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ORIGINAL RESEARCH

A Study on $^{8-18}$Be Isotopes Used on Neutron Multiplier in Reactor Design

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Abstract Neutronic characterization and development of structural materials, neutron multiplier materials, tritium breeders are primarily important for fusion and hybrid reactors. In order to improve neutron economy, beryllium, lead, bismuth, zirconium are considered and used as neutron multiplier materials in fusion and hybrid reactor design. In this study, rms charge radii, neutron radii, mass radii and neutron skin thickness were calculated for $^{8-18}$Be isotopes nuclei. The neutron and proton density are calculated for Be isotopes. The results obtained were compared with the experimental and theoretical results of other researchers by using Hartree–Fock method with an effective interaction with Skyrme forces.

Keywords $^{8-18}$Be isotopes · Neutron and proton density · Skyrme force · rms radii · Hartree–Fock calculations

Introduction

In the next century the world will face the need for new energy sources. Fusion serves an inexhaustible energy for humankind. Nuclear fusion can be one of the most attractive sources of energy from the viewpoint of safety and minimal environmental impact. Fusion will not produce CO_2 or SO_2 and thus will not contribute to global warming or acid rain [1]. And also; there are not radioactive nuclear waste problems in the fusion reactors. The fusion–fission hybrid is a combination of the fusion and fission processes [2–4]. In the fusion–fission hybrid reactor, tritium self-sufficiency must be maintained for a commercial power plant [2–4].

Neutronic characterization and development of structural materials, neutron multiplier materials, tritium breeders are primarily important for fusion and hybrid reactors. The (n, 2n) reactions of the selected blanket materials can play a key role for multiplying neutrons in reactor environment. In order to improve neutron economy, beryllium (Be), lead (Pb), bismuth (Bi), zirconium (Zr) are considered and used as neutron multiplier materials in fusion and hybrid reactor design. The Hartree–Fock method with an effective interaction with Skyrme forces is widely used for studying the properties of nuclei [5–7]. This method is successfully used for a wide range of nuclear characteristics such as binding energy, single particle energy, mass rms radii, neutron rms radii, proton rms radii, charge rms radii, neutron and proton density, electromagnetic multipole moments, etc. [8–11]. In this study, by using Hartree–Fock approximation with effective SKM* Skyrme force parameter, charge rms radii, mass rms radii, proton rms radii, neutron rms radii, neutron skin thickness, neutron and proton density were calculated for $^{8-18}$Be isotopes nuclei. The calculated results were compared with the experimental and theoretical results of other studies.

Calculations of the Total Energy of Nucleus

The Hartree–Fock equations and pairing equations are derived variationally from the total energy functional of the nucleus [5–7],

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$$\mathbf{E} = \mathbf{E_{Skyrme}} + \mathbf{E_{Coulomb}} + \mathbf{E_{pair}} - \mathbf{E_{cm}} \quad (1)$$

where $\mathbf{E}$ is the total energy of the nucleus, $\mathbf{E_{Skyrme}}$ is the energy of the Skyrme interaction, $\mathbf{E_{Coulomb}}$ is the Coulomb interaction energy, $\mathbf{E_{pair}}$ is the two nucleon interaction pairing energy and $\mathbf{E_{cm}}$ is the correction for the spurious center-of-mass motion of the mean field. $\mathbf{E_{Skyrme}}$ energy is calculated by using the effective Skyrme force [6].

The Coulomb interaction's infinite range makes it very consuming to evaluate the exchange part exactly and makes the exchange contribution only a small fraction of the total Coulomb energy, thus to preserving the simplicity of the Skyrme-Hartree–Fock with equation the Coulomb-exchange part treated in the Slater approximation [6]. The Coulomb energy is given by

$$E_{Coul} = \frac{1}{2}e^2 \int d^3rd^3r' \rho_C(\vec{r}) \frac{1}{\left|r - \vec{r'}\right|} \rho_C(\vec{r'}) + E_{Coul,exch} \quad (2)$$

$$E_{Coul,exch} = -\frac{3}{4}(\frac{3}{\pi})^{1/3} 4\pi \int_0^\infty drr^2 \rho_{pr}^{4/3}. \quad (3)$$

where e is the charge of the electron, $\rho_c(r)$ is the charge density and ρ_{pr} is the proton density. In the direct term, the nuclear charge distribution includes in folding with the finite size of the proton. The nuclear charge density is a most useful observable for analyzing nuclear structure: it provides information about the nuclear shape and can be determined by clear-cut procedures from the cross section for elastic electron scattering [12]. To compute the observable charge density from the Hartree–Fock results, one has to take into account that the nucleons themselves have an intrinsic electromagnetic structure [13]. Thus one needs to fold the proton and neutron densities from the Hartree–Fock method with the intrinsic charge density of the nucleons. Folding becomes a simple product in Fourier space, so that it is transformed the densities to the so-called form factors

$$F_q(k) = 4\pi \int_0^\infty r^2 j_0(kr) \rho_q(r) dr \quad (4)$$

where j_0 is the spherical Bessel function of zeroth order. In fact, the form factor is closer to experiment because in the Born approximation it directly represent the amplitude for scattering at momentum transfer $\hbar k$. The charge form factor is then given by

$$F_C(k) = \sum_q \left[F_q(k)\, G_{E,q}(k) + F_{ls,q}(k)\, G_M(k)\right] \exp\left(\frac{1}{8}(\hbar k)^2 \Big/ \left\langle p_{cm}^2 \right\rangle\right). \quad (5)$$

where $F_{ls,q}$ is the form factor of the spin–orbit current ∇J (accounting for magnetic contributions to the charge density), $G_{E,q}$ are the electric form factors of the nucleons, G_M is the magnetic form factor of the nucleons (assumed to be equal for both species), and the exponential factor takes into account an unfolding of the spurious vibrations of the nuclear center of mass in the harmonic approximation. The charge density is obtained from the charge form factor by the inverse Fourier–Bessel transform

$$\rho_{char}(r) = \frac{1}{2\pi^2} \int k^2 j_0(kr)\, F_C(k)\, dk. \quad (6)$$

Other information can be drawn directly from the form factor. Alternative information on the overall nuclear size is given by the root-mean-square (r.m.s) radius r, which is determined from the curvature of the form factor at $k \to 0$ as

$$r = 3\left(\frac{d^2}{dk^2} F_C(k)|_{k=0}\right) \Big/ F_C(0). \quad (7)$$

It does not carry much new information because it can be related to R and σ approximately as $r = \sqrt{R^2 + 3\sigma^2}$ [14]. The parameterization in terms of R and σ is preferable because the diffraction radius R is very stable against correlations and depends smoothly on the particle number A, whereas the surface thickness σ is sensitive to shell effects and correlations from low energy modes. The simplicity of the ansatz allows the expectation values of the energy for Slater determinants to be evaluated in terms of a few nucleon densities,

$$\rho_q(\vec{r}) = \sum_{\beta \in q} w_\beta \phi_\beta(\vec{r})^+ \phi_\beta(\vec{r}) \quad (8)$$

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. Completely filled shells have $\omega_\beta = 1$, but fractional occupancies occur for nonmagic nuclei; these are determined by the pairing scheme. We restrict consideration to the (stationary) ground state of spherical nuclei. The single-particle wave functions can be separated as

$$\phi_\beta(\vec{r}) = \frac{R_\beta(r)}{r} Y_{j_\beta l_\beta m_\beta}(\theta, \varphi) \quad (9)$$

The functions $Y_{j_\beta l_\beta m_\beta}$are spinor spherical harmonics [15]. The radial wave functions R_β are independent of the m_β quantum number. The factor $1/1r$. has been separated to simplify the overlap integrals to simple r-integration.

$$\left\langle \varphi_\beta \,\middle|\, \varphi'_\beta \right\rangle = \delta_{j_\beta j'_\beta} \delta_{l_\beta l'_\beta} \delta_{m_\beta m'_\beta} \int_0^\infty dr R_\beta(r) R'_\beta(r). \quad (10)$$

The nucleon densities in spherical representation are

$$\rho_q(r) = \sum_{n_\beta j_\beta l_\beta} w_\beta \frac{2j_\beta + 1}{4\pi} \left(\frac{R_\beta}{r}\right)^2. \quad (11)$$

The rms radii for protons and neutrons are defined as

$$\left\langle r_q^2 \right\rangle = \int_0^{R_{box}} r^2 \rho_q^2(r) d^3 r. \quad (12)$$

Results and Discussion

We have used the Skyrme interaction parameters for calculations. The Skyrme force parameters can be finding from the reference [6–9]. We have used for calculations with the program HAFOMN (http://www.phys.washington.edu/users/bulgac/Koonin/Skyrme_Hartree_Fock/skhafo.for). In these calculations, the pairing equations are solved by Newton's tangential iteration. For description of the systems consisting of an odd number of particles, we have used the filling approximation. The Hartree–Fock and pairing equations are coupled, and they are solved by simultaneous iteration of the wave functions and the occupation weight sw_β. Completely filled shells have $w_\beta = 1$, but fractional occupancies occur for nonmagic nuclei.

In this study, we have calculated by using the Hartree–Fock method with an effective interaction with Skyrme forces parameters for the Be isotopes and compared with experimental data experimental rms nuclear charge radii in Table 1. Although the Be nuclei has constant ($Z = 4$) proton number, it can be seen that the calculated with Skyrme force nuclear charge rms radii of Be isotopes decrease about from 2.3–2.5 fm (for ^{8}Be) to 2.1–2.4 fm (for ^{18}Be) in Table 2. Theoretically the calculated charge rms values are quite consistent with the theoretical calculations with all the Skyrme forces parameters. Also in Table 1, the nuclear charge rms values calculated by using Skyrme forces have been compared with the values of radius $r_o A^{1/3}$ in liquid-drop model in which the number of nucleons per unit volume is roughly constant. The value of r_o has been taken as 1.25 fm from electron scattering experiments. On the contrary of Hartree–Fock calculations with Skyrme forces, the radius values in liquid-drop model have been increased from 2.5 fm (for ^{8}Be) to 3.3 fm (for ^{18}Be) depending on the mass number A. We have clearly shown that there are important differences between the values of calculated with Quantum mechanical Skyrme Hartree–Fock model and $r_0 A^{1/3}$ in liquid-drop model. Theoretical values of two different averaging procedures, a refined Evaluated-1 (R_{for}) and a simpler Evaluated-1 (R_{exc}),

Table 2 Calculated nuclear mass rms radii (in fm)

	SI	SIII	SVI	T3	SKM	SKM*	$r_0 A^{1/3}$
^{8}Be	2.061	2.253	2.382	2.199	2.242	2.278	2.500
^{9}Be	2.140	2.312	2.262	2.293	2.308	2.341	2.600
^{10}Be	2.218	2.360	2.334	2.363	2.357	2.389	2.693
^{11}Be	2.366	2.483	2.466	2.520	2.517	2.545	2.779
^{12}Be	2.474	2.559	2.558	2.614	2.605	2.630	2.861
^{13}Be	2.724	2.801	2.791	2.823	2.817	2.840	2.939
^{14}Be	2.848	2.927	2.909	2.940	2.933	2.954	3.012
^{15}Be	2.987	3.072	3.046	3.072	3.060	3.080	3.082
^{16}Be	3.072	3.159	3.130	3.162	3.144	3.164	3.149
^{17}Be	3.140	3.228	3.198	3.240	3.215	3.234	3.214
^{18}Be	3.197	3.286	3.256	3.309	3.279	3.297	3.275

Table 1 Calculated nuclear charge rms radii (in fm and $r_0 = 1.25$ fm)

	SI	SIII	SVI	T3	SKM	SKM*	$r_0 A^{1/3}$	Other calculations and Exp.
^{8}Be	2.295	2.422	2.172	2.463	2.477	2.512	2.500	
^{9}Be	2.259	2.376	2.345	2.400	2.414	2.446	2.600	2.620 ± 0.091 (Exp) [16] 2.5180 ± 0.0114(R_{for}) [17, 18] 2.5180 ± 0.0119 (R_{exc}) [17] 2.519 ± 0.012 (Eval.) [17]
^{10}Be	2.245	2.352	2.329	2.366	2.377	2.408	2.693	
^{11}Be	2.271	2.377	2.355	2.406	2.422	2.451	2.779	
^{12}Be	2.290	2.390	2.371	2.418	2.438	2.465	2.861	
^{13}Be	2.240	2.350	2.328	2.387	2.410	2.438	2.939	
^{14}Be	2.227	2.336	2.316	2.378	2.404	2.431	3.012	
^{15}Be	2.212	2.324	2.305	2.373	2.401	2.429	3.082	
^{16}Be	2.201	2.313	2.294	2.365	2.396	2.423	3.149	
^{17}Be	2.191	2.305	2.286	2.359	2.391	2.419	3.214	
^{18}Be	2.182	2.299	2.278	2.354	2.387	2.415	3.275	

Table 3 Calculated nuclear neutron rms radii (in fm)

	SI	SIII	SVI	T3	SKM	SKM*	Other calculations	Exp.
^{8}Be	2.051	2.243	2.161	2.187	2.227	2.263		
^{9}Be	2.195	2.363	2.316	2.351	2.341	2.373		
^{10}Be	2.299	2.438	2.416	2.455	2.420	2.451		
^{11}Be	2.499	2.603	2.593	2.656	2.634	2.662	3.65 [17]	2.73 ± 0.05 [20, 22]
^{12}Be	2.621	2.690	2.697	2.763	2.737	2.762		
^{13}Be	2.940	3.001	2.994	3.028	3.008	3.029		
^{14}Be	3.073	3.142	3.123	3.157	3.137	3.156	2.95 [19]	3.22 ± 0.19 [21]
^{15}Be	3.229	3.305	3.277	3.301	3.277	3.295		
^{16}Be	3.310	3.390	3.358	3.390	3.360	3.378		
^{17}Be	3.370	3.454	3.421	3.465	3.428	3.446		
^{18}Be	3.419	3.505	3.472	3.530	3.487	3.504		

and experimental values for ^{9}Be nucleus have been given in Table 1. The values calculated with SKM* are closer to those two values.

We have calculated the nuclear mass rms radii by using the Hartree–Fock with Skyrme forces parameters for the Be isotopes without discriminating neutron and proton in Table 2. From Table 2, it has been shown that the values of nuclear mass rms radii calculated from Quantum mechanical Skyrme forces are come close to those of radius $r_0A^{1/3}$ in liquid-drop model, with the increasing of the mass number A. The calculated neutron rms radii with the Skyrme Hartree–Fock model have been given in Table 3. The obtained values have approximately been increased from 2.2 fm (for ^{8}Be) to 3.5 fm (^{18}Be) with the increasing of the number of neutron. If ^{12}Be nucleus is assumed as core, ^{11}Be and ^{14}Be are one and two neutron halos, respectively. The experimental values of neutron rms radii for ^{11}Be and ^{14}Be are 2.73 ± 0.05 and 3.22 ± 0.19 fm, respectively. It is seen that, the values of neutron rms radii calculated with using of SKM* parameters are very agreement with the experimental values.

The other theoretical results of other studies for ^{11}Be and ^{14}Be nuclei are also given in Table 3. In this study, it can be seen that the results obtained with SKM* for away from closed-shell configuration are in good agreement with those of experimental values in during of comparing to the other theoretical studies because of taking into consideration the fission barriers and heavy deformed nuclei. Finally, the proton rms radii with the Skyrme Hartree–Fock model have been calculated for Be isotopes and given in Table 4. As it has been given in Tables 1 and 4, we can say that the values of charge-rms radii calculated for all Skyrme parameters (in Table 1) are bigger than those of the proton rms radii (in Table 4). The values of charge rms radii have been decreased with the increasing of mass number A but those of the proton rms radii have been increased.

Table 4 Calculated nuclear proton rms radii and the neutron skin thickness ***t*** of Be isotopes for SKM* parameter (in fm)

	SI	SIII	SVI	T3	SKM	SKM*	*t* (SKM*)
^{8}Be	2.071	2.264	2.182	2.210	2.257	2.294	−0.031
^{9}Be	2.071	2.246	2.191	2.218	2.266	2.301	0.072
^{10}Be	2.090	2.238	2.205	2.218	2.260	2.292	0.159
^{11}Be	2.111	2.259	2.225	2.262	2.297	2.328	0.334
^{12}Be	2.149	2.276	2.255	2.286	2.316	2.344	0.418
^{13}Be	2.159	2.288	2.266	2.294	2.329	2.358	0.671
^{14}Be	2.183	2.303	2.285	2.313	2.347	2.375	0.781
^{15}Be	2.187	2.316	2.293	2.329	2.364	2.393	0.902
^{16}Be	2.210	2.332	2.313	2.347	2.380	2.408	0.970
^{17}Be	2.231	2.348	2.330	2.364	2.396	2.424	1.022
^{18}Be	2.250	2.364	2.347	2.381	2.412	2.439	1.065

A quantity of both theoretical and experimental interest, the neutron skin thickness ***t***, can then be defined as the difference between the neutron rms radius and the proton rms radius

$$t = r_n - r_p \tag{13}$$

Also, theoretically with SKM* parameters calculated the neutron skin thickness ***t*** values were given in Table 4. It has been shown from Table 4 that the neutron skin thickness ***t*** values have increased from 0.031 fm (for ^{8}Be) to 1.065 fm (for ^{18}Be) by increasing the neutron number. These values for halo nuclei have been calculated as 0.334 fm (for ^{11}Be) and 0.781 fm (for ^{14}Be).

We have calculated the proton and neutron densities for the Be isotopes in Figs. 1, 2, 3 and 4. ^{8}Be has the same proton and neutron number ($N = Z$) and the last two neutron of that are present in the $1P_{3/2}$ sub-shell. The proton and neutron density values of ^{8}Be nuclei are close to each other from center ($r = 0$) to surface (in Fig. 1). The ^{8}Be nuclei have not the neutron number of closed sub-shell.

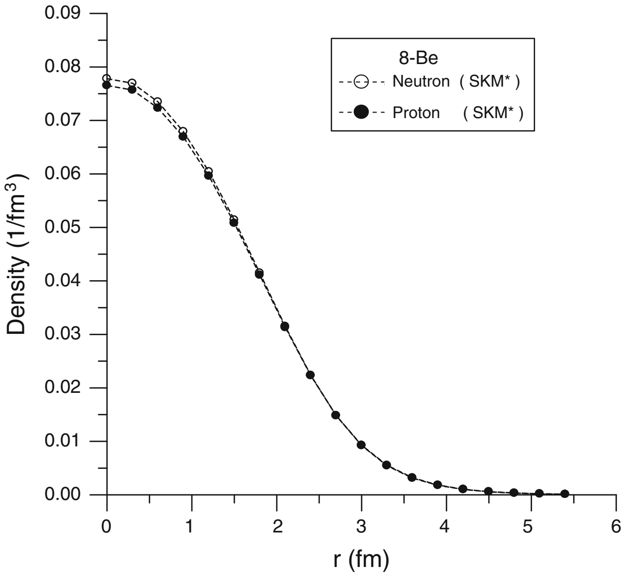

Fig. 1 Calculated using the SKM* parameter neutron and proton densities of 8-Be isotope

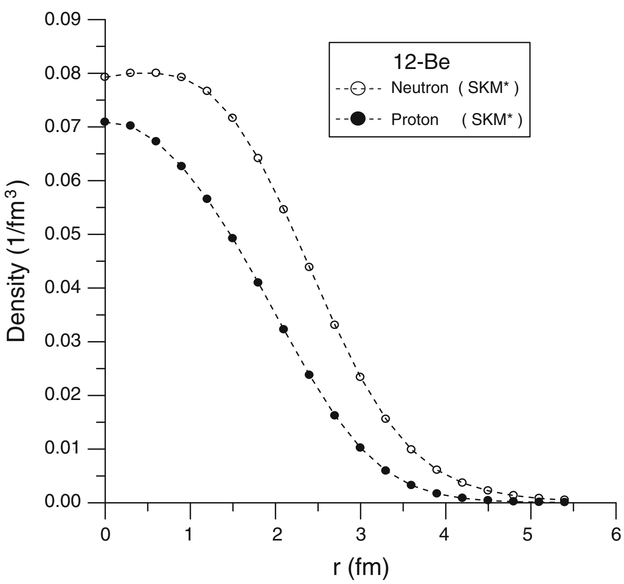

Fig. 2 Calculated using the SKM* parameter neutron and proton densities of 12-Be isotope

The $1D_{5/2}$ level is completely filled by neutrons for ^{18}Be nuclei. Both $1P_{3/2}$ and $1P_{1/2}$ sub-shell levels for ^{12}Be nucleus are also completely filled by neutrons. ^{12}Be and ^{18}B nuclei have spherical properties due to being the sub-shell filled completely by neutrons. The neutron and proton densities of those nuclei have been given in Figs. 1, 2, 3 and 4. ^{14}Be nucleus is far away from closed-shell configurations. The Skyrme-Hartree–Fock method is the useful for calculating of the spherical nuclei because this force is central and has zero range interactions. These means that the interactions are only dependence of radial and there is

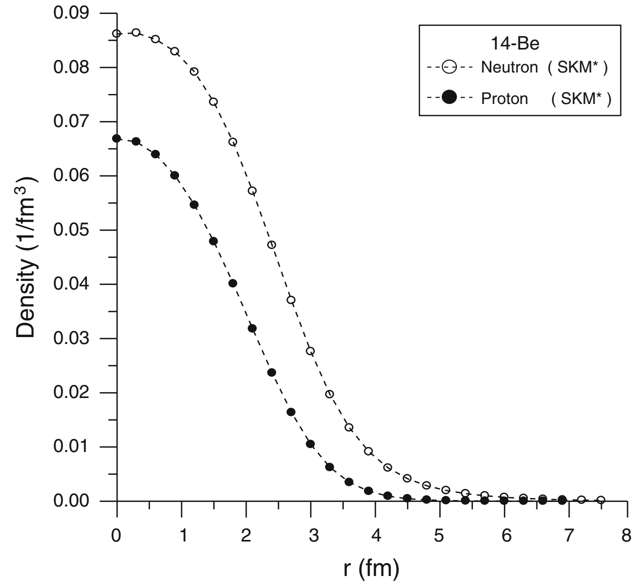

Fig. 3 Calculated using the SKM* parameter neutron and proton densities of 14-Be isotope

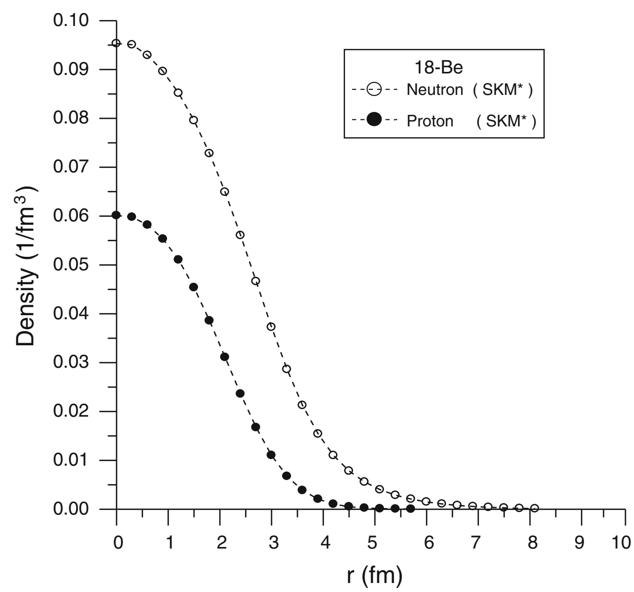

Fig. 4 Calculated using the SKM* parameter neutron and proton densities of 18-Be isotope

not dependence of angular. We have also draw the comparison of the calculated using only the SKM* parameter neutron and proton densities of Be in Figs. 1, 2, 3 and 4. The proton density for all Be isotopes changes from center ($r = 0$) to 4–5 fm. On the other hand, the neutron density changes from 4–5 fm (for ^{8}Be) to 7–8 fm (for ^{18}Be). The difference between the neutron and proton densities in center is nearly come to zero for $Z = N$ (^{8}Be). However, this difference has proportionally been large by increasing of the neutron number.

Summary and Conclusions

In this study, rms charge radii, neutron radii, mass radii, neutron-proton density and neutron skin thickness were calculated for $^{8-18}$Be isotopes nuclei. The calculated results have been also compared with the available experimental values in literature. The results can be summarized and concluded as follows:

1. The calculated nuclear charge rms radii of Be isotopes decrease about from 2.3 fm–2.5 (for ^{8}Be) to 2.1–2.4 fm (for ^{18}Be).
2. The radius values in liquid-drop model have been increased from 2.5 fm (for ^{8}Be) to 3.3 fm (for ^{18}Be) depending on the mass number *A*.
3. The calculated neutron rms radii values have approximately been increased from 2.2 fm (for ^{8}Be) to 3.5 fm (^{18}Be) with the increasing of the number of neutron.
4. The values of charge rms radii have been decreased with the increasing of mass number *A* but those of the proton rms radii have been increased.
5. The neutron skin thickness values have increased from 0.031 fm (for ^{8}Be) to 1.065 fm (for ^{18}Be) by increasing the neutron number.
6. The Skyrme-Hartree–Fock method is the useful for calculating of the spherical nuclei because this force is central and has zero range interactions.

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