'_1) \left[ \tilde{\tau}_q - \frac{1}{2} \Delta \tilde{\rho}_q \right] + \frac{1}{4} t'_2 (1 - x'_2) \rho' \rho_q \]

The form factors of spin-orbit fields and its pairing respectively can be approached by using

\[ B_q = -\frac{1}{8} (t_1 x_1 + t_2 x_2) J + \frac{1}{8} (t_1 - t_2) J_q + W_0 [\rho + \rho_q] \]

\[ \tilde{B}_q = \left[ \frac{1}{2} t'_2 (1 + x'_2) + W'_0 \right] \tilde{J}_q \]

where \( t'_0, t'_1, t'_2, t'_3, x'_0, x'_1, x'_2, x'_3, W'_0 \), and \( \gamma' \) are the parameter in the particle-particle channel of Skyrme force parameters implemented in the HFBRAD code [9].

2.2. The Numerov method in HFB equation

The matrix form of the fields can be defined as

\[ \mathcal{M} = \left( \begin{array}{cc} M & \tilde{M} \\
\tilde{M} & \tilde{M} \end{array} \right), \quad \mathcal{U} = \left( \begin{array}{cc} U - \lambda & \tilde{U} \\
\tilde{U} & -U + \lambda \end{array} \right) \]

\[ \mathcal{U}_{so} = \left( \begin{array}{cc} B & \tilde{B} \\
\tilde{B} & -B \end{array} \right) \left( j (j+1) - \ell (\ell+1) - \frac{3}{4} \right) \]

The HFB equations can be written as

\[ \left[ -\frac{d}{dr} \mathcal{M} \frac{d}{dr} + \mathcal{U} + \mathcal{M} \frac{\ell (\ell+1)}{r^2} + \mathcal{M}' \frac{1}{r} + \mathcal{U}_{so} \right] \left( \begin{array}{c} u_1 \\
u_2 \end{array} \right) = E \left( \begin{array}{c} u_1 \\
u_2 \end{array} \right) \]

This equation can be written as an equation with no differential operator in the coupling terms and no first order derivative, i.e.

\[ -M^* \frac{d^2}{dr^2} f_1 + V f_1 + W f_2 = E f_1 \]

\[ M^* \frac{d^2}{dr^2} f_2 + V f_2 + W f_1 = E f_2 \]

This last form, with no first order derivative of the functions, is particularly suitable for numerical integration by the Numerov algorithm. In this study, it is used the Numerov (Cowell) method as the standard technique to solve the integration of second-order differential equations [9, 12].

Consider the function \( y(r) \) as the solution of the differential equation

\[ y'' = F(y, r) \]
Based on the Numerov algorithm, it is used the finite difference formula for three consecutive points on a mesh with step $h$

$$y_{n+1} - 2y_n + y_{n-1} = \frac{h^2}{12} \left( y''_{n-1} + 10y''_n + y''_{n+1} \right) + O(h^6) \quad (24)$$

where $O(h^6)$ is the error in this relation. Combining eq. (24) with eq. (23), it can be obtained the relation

$$\left(1 - \frac{h^2}{12} F_{n+1}\right)y_{n+1} - 2 \left(1 + \frac{5h^2}{12} F_n \right)y_n + \left(1 - \frac{h^2}{12} F_{n-1}\right)y_{n-1} = 0 \quad (25)$$

In this study, to perform numerical calculation, the HFBRAD code [9] has been utilized with SIII set parameters. The SIII set parameters are set up by the adjustment of Skyrme interaction parameters through the binding energy and charge radii fittings of some semi-magic nuclei. The SIII set parameters work well for nuclei close to sphericity with small deformations [13]. In this study, the grid has been set at 0.1 fm with 400 mesh point. The side purpose of this study is to observe the precision of HFBRAD code in calculation of nuclear energy for nuclei far from stability. The calculation results have been compared with the related experiment data [14, 15].

3. Results and Discussion

3.1. Total Energy and Nuclear Radii

The calculation results of total energy for each nucleus investigated in this study are shown in Table 2. From Table 2, it can be seen that the calculation results are in good agreement with the experiment results with 0.687%-0.952% of discrepancies. The total energy of $^{233}$Th is almost similar with that of $^{233}$U although $^{233}$Th and $^{233}$U have different numbers of proton and neutron ($^{233}$Th has 90 protons with 143 neutrons and $^{233}$U has 92 protons with 141 neutrons). It is also similar for the cases of $^{238}$U with $^{238}$Pu and $^{241}$Pu with $^{241}$Am.

| Nucleus | Exp. [14] (MeV) | This study (MeV) | discr.* (%) | Nucleus | Exp. [14] (MeV) | This study (MeV) | discr.* (%) |
|---------|----------------|----------------|-------------|---------|----------------|----------------|-------------|
| $^{232}$Th | -1766.686 | -1753.916 | 0.723 | $^{238}$Pu | -1801.268 | -1784.689 | 0.920 |
| $^{233}$Th | -1771.472 | -1759.187 | 0.693 | $^{239}$Pu | -1806.914 | -1790.722 | 0.896 |
| $^{235}$U | -1771.721 | -1759.541 | 0.687 | $^{240}$Pu | -1813.449 | -1796.708 | 0.923 |
| $^{235}$U | -1783.863 | -1771.033 | 0.719 | $^{241}$Pu | -1818.690 | -1802.649 | 0.882 |
| $^{238}$U | -1801.689 | -1787.934 | 0.763 | $^{241}$Am | -1817.929 | -1800.632 | 0.952 |

*discrepancy

The charge, mass, proton, and neutron radii for each nucleus have been also calculated. The calculation results are shown in Table 3. As well as the results of total energies, the calculation results of charge radii are also in good agreement with the related experiment results. From Table 3, it can be indicated that the charge, mass, and proton radii increase accordingly with the increase of nucleon number. From those results above, the obtained results of HFBRAD code are in good agreement with the related experiment results. It is indicated that the HFBRAD code can be a useful tool to investigate the ground state properties of nuclei used on nuclear reactor, especially heavy nuclei.
Table 3. The nuclear radii of fuel elements (the units of radii and neutron skin are in fm).

| Nucleus  | Neutron number | Charge radius Exp. [15] | Charge | Radius | Proton | Neutron | Neutron skin thickness |
|----------|----------------|-------------------------|--------|--------|--------|---------|----------------------|
| ^{232}\text{Th} | 142 | 5.7848±0.0124 | 5.8099 | 5.8306 | 5.7546 | 5.8783 | 0.1237 |
| ^{233}\text{Th} | 143 | 5.8203±0.0049 | 5.8335 | 5.8420 | 5.7784 | 5.8831 | 0.1275 |
| ^{235}\text{U} | 143 | 5.8337±0.0041 | 5.8456 | 5.8591 | 5.7906 | 5.9029 | 0.1123 |
| ^{238}\text{U} | 146 | 5.8571±0.0033 | 5.8630 | 5.8842 | 5.8082 | 5.9315 | 0.1234 |
| ^{239}\text{Pu} | 144 | 5.8535±0.0378 | 5.8771 | 5.8838 | 5.8224 | 5.9235 | 0.1011 |
| ^{240}\text{Pu} | 145 | 5.8601±0.0378 | 5.8829 | 5.8920 | 5.8283 | 5.9330 | 0.1047 |
| ^{241}\text{Pu} | 146 | 5.8701±0.0379 | 5.8886 | 5.9002 | 5.8340 | 5.9424 | 0.1084 |
| ^{241}\text{Am} | 147 | 5.8748±0.0379 | 5.8943 | 5.9083 | 5.8397 | 5.9517 | 0.1119 |

3.2. The Profiles of Density and Potential

In this study, it is also investigated the profiles of density and potential for each fuel element to understand its distribution. In Figure 1, it can be seen that neutron densities are larger than proton densities because neutron numbers in each observed nucleus are larger than proton numbers. Proton densities of all observed nuclei in this study are similar to each other and so are the neutron densities. The widths of proton densities for all nuclei are almost similar to each other and so are the widths of neutron densities. The densities of proton and neutron decreased drastically in radius 5-10 fm and approached to zero smoothly at r \geq 10 fm.

In Figure 2, it can be seen that neutron potentials are deeper than that of proton in radius.
0-5 fm. In other hand, proton potentials are larger than neutron potential in \( r \geq 10 \) fm. Proton potentials of all observed nuclei in this study are similar to each other and so are the neutron potentials. The widths of proton and neutron potentials are almost similar. From those results above, it can be seen that the results of this study are in good agreement with the results of the related experiment.

4. Summary

In this study, it has been performed the investigation of the total energy, nuclear radii, and neutron skin thickness of nuclear reactor fuel elements, especially \(^{232,233}\)Th, \(^{233,235,238}\)U, \(^{238-241}\)Pu, and \(^{241}\)Am, by using Skyrme-Hartree-Fock-Bogoliubov method. Both proton and neutron densities were calculated by using SIII set parameters. The obtained results of this study have achieved the good agreement with the related experiment results as well as the results of HFBRAD code. It can be indicated that SHFB method applied in the HFBRAD code can be a useful tool to investigate the ground-state properties of nuclei far from stability.

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