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Investigation of some nuclear structure properties of ^{213}Bi, ^{201}Tl, ^{188}Re, ^{186}Re, ^{133}Xe, ^{131}I, ^{125}I, ^{123}I, ^{111}In, ^{94}Tc, ^{90}Y, ^{67}Ga, ^{67}Cu, ^{62}Cu, ^{61}Cu, ^{55}Co, and ^{48}V nuclei used in SPECT in axial deformation

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Abstract: The present work mainly purposed to investigate significant nuclear structure properties nuclei used in single photon emission computed tomography (SPECT), in addition to ground state nuclear properties such as the binding energy per particle, the root mean square (rms) charge, and proton and neutron radii. Besides, we calculated the neutron skin thicknesses (NST), the proton, neutron quadrupole moments (Q_P, Q_N), quadrupole deformation parameter (β_2), and the proton and neutron pairing energies (P_P, P_N) to determine shapes and deformations of SPECT nuclei including odd-odd or odd-even/even-odd nuclei in axial symmetry for Skyrme and Gogny interactions. To analyze the accuracy of the calculated results, the calculated results were compared with available experimental and the theoretical finite-range liquid-drop model (FRDM), and discussed for 12 different force interactions. Notably, the results provide thorough nuclear data to the literature for deformed nuclei of SPECT.

Key words: Nuclear structure, Skyrme and Gogny forces, deformation, SPECT

1. Introduction

The structure and properties of nuclei have been explained by nuclear structure [1–6] and reaction theories [7–12] such as Hartree–Fock–Bogoliubov (HFB) approach for the determination of nuclear properties of spherical nuclei, e.g., the root mean square (rms) charge, proton, neutron radii and the binding energies [1–5]. For accurate determination of nuclear structure and properties of nuclei, many force interactions such as SKM*, SLY4, DS1 etc. have been derived under the leadership of Skyrme and Gogny based on theoretical formulation that can describe the structure of even-even nuclei. However, the recent development of new codes with HFB framework has made it possible to calculate the nuclear structure and properties for both even-even and odd-odd/odd-even nuclei through blocking of quasiparticles approach. At the present time, one of these codes is HFBTHO (3.00), the newest version [6], which is available for quadrupole deformation parameter (β_2), the neutron and proton pairing energies, the proton and neutron quadrupole moment calculations in addition to the binding energies, the charge, proton, and neutron radii. In fact, the code including HFB solutions for deformed nuclei inharmonic oscillator (HO) potential is carried out in axial symmetry, and this code includes not only Skyrme force parameters but also Gogny force parameters, such as D1S, D1p, D1, and D1N [6]. For the aims described above, such a code can be exploited when establishing the nuclear structure properties of nuclei used in single photon emission computed tomography (SPECT) because the nuclei used in SPECT are

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generally odd-odd or odd-even/even-odd deformed nuclei. Moreover, determining of the ground state nuclear structure properties of nuclei is important as these properties such as quadrupole deformation parameters (β_2), the quadrupole moments, pairing energy, neutron skin thickness etc. keep informed about shape and surface of nuclei in accordance with the purpose of the nuclear physics. To calculate the nuclear properties of nuclei which have not been calculated up to now, HFBTHO, which may calculate the properties of odd-odd or odd-even nuclei in axial deformation, allows to meet deficiency in the literature. For the medical nucleus selection, the calculations of SPECT nuclei are suitable for odd nuclei, and although the studies including the nuclear properties of PET nuclei, and the nuclei used in nuclear batteries [2] are available in the literature, there are not any calculations for SPECT nuclei. Additionally, the obtained results via new version of the code HFBTHO 3.00 pave the way for understanding of axial approach, and Skyrme, Gogny interactions used in code.

Furthermore, it is important to understand nuclear structure of medical nuclei, because these nuclei are produced by charged particle induced reactions**,** including preequilibrium (PEQ) reaction mechanism at about 14–15 MeV [13], where initial exciton numbers act a part significant because initial exciton numbers are obtained from proton and neutron density radii. Accordingly, proton and neutron radii of each nucleus should be known for all the force parameters. The proton and neutron initial exciton numbers (X_p and X_n) dependent on proton and neutron radii of nuclei and these numbers can be effectively used in proton induced reactions with PEQ reaction mechanism to produce medical radioisotope [13,14]. Besides, in terms of structure of nucleus, the neutron thicknesses ($S_n \equiv \langle r_n^2 \rangle^{1/2} - \langle r_p^2 \rangle^{1/2}$) obtained from the difference between proton and neutron radii provide understanding of the asymmetry of neutron and proton dispersion in the nucleus, and the features of equation of state (EOS) for dissymmetrical nuclear matter, and the interaction and neutron abrasion cross-sections in heavy ion collisions [15–21].

In this paper, the ground state nuclear structure and properties of nuclei used in SPECT, ^{213}Bi, ^{201}Tl, ^{188}Re, ^{186}Re, ^{133}Xe, ^{131}I, ^{125}I, ^{123}I, ^{111}In, ^{94}Tc, ^{90}Y, ^{67}Ga, ^{67}Cu, ^{62}Cu, ^{61}Cu, ^{55}Co and ^{48}V have been calculated in axial deformation for Skyrme and Gogny force parameters, S3, SKM*, SKP, SKX, SLY4, HFB9, UNEDF0, UNEDF1 [22–29] and D1, D1N, D1p, D1S [30–33], respectively. For this aim, based on Skyrme and Gogny force parameters, the neutron, proton pairing energies and quadrupole moments, the binding energy, the rms charge, proton and neutron radii, the quadrupole deformation parameter, and the neutron skin thickness (NST) obtained by the HFBTO code were compared with the experimental data [34,35] and the theoretical results of the finite-range liquid-drop model (FRDM) [36].

2. Theoretical framework

To investigate the nuclear structure and properties of SPECT nuclei, Skyrme and Gogny's force interactions were used based on axial deformations. In addition to even-even nuclei, the nuclear properties of odd-odd nuclei are also determined, and in order to compensate such a need in the axial deformation, the blocking of quasiparticles approach in the Equal Filling Approximation (EFA), which is an ideal approximation to exact blocking, can be recommended in the calculation of nuclear properties of both odd-odd and odd-even nuclei. For each iteration in the code, the mean field Hamiltonian that ensures a sequence equivalent single-particle states is diagonalized. The code defines index of quasiparticles to be blocked by taking into account the overlap between quasiparticle wave function and single particle wave function based on the Nilsson quantum numbers supplied in input of the code [6,37,38].

Each force interaction of Skyrme and Gogny is presented together with the parameter values in Tables 1 and 2 [1–3,6].

2.1. Hartree–Fock–Bogolyubov method for Skyrme forces

HFB approach is given in the form of local energy density functional [6,37,38]:

$$E\left[\rho,\tilde{\rho}\right]=\int d^{3}\vec{r}\mathrm{H}\left(\vec{r}\right), \tag{1}$$

where, $\mathrm{H}\left(\vec{r}\right)$ consists of two Hamiltonians, which are the sum of mean field ($H\left(\vec{r}\right)$) and pairing energy densities ($\tilde{H}(\vec{r})$):

$$\mathrm{H}\left(\vec{r}\right)=H\left(\vec{r}\right)+\tilde{H}\left(\vec{r}\right), \tag{2}$$

$$\begin{aligned}
H\left(\vec{r}\right) &= \frac{\hbar^{2}}{2m}\tau+\frac{1}{2}t_{0}\left[\left(1+\frac{1}{2}x_{0}\right)\rho^{2}-\left(\frac{1}{2}+x_{0}\right)\sum_{q}\rho_{q}^{2}\right]\\
&+\frac{1}{2}t_{1}\left[\left(1+\frac{1}{2}x_{1}\right)\rho\left(\tau-\frac{3}{4}\Delta\rho\right)-\left(\frac{1}{2}+x_{1}\right)\sum_{q}\rho_{q}\left(\tau_{q}-\frac{3}{4}\Delta\rho_{q}\right)\right]\\
&+\frac{1}{2}t_{2}\left[\left(1+\frac{1}{2}x_{2}\right)\rho\left(\tau+\frac{1}{4}\Delta\rho\right)-\left(\frac{1}{2}+x_{2}\right)\sum_{q}\rho_{q}\left(\tau_{q}+\frac{1}{4}\Delta\rho_{q}\right)\right]\\
&+\frac{1}{12}t_{3}\rho^{\alpha}\left[\left(1+\frac{1}{2}x_{3}\right)\rho^{2}-\left(\frac{1}{2}+x_{3}\right)\sum_{q}\rho_{q}^{2}\right]-\frac{1}{8}\left(t_{1}x_{1}+t_{2}x_{2}\right)\sum_{ij}\vec{J}_{ij}^{2}\\
&+\frac{1}{8}\left(t_{1}-t_{2}\right)\sum_{q,ij}\vec{J}_{q,ij}^{2}-\frac{1}{2}W_{0}\sum_{ijk}\varepsilon_{ijk}\left[\rho\nabla_{k}\vec{J}_{ij}+\sum_{q}\rho_{q}\nabla_{k}\vec{J}_{q,ij}\right],
\end{aligned} \tag{3}$$

and,

$$\tilde{H}\left(\vec{r}\right)=\frac{1}{2}V_{0}\left[1-V_{1}\left(\frac{\rho}{\rho_{0}}\right)^{\gamma}\right]\sum_{q}\tilde{p}_{q}^{2}. \tag{4}$$

In Eq. (4), the index q is proton (p) or neutron (n) densities, and γ called as power of density for pairing represents a constant for each force parameter given by Table 1. $H\left(\vec{r}\right)$ and $\tilde{H}\left(\vec{r}\right)$ in Eqs. (3) and (4) rely on $J_{i,j}\left(\vec{r}\right)$, q, $\tau\left(\vec{r}\right)$,$\rho\left(\vec{r}\right)$ and $\tilde{\rho}\left(\vec{r}\right)$,which they are spin-current density, proton or neutron densities, kinetic energy density, the local particle and pairing densities, respectively.

$$\rho\left(\vec{r}\right)=\rho\left(\vec{r},\vec{r}\right),\ \tilde{\rho}\left(\vec{r}\right)=\tilde{\rho}\left(\vec{r},\vec{r}\right), \tag{5}$$

$$\tau\left(\vec{r}\right)=\nabla_{\vec{r}}\nabla_{\vec{r}'}\rho\left(\vec{r},\vec{r}'\right)|_{\vec{r}'=\vec{r}},\vec{J}_{ij}\left(\vec{r}\right)=\frac{1}{2i}\left(\nabla_{i}-\nabla_{i}'\right)\rho_{j}\left(\vec{r},\vec{r}'\right)|_{\vec{r}'=\vec{r}}, \tag{6}$$

where $\rho\left(\vec{r},\vec{r}'\right)$, $\rho_{i}\left(\vec{r},\vec{r}'\right)$, $\tilde{\rho}\left(\vec{r},\vec{r}'\right)$ and $\tilde{\rho}_{i}\left(\vec{r},\vec{r}'\right)$ can be expressed by the spin-dependent one-body density matrices as follow:

$$\rho\left(\vec{r}\sigma,\vec{r}'\sigma'\right)=\frac{1}{2}\rho\left(\vec{r},\vec{r}'\right)\delta_{\sigma\sigma'}+\frac{1}{2}\sum_{i}\left(\sigma\left|\sigma_{i}\right|\sigma'\right)\rho_{i}\left(\vec{r},\vec{r}'\right), \tag{7}$$

$$\tilde{\rho}\left(\vec{r}\sigma,\vec{r}^{'}\sigma^{'}\right)=\frac{1}{2}\tilde{\rho}\left(\vec{r},\vec{r}^{'}\right)\delta_{\sigma\sigma^{'}}+\frac{1}{2}\sum_{i}\left(\sigma\left|\sigma_{i}\right|\sigma^{'}\right)\tilde{\rho}_{i}\left(\vec{r},\vec{r}^{'}\right). \tag{8}$$

In Eq. (8), the pairing density matrix $\tilde{\rho}$ is used instead of the pairing tensor (κ):

$$\tilde{\rho}\left(\vec{r}\sigma,\vec{r}^{'}\sigma^{'}\right)=-2\sigma^{'}\kappa\left(\vec{r},\sigma,\vec{r}^{'},-\sigma^{'}\right). \tag{9}$$

The variation in energy in Eq. (1) for Skyrme HFB approach is expressed as:

$$\sum_{\sigma}^{'}\begin{pmatrix} h\left(\vec{r},\sigma,\sigma^{'}\right) & \tilde{h}\left(\vec{r},\sigma,\sigma^{'}\right)\\ \tilde{h}\left(\vec{r},\sigma,\sigma^{'}\right) & -h\left(\vec{r},\sigma,\sigma^{'}\right)\end{pmatrix}\begin{pmatrix} U\left(E,\vec{r}\sigma^{'}\right)\\ V\left(E,\vec{r}\sigma^{'}\right)\end{pmatrix}=\begin{pmatrix} E+\lambda & 0\\ 0 & E-\lambda\end{pmatrix}\begin{pmatrix} U\left(E,\vec{r}\sigma\right)\\ V\left(E,\vec{r}\sigma\right)\end{pmatrix}. \tag{10}$$

In Eq. (10), $h\left(\vec{r},\sigma,\sigma^{'}\right)$ and $\tilde{h}\left(\vec{r},\sigma,\sigma^{'}\right)$ are local fields calculated in coordinate space via the following equations:

$$h_{q}\left(\vec{r},\sigma,\sigma^{'}\right)=-\nabla M_{q}\nabla+U_{q}+\frac{1}{2i}\sum_{ij}\left(\nabla_{i}\sigma_{j}B_{q,ij}+B_{q,ij}\nabla_{i}\sigma_{j}t\right),\ \tilde{h}_{q}\left(\vec{r},\sigma,\sigma^{'}\right)=V_{0}\left(1-V_{1}\left(\frac{\rho}{\rho_{0}}\right)^{\gamma}\right)\tilde{\rho}_{q}. \tag{11}$$

In Eq. (11), M_q, $B_{q,ij}$ and U_q are given by [3,24,25, 37,38]

$$M_{q} = \frac{\hbar^{2}}{2m}+\frac{1}{4}t_{1}\left[\left(1+\frac{1}{2}x_{1}\right)\rho-\left(x_{1}+\frac{1}{2}\right)\rho_{q}^{2}\right]+\frac{1}{4}t_{2}\left[\left(1+\frac{1}{2}x_{2}\right)\rho-\left(x_{2}+\frac{1}{2}\right)\rho_{q}^{2}\right], \tag{12}$$

$$B_{q,ij} = -\frac{1}{4}\left(t_{1}x_{1}+t_{2}x_{2}\right)\vec{J}_{ij}+\frac{1}{4}\left(t_{1}-t_{2}\right)\vec{J}_{q,ij}+\frac{1}{2}W_{0}\sum_{ijk}\varepsilon_{ijk}\nabla_{k}\left(\rho+\rho_{q}\right), \tag{13}$$

$$\begin{aligned} U_{q} = {} & t_{0}\left[\left(1+\frac{1}{2}x_{0}\right)\rho-\left(x_{0}+\frac{1}{2}\right)\rho_{q}\right]+\frac{1}{4}t_{1}\left[\left(1+\frac{1}{2}x_{1}\right)\left(\tau-\frac{3}{4}\Delta\rho\right)-\left(x_{1}+\frac{1}{2}\right)\left(\tau_{q}-\frac{3}{2}\Delta\rho_{q}\right)\right]\\ & +\frac{1}{4}t_{2}\left[\left(1+\frac{1}{2}x_{2}\right)\left(\tau+\frac{1}{2}\Delta\rho\right)+\left(x_{2}+\frac{1}{2}\right)\left(\tau_{q}+\frac{1}{2}\Delta\rho_{q}\right)\right]\\ & +\frac{1}{12}t_{3}\rho^{\alpha}\left[\left(1+\frac{1}{2}x_{3}\right)\left(2+\alpha\right)\rho-\left(x_{3}+\frac{1}{2}\right)\left(2\rho_{q}+\frac{\alpha}{\rho}\sum_{q}^{'}\rho_{q^{'}}^{2}\right)\right]\\ & -\frac{\gamma V_{0}V_{1}}{2\rho}\left(\frac{\rho}{\rho_{0}}\right)^{\gamma}\sum_{q}\tilde{\rho}_{q}^{2}-\frac{1}{2}W_{0}\sum_{ijk}\varepsilon_{ijk}\nabla_{k}\left[\vec{J}_{ij}+\vec{J}_{q,ij}\right]. \end{aligned} \tag{14}$$

2.2. Hartree–Fock–Bogolyubov method for Gogny forces

On the other hand, in the presence of the theory of Gogny, the force interactions are applied in Eq. (1) where $\hat{P}_{\sigma}$ and $\hat{P}_{\tau}$ represent spin and isospin exchange operators. The parameters for D1S, D1p, D1, D1N force interactions can be clearly found in Table 2 [6,30–33].

$$\begin{aligned} \hat{V}\left(\vec{r}_{1},\vec{r}_{2}\right) = {} & \sum_{i=1,2}e^{-\left(\vec{r}_{1}-\vec{r}_{2}\right)^{2}/\mu_{i}^{2}}\left(W_{i}+B_{i}\hat{P}_{\sigma}-H_{i}\hat{P}_{\tau}-M_{i}\hat{P}_{\sigma}\hat{P}_{\tau}\right)+t_{0}\left(1+x_{0}\hat{P}_{\sigma}\right)\rho^{\alpha}\left(\frac{\vec{r}_{1}+\vec{r}_{2}}{2}\right)\delta\left(\vec{r}_{1}-\vec{r}_{2}\right)\\ & +iW_{LS}\left(\vec{\sigma}_{1}+\vec{\sigma}_{2}\right)\left(\vec{\nabla}_{1}-\vec{\nabla}_{2}\right)\times\delta\left(\vec{r}_{1}-\vec{r}_{2}\right)\left(\vec{\nabla}_{1}-\vec{\nabla}_{2}\right). \end{aligned} \tag{15}$$

However, to apply Gogny force interactions to HFB, particular changes are needed in matrix elements to avoid defile of the finite range part in the Gogny functional where includes high computation time in each iteration, for this aim, matrix elements of the antisymmetrized potential are given by the matrix elements that can be expressed via the pairing matrix tensor κ or the density matrix ρ:

$$\Gamma_{\vec{n}_1\vec{n}_3} = \sum_{\vec{n}_2\vec{n}_4} \left\langle \vec{n}_1\vec{n}_2 \,|\, \hat{V}\hat{A} \,|\, \vec{n}_3\vec{n}_4 \right\rangle \rho_{\vec{n}_4\vec{n}_2}, \tag{16}$$

$$\Delta_{\vec{n}_1\vec{n}_2} = \frac{1}{2} \sum_{\vec{n}_3\vec{n}_4} \left\langle \vec{n}_1\vec{n}_2 \,|\, \hat{V}\hat{A} \,|\, \vec{n}_3\vec{n}_4 \right\rangle \kappa_{\vec{n}_3\vec{n}_4}. \tag{17}$$

In Eq. (17), the basis composed of the states ($|n\rangle$, $|\tilde{n}\rangle$) and in such a basis, the pairing matrix tensor equals to zero ($\kappa_{\vec{n}_3\vec{n}_4} = \kappa_{\bar{\vec{n}}_3\bar{\vec{n}}_4} = 0$). In configuration space, the pairing density $\tilde{\rho}$ and the pairing field $\tilde{h}$ are convenient compared to the pairing tensor κ and Δ:

$$\tilde{\rho}_{\vec{n}_3\vec{n}_4} = -2\sigma_{\vec{n}_4}\kappa^*_{\bar{\vec{n}}_3\bar{\vec{n}}_4}, \tag{18}$$

$$\tilde{h}_{\vec{n}_1\vec{n}_2} = -2\sigma_{\vec{n}_2}\Delta^*_{\bar{\vec{n}}_1\bar{\vec{n}}_2}. \tag{19}$$

After using these, to make facilitation, pairing field $\tilde{h}$ and pairing density being real and symmetric can be given by:

$$\tilde{h}_{\vec{n}_1\vec{n}_2} = \frac{1}{2} \sum_{\vec{n}_3\vec{n}_4} \left\langle \vec{n}_1\bar{\vec{n}}_2 \,|\, \hat{V}\hat{A} \,|\, \vec{n}_3\bar{\vec{n}}_4 \right\rangle \sigma_{\vec{n}_2}\sigma_{\vec{n}_4}\tilde{\rho}_{\vec{n}_3\vec{n}_4}. \tag{20}$$

In Eq. (20), $\hat{A}$ is the antisymmetrization operator $(1 - \hat{P}_r\hat{P}_\sigma\hat{P}_\tau)$ and, each basis state " $|n\rangle$ " is represented by the quantum numbers of Harmonic oscillator, and $\hat{V}\hat{A}$ can be given by isospin direct and isospin exchange with ID and IE labels:

$$\hat{V}_i\hat{A} = V_i(\vec{r}) \left(W_i + B_i\hat{P}_\sigma - H_i\hat{P}_\tau - M_i\hat{P}_\sigma\hat{P}_\tau\right) \left(1 - \hat{P}_\sigma\hat{P}_\tau\hat{P}_r\right) \equiv \hat{V}_i^{ID} - \hat{V}_i^{IE}\hat{P}_r. \tag{21}$$

Gogny force expressions applied in HFB can be found out Perez et al.'s study in more detail.

In terms of calculations, in addition to knowledge mentioned above, it is important to note that the calculations include linear constraint method for multi-constraint calculations based upon the approximation of the random phase approximation (RPA) matrix, especially on the nuclear shape where the constraints permit probing the potential energy surface of the nucleus, such as the definition of shape fission or isomers [6,37,38].

Table 1. Parameters of Skyrme forces used in HFBTHO code.

Forces	t_0 (MeVfm^3)	t_1 (MeVfm^5)	t_2 (MeVfm^5)	t_3 (MeVfm^3)	x_0	x_1	x_2	x_3	γ
S3	-1128.750	395.000	-95.000	14000.000	0.450	0.000	0.000	1.000	1
SKM*	-2645.000	410.000	-135.000	15595.000	0.900	0.000	0.000	0.000	1/6
SKP	-2931.696	320.618	-337.409	18708.960	0.292	0.653	-0.537	0.181	1/6
SLY4	-2488.913	486.818	-546.395	13777.000	0.834	-0.344	-1.000	1.354	1/6
SKX	-1445.300	246.900	-131.800	12103.890	0.340	0.580	0.127	0.300	1/2
HFB9	-2043.918	411.599	-194.189	12497.170	0.515	-0.954	-0.332	0.899	1/4
UNEDF0	-1883.688	277.500	608.431	13901.948	0.974	-1.778	-1.677	-0.381	1/3.106
UNEDF1	-2078.328	239.400	1575.120	14263.650	0.537	-5.077	-1.367	-0.162	1/3.703

Table 2. Parameters of Gogny forces used in HFBTHO code.

Forces	i	r_i (fm)	W_i(MeV)	B_i (MeV)	H_i(MeV)	M_i(MeV)	t_0 (MeVfm^4)	x_0	α
D1	1	0.7	-402.4	-100.00	-496.20	-23.56	8100.0	1.0	1/3
	2	1.2	-21.30	-11.77	37.27	-68.81			
D1N	1	0.8	-2047.61	1700.00	-2414.93	1519.35	9657.0	1.0	1/3
	2	1.2	293.02	-300.78	414.59	-316.84			
D1P	1	0.7	-402.40	-100.0	-496.20	-23.56	8100.0	1.0	1/3
	2	1.2	-21.30	-11.77	32.27	-68.81			
D1S	1	0.7	-1720.30	1300.00	-1813.53	1397.60	8343.6	1.0	1/3
	2	1.2	103.64	-163.48	162.81	-223.93			

3. Results and discussion

In the present work, in order to study the effect of the axial deformation in the SPECT nuclei, investigations of ground state nuclear structure properties of ^{213}Bi, ^{201}Tl, ^{188}Re, ^{186}Re, ^{133}Xe, ^{131}I, ^{125}I, ^{123}I, ^{111}In, ^{94}Tc, ^{90}Y, ^{67}Ga, ^{67}Cu, ^{62}Cu, ^{61}Cu, ^{55}Co, and ^{48}V nuclei used in SPECT have been performed by Skyrme and Gogny force interactions. Thus we calculated the binding energies, the rms charge, proton and neutron radii, NST, the proton and neutron quadrupole moments (Q_P and Q_N), quadrupole deformation parameter (β_2), and the proton and neutron pairing energies (P_P and P_N). The Skyrme and Gogny force parameters used in the calculations of nuclear properties of each SPECT nucleus are S3, SKM*, SKP, SKX, SLY4, HFB9, UNEDF0, UNEDF1 and D1, D1N, D1p, D1S, respectively. To analyze and discuss the accuracy of the obtained results, the calculated results for Skyrme and Gogny force parameters were also compared with experimental data and the theoretical results in the literature e.g. FRDM.

HFB approach with Skyrme and Gogny interactions in axial deformation was implemented by HFTHO 3.00 code which allows the calculation of nuclear structure properties of all nuclei. To understand how to work each force parameter of interactions in the HFBTHO, we calculated for SPECT nuclei and the obtained results compared with the experimental results in the literature. In addition to the related calculations in this work, in the literature, the comparisons of Gogny and Skyrme interactions may also be analyzed in detail [39].

3.1. Binding energies per particle

In order to determine the nuclear structure properties of SPECT nuclei, we calculated the binding energies per particle of ^{213}Bi, ^{201}Tl, ^{188}Re, ^{186}Re, ^{133}Xe, ^{131}I, ^{125}I, ^{123}I, ^{111}In, ^{94}Tc, ^{90}Y, ^{67}Ga, ^{67}Cu, ^{62}Cu, ^{61}Cu, ^{55}Co, and ^{48}V nuclei via two different approaches, Gogny and Skyrme force parameterizations. The calculated results were then compared with the experimental data and FRDM results as presented in Table 3. It is obvious that Gogny's D1, D1N and D1p force parameter results get away from the experimental data and other results, except for ^{131}I, ^{90}Y and ^{67}Ga nuclei. However, D1S force parameter is closer to the experimental data and Skyrme force results. It is seen that the results of FRDM are consistent with the experimental data, however, there are a few exceptional circumstances. The binding energy result of ^{67}Ga for UNEDF0 force parameter is the same value with the experimental data. Similarly, in terms of HFB9, this result is more consistent than FRDM result. The SKP interaction results show that ^{213}Bi, ^{201}Tl, ^{188}Re, ^{133}Xe, ^{131}I, ^{125}I, ^{123}I, ^{111}In, ^{90}Y and ^{55}Co nuclei are in good agreement with the experimental data compared to other Skyrme parameters and Gogny parameters. In particular, for ^{213}Bi nucleus, SKP has a better result than FRDM, in addition to ^{213}Bi, it is clear that the binding energy result (8.421 MeV) of ^{131}I is fairly closer to the experimental data (8.423

MeV). Among the SPECT nuclei, Gogny's D1S force parameter only gives more suitable result for ^{186}Re than those of Skyrme force parameters. Further, for an accurate determination of the calculated results, when taking into account deviations between the calculated results and the available experimental data, Gogny's D1S force parameter for all nuclei has a deviation from 0.013 MeV (^{186}Re) to 0.452 MeV (^{62}Cu), and the maximum deviation of FRDM is 0.021 MeV for ^{61}Cu and the deviations of ^{201}Tl and ^{111}In are zero. Among the Skyrme interactions, SKP parameter has fairly low deviations e.g., 0.001 MeV (^{213}Bi), 0.002 MeV (^{131}I), and UNEDF0 is in good agreement with experimental results and has minimum deviations after SKP, especially in ^{67}Ga (0 MeV), ^{213}Bi (0.009 MeV), ^{94}Tc (0.020 MeV), ^{90}Y (0.090 MeV), ^{67}Cu (0.008 MeV). Based on the mean deviation rate, the SKP has the lowest rate ~0.055 MeV and this rate is less than UNEDF0 (0.093 MeV). On the basis of our results, when compared with the force interactions among themselves, it can be clearly said that Skyrme's SKP parameter in axial deformation is in good agreement with the experimental results compared to other force parameters in regarding the binding energy per particle.

3.2. Charge, proton and neutron density radii

To determine the rms charge, proton and neutron density radii in axial deformation, we have utilized Gogny and Skyrme force parameters based on Hartree–Fock–Bogolyubov approach and the calculated results for 12 different force parameters are illustrated in Tables 4, 5 and 6 together with the experimental results in the literature. In the rms charge density radii used in SPECT nuclei, contrary to the binding energy, it has been noted that Gogny's force parameters have given suitable results in Table 4 when compared with the available experimental results. For only ^{201}Tl, Gogny's D1p force parameter is consistent with the experimental data, and on the other hand the rms charge result of ^{213}Bi for UNEDF1 parameter is the closest to the experimental result. Additionally, SKX results of ^{201}Tl, ^{133}Xe and ^{90}Y nuclei are in good agreement with the experimental results compared to the other parameters. In the deviations of the charge radii, Gogny's D1, D1N, D1p interactions for ^{213}Bi and ^{201}Tl nuclei have small deviations compared to the binding energies, 0.007 fm, 0.065 fm, 0.006 fm and 0.060 fm, 0.055 fm, 0.006 fm, respectively. In addition to SKX, the deviations of UNE results with available experimental results also are low values ^{213}Bi (0.010 fm), ^{133}Xe (0.008 fm) and ^{90}Y (0.009 fm). Furthermore, the based on the calculated results and the experimental results in Table 4, the minimum mean deviation values are 0.0114 fm (SKX), 0.0126 fm (UNEDF1) and 0.0136 fm (UNEDF0). According to these results, it is important to note that such a result of SKX interaction was also acceptable for PET nuclei in Artun's previous study [3].

In addition to the rms charge radii, the rms proton and neutron density radii are calculated to observe the NST of the SPECT nuclei. The obtained the rms proton and neutron density radii are shown in Tables 5 and 6, respectively. It is well known that the experimental or theoretical proton and neutron density radii results for odd-odd and odd-even/even-odd nuclei are not available in the literature. Further, all SPECT nuclei are almost both odd-odd and odd-even/even-odd nuclei. Therefore, data of this study are quite important for literature. For this aim, in the following, in order to assess the deformation of the SPECT nuclei, NSTs, the quadrupole deformation parameters, the proton and neutron quadrupole moments, and pairing energies were calculated in axial symmetry.

Table 3. Binding energies per particle for SPECT nuclei.

Nuclei	D1	D1N	D1p	D1S	S3	SKM*	SKP	SKX	SLY4	HFB9	UNEDF0	UNEDF1	FRDM	EXP.
^{213}Bi	6.254	5.479	6.008	7.809	7.742	7.771	7.790	7.951	7.755	7.795	7.782	7.771	7.789	7.791
^{201}Tl	5.934	6.753	6.883	7.912	7.794	7.814	7.875	8.046	7.831	7.866	7.850	7.844	7.891	7.891
^{188}Re	6.503	5.217	3.484	7.931	7.875	7.883	7.934	8.076	7.837	7.878	7.849	7.855	7.969	7.967
^{186}Re	7.162	5.972	5.932	7.968	7.883	7.894	7.948	8.118	7.887	7.894	7.915	7.864	7.984	7.981
^{133}Xe	6.204	6.796	7.427	8.431	8.331	8.354	8.422	8.593	8.345	8.386	8.356	8.342	8.412	8.413
^{131}I	8.323	9.424	8.538	8.408	8.319	8.354	8.421	8.593	8.319	8.370	8.356	8.336	8.422	8.423
^{125}I	12.981	12.688	12.879	8.418	8.251	8.340	8.454	8.630	8.317	8.368	8.340	8.350	8.448	8.450
^{123}I	11.553	14.036	13.313	8.412	8.302	8.328	8.422	8.628	8.344	8.358	8.371	8.346	8.448	8.449
^{111}In	2.523	2.257	2.783	8.546	8.410	8.450	8.536	8.747	8.462	8.481	8.486	8.435	8.522	8.522
^{94}Tc	5.058	4.576	5.995	8.745	8.186	8.303	8.340	8.727	8.262	8.342	8.589	8.452	8.613	8.609
^{90}Y	8.638	8.852	8.646	8.646	8.570	8.547	8.660	8.819	8.601	8.618	8.603	8.593	8.688	8.693
^{67}Ga	8.004	8.137	8.130	8.802	8.598	8.693	8.781	8.988	8.670	8.707	8.708	8.654	8.697	8.708
^{67}Cu	1.204	2.892	4.428	8.847	8.676	8.752	8.808	9.042	8.749	8.767	8.745	8.703	8.731	8.737
^{62}Cu	7.129	6.277	6.534	8.266	8.038	8.255	8.424	8.629	8.320	8.307	8.338	8.361	8.699	8.718
^{61}Cu	7.651	6.726	6.738	8.537	8.320	8.523	8.613	8.890	8.516	8.622	8.585	8.460	8.695	8.716
^{55}Co	6.583	6.089	6.702	8.587	8.422	8.491	8.613	8.789	8.275	8.487	8.603	8.384	8.676	8.670
^{48}V	4.407	4.958	4.154	8.254	8.098	7.776	8.391	8.506	8.240	8.158	8.305	8.174	8.631	8.623

Table 4. Charge density radii for SPECT nuclei.

Nuclei	D1	D1N	D1p	D1S	S3	SKM*	SKP	SKX	SLY4	HFB9	UNEDF0	UNEDF1	EXP.
^{213}Bi	5.552	5.624	5.553	5.528	5.627	5.551	5.569	5.545	5.563	5.561	5.549	5.560	5.559
^{201}Tl	5.517	5.512	5.463	5.466	5.546	5.483	5.501	5.468	5.493	5.490	5.481	5.485	5.457
^{188}Re	5.385	5.487	5.544	5.425	5.489	5.412	5.398	5.397	5.431	5.424	5.356	5.366	——
^{186}Re	5.336	5.422	5.366	5.403	5.480	5.409	5.397	5.386	5.425	5.423	5.407	5.354	——
^{133}Xe	4.914	4.914	4.841	4.795	4.863	4.799	4.827	4.780	4.812	4.812	4.791	4.793	4.783
^{131}I	4.824	4.774	4.794	4.768	4.836	4.773	4.797	4.759	4.789	4.779	4.761	4.771	——
^{125}I	4.590	4.600	4.619	4.734	4.851	4.737	4.761	4.721	4.762	4.742	4.732	4.726	——
^{123}I	4.627	4.584	4.575	4.722	4.783	4.724	4.756	4.707	4.740	4.729	4.715	4.712	——
^{111}In	4.776	4.837	4.749	4.565	4.633	4.576	4.605	4.563	4.587	4.580	4.569	4.574	4.586
^{94}Tc	4.586	4.624	4.600	4.354	4.435	4.490	4.425	4.353	4.405	4.378	4.363	4.367	——
^{90}Y	4.211	4.220	4.212	4.310	4.326	4.294	4.314	4.263	4.293	4.294	4.266	4.269	4.257
^{67}Ga	3.957	3.939	3.963	3.981	4.005	3.964	3.994	3.941	3.991	3.974	3.959	3.941	——
^{67}Cu	4.196	4.126	4.040	3.919	3.967	3.917	3.954	3.901	3.932	3.927	3.926	3.913	——
^{62}Cu	3.999	4.083	3.948	3.943	4.089	3.914	3.939	3.896	3.945	3.929	3.918	3.885	——
^{61}Cu	3.943	3.995	3.922	3.900	4.080	3.874	3.912	3.882	3.931	3.922	3.872	3.870	——
^{55}Co	3.895	4.021	3.872	3.758	3.882	3.843	3.808	3.747	3.961	3.866	3.798	3.844	——
^{48}V	3.818	3.938	3.817	3.693	3.714	3.703	3.773	3.613	3.794	3.799	3.668	3.725	——

3.3. Neutron skin thickness

Here, the NSTs of the SPECT nuclei are estimated via the rms proton and neutron density radii obtained from Tables 5 and 6. NST results are shown in Table 7 for each force interaction. As expected, ^{213}Bi nucleus has generally the maximum NSTs compared to the other nuclei. As Gogny's some force interactions for ^{131}I, ^{125}I and ^{94}Tc nuclei are negative values, all Skyrme interaction results are positive values. However, for ^{62}Cu, ^{61}Cu, ^{55}Co and ^{48}V nuclei, some Gogny and Skyrme force interactions give negative NST values. On the other hand, NST value of ^{55}Co is negative for both Gogny and Skyrme force interactions. SKM* and UNEDF0 interactions of ^{62}Cu and ^{61}Cu nuclei approach to zero NST values. Further, NST values of ^{90}Y for all force interactions are fairly big compared to the mass number of Y nucleus, and this nucleus has almost values the equivalent to that of ^{125}I.

3.4. Quadrupole deformation parameter

For comprehending the shapes and skin thickness of SPECT nuclei, the investigations of quadrupole deformation parameters (β_2) of the nuclei have fairly significant role in the nuclear structure. Therefore, the quadrupole deformation parameters of nuclei used in SPECT are calculated in axial symmetry for 12 different force interactions, as shown in Table 8. In the quadrupole deformation parameter calculation, besides Gogny and Skyrme calculations, FRDM and FRDM* results (* represents the calculated quadrupole deformation parameter in the Nilsson perturbed-spheroid parameterization) are also available in Table 8.

On the other hand, the quadrupole deformation parameter calculations of SPECT nuclei with odd-odd and odd-even/even-odd numbers provide nuclear structure data to the literature, especially including knowledge about shapes of nuclei as oblate and prolate, as it is indicated in Tables 9 and 10, the positive results represent prolate basis. It is clear that the quadrupole deformation parameter of ^{67}Cu for both force interactions and

Table 5. Proton density radii for SPECT nuclei.

Nuclei	D1	D1N	D1p	D1S	S3	SKM*	SKP	SKX	SLY4	HFB9	UNEDF0	UNEDF1
^{213}Bi	5.496	5.568	5.497	5.472	5.572	5.495	5.513	5.489	5.507	5.505	5.492	5.504
^{201}Tl	5.459	5.454	5.405	5.408	5.489	5.425	5.444	5.410	5.435	5.433	5.423	5.428
^{188}Re	5.327	5.430	5.487	5.367	5.431	5.354	5.340	5.339	5.373	5.365	5.298	5.307
^{186}Re	5.277	5.364	5.307	5.344	5.422	5.350	5.339	5.327	5.367	5.365	5.349	5.294
^{133}Xe	4.849	4.850	4.775	4.729	4.798	4.733	4.761	4.714	4.746	4.746	4.725	4.727
^{131}I	4.758	4.708	4.728	4.701	4.770	4.706	4.731	4.692	4.723	4.713	4.694	4.704
^{125}I	4.519	4.529	4.549	4.665	4.784	4.668	4.693	4.652	4.694	4.673	4.664	4.658
^{123}I	4.556	4.513	4.503	4.653	4.715	4.654	4.687	4.638	4.671	4.659	4.646	4.643
^{111}In	4.707	4.768	4.679	4.492	4.562	4.504	4.534	4.490	4.515	4.508	4.497	4.502
^{94}Tc	4.513	4.552	4.527	4.277	4.359	4.415	4.349	4.276	4.329	4.302	4.286	4.291
^{90}Y	4.133	4.142	4.134	4.234	4.251	4.217	4.238	4.186	4.217	4.218	4.189	4.192
^{67}Ga	3.872	3.854	3.878	3.897	3.920	3.879	3.910	3.856	3.906	3.889	3.874	3.855
^{67}Cu	4.117	4.047	3.959	3.835	3.884	3.834	3.870	3.817	3.848	3.843	3.842	3.829
^{62}Cu	3.915	4.000	3.862	3.857	4.006	3.858	3.853	3.809	3.860	3.843	3.831	3.797
^{61}Cu	3.857	3.910	3.835	3.813	3.996	3.786	3.825	3.794	3.845	3.835	3.784	3.782
^{55}Co	3.806	3.935	3.783	3.666	3.794	3.753	3.718	3.655	3.874	3.777	3.708	3.754
^{48}V	3.729	3.851	3.727	3.601	3.622	3.610	3.683	3.518	3.704	3.709	3.575	3.634

Table 6. Neutron density radii for SPECT nuclei.

Nuclei	D1	D1N	D1p	D1S	S3	SKM*	SKP	SKX	SLY4	HFB9	UNEDF0	UNEDF1
^{213}Bi	5.762	5.897	5.782	5.617	5.701	5.674	5.665	5.650	5.676	5.668	5.693	5.688
^{201}Tl	5.600	5.602	5.538	5.519	5.587	5.561	5.561	5.535	5.567	5.558	5.579	5.568
^{188}Re	5.445	5.578	5.619	5.506	5.538	5.504	5.475	5.477	5.517	5.504	5.473	5.469
^{186}Re	5.419	5.534	5.467	5.454	5.520	5.488	5.462	5.455	5.499	5.493	5.506	5.445
^{133}Xe	4.889	4.914	4.852	4.864	4.923	4.893	4.901	4.867	4.901	4.898	4.904	4.903
^{131}I	4.743	4.754	4.769	4.826	4.887	4.864	4.872	4.838	4.869	4.859	4.872	4.876
^{125}I	4.561	4.567	4.528	4.750	4.838	4.778	4.787	4.749	4.795	4.774	4.785	4.784
^{123}I	4.578	4.568	4.505	4.722	4.777	4.746	4.763	4.718	4.757	4.744	4.744	4.752
^{111}In	4.869	4.957	4.865	4.550	4.611	4.579	4.591	4.548	4.587	4.575	4.577	4.588
^{94}Tc	4.595	4.485	4.383	4.303	4.382	4.417	4.374	4.311	4.375	4.388	4.348	4.338
^{90}Y	4.357	4.335	4.334	4.315	4.335	4.320	4.329	4.289	4.318	4.319	4.326	4.313
^{67}Ga	3.952	3.947	3.887	3.922	3.942	3.917	3.937	3.884	3.939	3.922	3.917	3.913
^{67}Cu	4.318	4.276	4.162	3.934	3.975	3.957	3.975	3.918	3.964	3.957	3.968	3.973
^{62}Cu	4.015	4.030	4.016	3.877	3.854	3.858	3.874	3.806	3.846	3.852	3.845	3.844
^{61}Cu	3.841	3.886	3.888	3.786	3.817	3.779	3.818	3.789	3.788	3.830	3.784	3.797
^{55}Co	3.767	3.787	3.800	3.622	3.672	3.646	3.677	3.621	3.649	3.691	3.677	3.687
^{48}V	3.896	3.799	3.893	3.651	3.671	3.596	3.641	3.614	3.714	3.692	3.597	3.590

the FRDM results is stated as an oblate nucleus, except for D1N. Based on the FRDM and force interactions, the quadrupole deformation parameter value of ^{213}Bi has lower values, and this nucleus is closer to sphericity

Table 7. Neutron skin thicknesses for SPECT nuclei.

Nuclei	D1	D1N	D1p	D1S	S3	SKM*	SKP	SKX	SLY4	HFB9	UNEDF0	UNEDF1
^{213}Bi	0.266	0.329	0.285	0.145	0.129	0.179	0.152	0.161	0.169	0.163	0.201	0.184
^{201}Tl	0.141	0.148	0.133	0.111	0.098	0.136	0.117	0.125	0.132	0.125	0.156	0.140
^{188}Re	0.118	0.148	0.132	0.139	0.107	0.150	0.135	0.138	0.144	0.139	0.175	0.162
^{186}Re	0.142	0.170	0.160	0.110	0.098	0.138	0.123	0.128	0.132	0.128	0.157	0.151
^{133}Xe	0.040	0.064	0.077	0.135	0.125	0.160	0.140	0.153	0.155	0.152	0.179	0.176
^{131}I	-0.015	0.046	0.041	0.125	0.117	0.158	0.141	0.146	0.146	0.146	0.178	0.172
^{125}I	0.042	0.038	-0.021	0.085	0.054	0.110	0.094	0.097	0.101	0.101	0.121	0.126
^{123}I	0.022	0.055	0.002	0.069	0.062	0.092	0.076	0.080	0.086	0.085	0.098	0.109
^{111}In	0.162	0.189	0.186	0.058	0.049	0.075	0.057	0.058	0.072	0.067	0.080	0.086
^{94}Tc	0.082	-0.067	-0.144	0.026	0.023	0.002	0.025	0.035	0.046	0.086	0.062	0.047
^{90}Y	0.224	0.193	0.200	0.081	0.084	0.103	0.091	0.103	0.101	0.101	0.137	0.121
^{67}Ga	0.080	0.093	0.009	0.025	0.022	0.038	0.027	0.028	0.033	0.033	0.043	0.058
^{67}Cu	0.201	0.229	0.203	0.099	0.091	0.123	0.105	0.101	0.116	0.114	0.126	0.144
^{62}Cu	0.100	0.030	0.154	0.020	-0.152	0.000	0.021	-0.003	-0.014	0.009	0.014	0.047
^{61}Cu	-0.016	-0.024	0.053	-0.027	-0.179	-0.007	-0.007	-0.005	-0.057	-0.005	0.000	0.015
^{55}Co	-0.039	-0.148	0.017	-0.044	-0.122	-0.107	-0.041	-0.034	-0.225	-0.086	-0.031	-0.067
^{48}V	0.167	-0.052	0.166	0.05	0.049	-0.014	-0.042	0.096	0.010	-0.017	0.022	-0.044

or to nucleus with small deformation compared to the other nuclei. ^{90}Y nucleus is specified as oblate, except for D1N, S3, and SLY4 force interactions. The contrary situation is valid for ^{133}Xe nucleus, which is prolate. The FRDM results and many force interactions for ^{48}V, ^{61}Cu, and ^{62}Cu nuclei are represented as prolate basis.

3.5. Proton and neutron quadrupole moments

In order to analyze the axial deformation via the HFBTHO code, another important nuclear structure property to determine the shape of nuclei as oblate or prolate is quadrupole moment. Hence, based on axial deformation, both proton (Q_P) and neutron (Q_N) quadrupole moments are presented in Tables 9 and 10 for Skyrme and Gogny force interactions. When total quadrupole moments ($Q = Q_N + Q_P$) of SPECT nuclei are investigated, the total quadrupole moment of ^{213}Bi for all force interactions are positive and it can be labeled as prolate ($Q > 0$). ^{67}Cu has negative Q value (oblate), except for D1 interaction, and as can be expected from quadrupole deformation parameter, ^{48}V, ^{61}Cu and ^{62}Cu nuclei are prolate due to $Q > 0$. Similarly, ^{201}Tl, ^{133}Xe, ^{94}Tc, and ^{67}Ga are labeled as prolate for most parameters. It can be said that the quadrupole moment results for Skyrme and Gogny force interactions are in good agreement with quadrupole deformation results shown in Table 8.

Table 8. Quadrupole deformation parameters (β_2) for SPECT nuclei.

Nuclei	D1	D1N	D1p	D1S	S3	SKM*	SKP	SKX	SLY4	HFB9	UNEDF0	UNEDF1	FRDM	FRDM*
^{213}Bi	0.077	0.044	0.079	0.007	0.015	0.014	0.012	0.016	0.013	0.015	0.022	0.023	-0.010	-0.010
^{201}Tl	0.095	0.085	0.080	0.064	0.015	0.046	0.022	0.043	0.060	0.071	0.078	-0.026	-0.050	-0.053
^{188}Re	-0.002	-0.000	0.129	0.262	0.210	0.196	0.107	0.198	0.206	0.201	-0.001	-0.002	0.190	0.209
^{186}Re	-0.003	0.000	-0.014	0.227	0.220	0.214	0.148	0.206	0.225	0.223	0.230	-0.003	0.200	0.221
^{133}Xe	0.176	0.173	0.165	0.082	0.081	0.015	0.021	-0.004	0.058	0.115	0.059	0.016	0.050	0.053
^{131}I	0.001	-0.098	-0.107	0.005	-0.002	0.001	0.003	0.010	0.018	-0.016	0.004	-0.003	0.030	0.032
^{125}I	0.003	0.002	0.001	0.001	0.200	-0.002	0.002	-0.020	-0.073	-0.002	-0.039	0.005	-0.160	-0.166
^{123}I	0.015	0.002	0.001	0.001	-0.005	-0.004	-0.026	-0.008	-0.004	-0.002	0.001	-0.001	-0.180	-0.187
^{111}In	-0.003	-0.001	-0.007	-0.004	-0.003	-0.091	0.005	-0.004	-0.001	-0.003	0.010	-0.073	0.100	0.108
^{94}Tc	0.231	0.199	0.056	0.040	-0.047	0.137	-0.044	0.018	0.041	0.026	0.047	0.049	0.020	0.021
^{90}Y	-0.023	0.007	-0.018	-0.168	0.006	-0.084	-0.044	-0.032	0.005	-0.111	-0.004	-0.027	-0.020	-0.021
^{67}Ga	0.125	0.079	0.021	0.168	0.008	0.070	0.004	-0.007	0.103	0.097	0.063	-0.039	-0.240	-0.247
^{67}Cu	0.012	-0.093	-0.094	-0.082	-0.095	-0.074	-0.021	-0.061	-0.051	-0.072	-0.063	-0.093	-0.080	-0.084
^{62}Cu	0.282	0.293	0.208	-0.190	0.150	-0.099	-0.071	0.105	0.000	0.097	0.110	0.148	0.140	0.151
^{61}Cu	0.168	0.175	0.103	0.142	0.211	-0.032	-0.047	0.205	0.004	-0.220	0.070	0.134	0.140	0.150
^{55}Co	0.220	0.312	0.339	-0.041	0.119	0.120	-0.022	-0.060	0.162	0.242	-0.202	0.228	0.040	0.043
^{48}V	0.373	0.277	0.362	0.244	0.252	-0.075	0.289	-0.040	0.394	0.370	0.214	0.244	0.190	0.205

Table 9. Quadrupole moments of proton for SPECT nuclei.

Nuclei	D1	D1N	D1p	D1S	S3	SKM*	SKP	SKX	SLY4	HFB9	UNEDF0	UNEDF1
^{213}Bi	2.468	1.402	2.556	0.192	0.492	0.467	0.387	0.524	0.423	0.479	0.662	0.709
^{201}Tl	3.055	2.701	2.488	1.929	0.420	1.344	0.688	1.337	1.838	2.163	2.364	-0.770
^{188}Re	-0.008	0.025	3.848	7.095	6.112	5.597	3.013	5.597	5.932	5.727	-0.034	-0.058
^{186}Re	-0.044	0.016	-0.348	6.348	6.292	6.033	4.131	5.785	6.367	6.255	6.505	-0.070
^{133}Xe	2.889	2.862	2.659	1.372	1.336	0.284	0.358	-0.066	0.984	1.899	1.034	0.327
^{131}I	0.017	-1.536	-1.685	0.080	-0.044	-0.002	0.036	0.157	0.301	-0.279	0.057	-0.060
^{125}I	0.042	0.021	0.014	0.012	3.187	-0.037	0.024	-0.313	-1.126	-0.036	-0.601	0.069
^{123}I	0.213	0.019	0.019	0.007	-0.078	-0.066	-0.414	-0.126	-0.066	-0.030	0.007	-0.023
^{111}In	-0.057	-0.034	-0.119	-0.048	-0.041	-1.061	0.055	-0.050	-0.020	-0.045	0.104	-0.865
^{94}Tc	2.219	2.609	0.113	0.377	-0.487	1.586	-0.456	0.141	0.308	-0.032	0.462	0.470
^{90}Y	-0.170	0.039	-0.127	-1.521	0.043	-0.763	-0.394	-0.266	0.032	-1.004	-0.042	-0.211
^{67}Ga	0.785	0.480	0.127	1.047	0.041	0.418	0.023	-0.041	0.643	0.599	0.365	-0.212
^{67}Cu	0.051	-0.620	-0.590	-0.467	-0.530	-0.421	-0.132	-0.344	-0.307	-0.411	-0.361	-0.522
^{62}Cu	1.124	1.770	0.800	-1.024	1.323	-0.537	-0.393	0.640	0.015	0.609	0.627	0.824
^{61}Cu	0.847	1.089	0.482	0.789	1.622	-0.188	-0.265	1.107	0.048	-1.221	0.434	0.718
^{55}Co	1.028	2.054	1.693	-0.203	0.774	0.728	-0.115	-0.284	1.252	1.293	-0.971	1.155
^{48}V	1.236	1.166	1.184	0.814	0.847	-0.274	1.184	-0.199	1.608	1.512	0.774	0.943

Table 10. Quadrupole moments of neutron for SPECT nuclei.

Nuclei	D1	D1N	D1p	D1S	S3	SKM*	SKP	SKX	SLY4	HFB9	UNEDF0	UNEDF1
^{213}Bi	4.167	2.503	4.291	0.359	0.804	0.754	0.624	0.848	0.682	0.787	1.166	1.240
^{201}Tl	4.381	3.950	3.606	2.958	0.787	2.207	1.005	1.978	2.786	3.321	3.647	-1.221
^{188}Re	-0.112	-0.031	5.655	11.363	8.904	8.161	4.429	8.188	8.625	8.407	-0.056	-0.108
^{186}Re	-0.155	-0.040	-0.596	9.246	9.217	8.806	6.034	8.343	9.262	9.205	9.510	-0.128
^{133}Xe	4.118	4.083	3.789	1.809	1.882	0.317	0.479	-0.106	1.313	2.600	1.276	0.286
^{131}I	0.032	-2.078	-2.314	0.125	-0.040	0.021	0.074	0.229	0.396	-0.339	0.103	-0.056
^{125}I	0.059	0.034	0.015	0.031	4.110	-0.033	0.052	-0.394	-1.467	-0.029	-0.764	0.101
^{123}I	0.275	0.031	0.027	0.022	-0.090	-0.076	-0.505	-0.148	-0.065	-0.023	0.024	-0.015
^{111}In	-0.038	0.006	-0.121	-0.060	-0.044	-1.571	0.085	-0.056	-0.012	-0.051	0.178	-1.249
^{94}Tc	3.462	2.192	1.198	0.492	-0.577	1.571	-0.545	0.245	0.608	0.624	0.573	0.617
^{90}Y	-0.312	0.096	-0.237	-1.973	0.082	-0.988	-0.533	-0.390	0.069	-1.298	-0.040	-0.336
^{67}Ga	0.834	0.538	0.137	1.127	0.065	0.477	0.029	-0.046	0.703	0.658	0.438	-0.281
^{67}Cu	0.128	-0.754	-0.726	-0.583	-0.710	-0.539	-0.143	-0.424	-0.359	-0.518	-0.460	-0.682
^{62}Cu	2.344	1.930	1.727	-1.203	0.485	-0.603	-0.436	0.547	-0.010	0.520	0.636	0.869
^{61}Cu	1.073	0.953	0.696	0.793	0.856	-0.162	-0.266	1.160	0.001	-1.263	0.342	0.759
^{55}Co	1.163	1.172	1.686	-0.176	0.371	0.407	-0.096	-0.271	0.339	1.043	-0.940	1.037
^{48}V	2.052	1.289	2.004	1.130	1.184	-0.315	1.159	-0.109	1.677	1.556	0.889	0.986

3.6. Proton and neutron pairing energies

Besides the quadrupole deformation parameter and quadrupole moment, here, the proton pairing energy (P_P) and the neutron pairing energy (P_N) are calculated for each force interaction with Gogny and Skyrme, and

the obtained results are presented in Tables 11 and 12. For the calculations of proton and neutron pairing energies which assist in the understanding of some structural properties of nucleus, such as deformation (oblate, prolate), especially in nuclei close to $N = Z$ line and in the nuclei with magic number, the code implements the regularization of zero-range pairing interactions which are restricted to the case of functionals of the local pairing density [6,38]. When the proton pair energy of ^{213}Bi is paid attention, D1S, S3, SKM, SKX, SLY4, HFB9, UNEDF0 and UNEDF1 force interactions give zero value because of proton number of ^{213}Bi (Z = 83) approaching to magic number (Z = 82). The neutron pairing energy of ^{213}Bi is nonzero. In quadrupole deformation and moment sections above, we said that ^{213}Bi has small deformation with prolate, and this result is consistent with the pairing energies. Accordingly, based on Gongny's D1S interaction and Skyrme interactions, it can be said that ^{213}Bi has small deformation and this deformation is mostly caused by neutron deformation. Moreover, the shape of ^{213}Bi nucleus can be stated as prolate. Similar situation may be said for ^{67}Cu nucleus, which is in oblate (Q < 0) formation with neutron deformation. Furthermore, ^{111}In nucleus is stated as oblate with neutron deformation, and ^{94}Tc nucleus is stated as prolate with proton deformation.

Table 11. Proton pairing energies for SPECT nuclei.

Nuclei	D1	D1N	D1p	D1S	S3	SKM*	SKP	SKX	SLY4	HFB9	UNEDF0	UNEDF1
^{213}Bi	1.458	1.672	1.507	0.000	0.000	0.000	1.270	0.000	0.000	0.000	0.000	0.000
^{201}Tl	1.415	1.241	1.303	0.938	0.000	0.777	1.744	0.632	0.654	0.424	0.260	0.320
^{188}Re	2.030	2.040	1.945	0.962	0.556	0.882	2.250	0.715	0.708	0.481	0.662	0.656
^{186}Re	2.020	2.030	2.090	0.917	0.587	0.880	2.249	0.707	0.698	0.469	0.196	0.658
^{133}Xe	1.552	1.524	1.490	1.631	1.318	1.581	2.550	1.297	1.369	0.821	0.585	0.685
^{131}I	2.171	1.929	1.921	1.751	1.441	1.561	2.460	1.276	1.388	1.036	0.621	0.695
^{125}I	2.198	2.060	2.337	1.759	0.968	1.609	2.527	1.324	1.422	1.053	0.566	0.705
^{123}I	2.194	2.002	2.294	1.755	1.576	1.626	2.600	1.352	1.469	1.057	0.530	0.706
^{111}In	1.709	1.616	1.695	0.000	0.000	0.000	2.302	0.000	0.000	0.000	0.000	0.000
^{94}Tc	2.109	1.996	2.120	1.497	1.795	1.966	2.969	1.493	1.518	1.112	0.616	0.667
^{90}Y	1.244	1.651	1.509	1.577	1.636	1.745	2.711	1.342	1.150	0.977	0.608	0.430
^{67}Ga	1.189	1.026	1.620	0.757	1.571	1.118	2.827	1.290	1.017	0.523	0.000	0.283
^{67}Cu	1.935	1.726	1.758	0.000	0.000	0.000	2.567	0.000	0.000	0.000	0.000	0.000
^{62}Cu	1.678	1.368	1.374	1.496	0.000	1.636	3.258	0.812	0.000	0.000	0.000	0.255
^{61}Cu	1.602	1.238	1.506	1.007	0.768	1.543	3.213	1.187	0.000	0.838	0.000	0.084
^{55}Co	1.435	1.332	1.193	0.000	1.557	1.703	3.251	0.667	1.425	0.556	0.000	0.000
^{48}V	1.227	1.680	1.340	1.085	1.617	2.273	3.283	1.771	1.475	1.135	0.444	0.614

4. Conclusion

In this work, to investigate the nuclear structure and properties of ^{213}Bi, ^{201}Tl, ^{188}Re, ^{186}Re, ^{133}Xe, ^{131}I, ^{125}I, ^{123}I, ^{111}In, ^{94}Tc, ^{90}Y, ^{67}Ga, ^{67}Cu, ^{62}Cu, ^{61}Cu, ^{55}Co, and ^{48}V nuclei used in SPECT, HFB approach with Gogny and Skyrme force interactions was utilized in axial symmetry and we calculated the binding energies per particle, the rms charge, proton, neutron density radii, NSTs, the quadrupole deformation parameters, the proton and neutron quadrupole moments, and the proton and neutron pairing energies of SPECT nuclei for 12 different force interactions.

Table 12. Neutron pairing energies for SPECT nuclei.

Nuclei	D1	D1N	D1p	D1S	S3	SKM*	SKP	SKX	SLY4	HFB9	UNEDF0	UNEDF1
^{213}Bi	1.551	1.418	1.566	0.996	0.923	0.803	1.331	1.294	1.156	0.780	0.351	0.410
^{201}Tl	1.515	1.122	1.398	1.249	0.811	0.922	1.616	1.382	1.245	0.764	0.396	0.543
^{188}Re	2.091	1.842	1.987	0.597	0.390	0.608	1.860	1.429	0.933	0.516	0.728	0.773
^{186}Re	2.178	1.866	2.168	0.631	0.463	0.663	1.828	1.411	0.903	0.478	0.000	0.797
^{133}Xe	1.583	1.331	1.516	1.346	0.819	1.070	1.816	1.546	1.222	0.768	0.449	0.590
^{131}I	1.909	1.350	1.667	1.537	1.024	1.101	1.887	1.601	1.327	0.953	0.549	0.601
^{125}I	2.045	1.950	2.262	2.050	0.918	1.479	2.194	1.992	1.699	1.318	0.705	0.786
^{123}I	2.154	2.059	2.343	2.115	1.353	1.531	2.230	2.040	1.777	1.375	0.722	0.787
^{111}In	2.432	2.174	2.457	2.203	1.373	1.428	2.231	2.142	1.952	1.422	0.819	0.761
^{94}Tc	1.682	1.212	1.742	0.000	0.834	0.000	1.487	0.000	0.000	0.000	0.000	0.000
^{90}Y	1.817	1.231	1.558	0.931	0.826	0.603	1.553	1.354	1.148	0.615	0.366	0.377
^{67}Ga	2.095	1.998	2.380	1.824	1.320	1.353	1.983	1.946	1.727	1.255	0.632	0.699
^{67}Cu	2.417	1.927	2.237	1.935	1.097	1.483	2.108	1.994	1.737	1.309	0.566	0.385
^{62}Cu	1.699	1.499	1.873	1.410	1.252	1.161	1.912	1.892	1.654	1.177	0.317	0.187
^{61}Cu	1.934	1.716	2.166	1.580	1.021	0.000	1.685	1.589	1.311	0.955	0.001	0.441
^{55}Co	1.866	1.568	1.328	0.000	0.000	0.000	1.564	0.926	0.001	0.838	0.000	0.436
^{48}V	1.462	1.678	1.640	1.367	0.678	1.141	1.556	1.739	0.362	0.650	0.053	0.001

On the basis of our results, the calculated results showed that Gogny's D1S force interaction is more suitable than D1, D1N, D1p force parameters, and it is also found that Skyrme's SKX interaction for the rms charge radii is consistent with the experimental data compared to the other force parameters. In the case of the binding energy per particle, it is clearly said that Skyrme's SKP interaction and FRDM results were consistent with the experimental binding energy results.

Furthermore, the deformation and shape of SPECT nuclei were estimated on the basis of the quadrupole deformation parameter, the proton and neutron quadrupole moment, and the proton and neutron pairing energies. According to the obtained results, it has been noticed that ^{213}Bi nucleus is stated prolate with small deformation which is mostly caused by neutron deformation, whereas ^{67}Cu and ^{111}In nuclei are in oblate formations with neutron deformations. It was also found that ^{94}Tc nucleus is stated as prolate with proton deformation. On the other hand, while ^{201}Tl, ^{133}Xe, ^{67}Ga, ^{62}Cu, ^{61}Cu, and ^{48}V nuclei for most parameter are labeled as prolate, the ^{90}Y nucleus is specified as oblate. Moreover, it is obvious that the calculated data and the obtained results for SPECT nuclei provide thorough nuclear data for the literature, especially in the extending of nuclear structure and properties of odd-odd and odd-even/even-odd nuclei.

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