GROUND-STATE PROPERTIES OF AXIALLY DEFORMED Sr ISOTOPES IN SKYRME-HARTREE-FOCK-BOGOLIUBOV METHOD

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Binding energies, the mean-square nuclear radii, neutron radii, quadrupole moments and deformation parameters to axially deformed Strontium isotopes were evaluated using Hartree-Fock-Bogoliubov method. Shape coexistence was also discussed. The results were compared with experimental data and some estimates obtained within some nuclear models. The calculations were performed for Sly4 set of Skyrme forces and for a wide range of the neutron numbers of Sr isotopes.

Strontium isotopes exhibit many interesting nuclear properties. These nuclei which have neutron numbers close to magic number 50 are known well deformed. It is hard to describe theoretically because their rms radii and isotope shifts behave in a manner showing the change of the slope at the neutron magic nucleus A=88. So, Sr nuclei are attractive to study both experimentally and theoretically [1-5].

The aim of this work is to analyse some ground-properties of even Sr isotopes using Skyrme-Hartree-Fock-Bogoliubov method for a wide range of neutron numbers.

A two-body Hamiltonian of a system of fermions can be expressed in terms of a set of annihilation and creation operators ($c, c^{\dagger}$):

$$H = \sum_{n_1 n_2} e_{n_1 n_2} c^{\dagger}_{n_1} c_{n_2} + \tfrac{1}{4} \sum_{n_1 n_2 n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4} c^{\dagger}_{n_1} c^{\dagger}_{n_2} c_{n_4} c_{n_3}, \qquad (1)$$

where $\bar{v}_{n_1 n_2 n_3 n_4} = \langle n_1 n_2 | V | n_3 n_4 - n_4 n_3 \rangle$ are anti-symmetrized two-body interaction matrix elements. In the Hartree-Fock-Bogoliubov (HFB) method, the ground-state wave function $|\Phi\rangle$ is defined as the quasiparticle vacuum where the quasiparticle operators ($\alpha, \alpha^{\dagger}$) are connected to the original particle operators via the linear Bogoliubov transformation:

$$\alpha_k = \sum_n \left(U^*_{nk} c_n + V^*_{nk} c^{\dagger}_n \right),$$
$$\alpha^{\dagger}_k = \sum_n \left(V_{nk} c_n + U_{nk} c^{\dagger}_n \right) \qquad (2)$$

In terms of the normal ρ and pairing κ one-body density matrices, defined as

$$\rho_{nn'} = \langle \Phi | c^{\dagger}_{n'} c_n | \Phi \rangle = (V^* V^T)_{nn'},$$

$$\kappa_{nn'} = \langle \Phi | c_{n'} c_n | \Phi \rangle = (V^* U^T)_{nn'} \qquad (3)$$

the expectation value of the Hamiltonian (1) could be expressed as an energy functional

$$E[\rho, \kappa] = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle}$$
$$= Tr[(e + \tfrac{1}{2}\Gamma)\rho] - \tfrac{1}{2} Tr[\Delta \kappa^*], \qquad (4)$$

where

$$\Gamma_{n_1 n_3} = \sum_{n_2 n_4} \bar{v}_{n_1 n_2 n_3 n_4} \rho_{n_4 n_2}, \quad \Delta_{n_1 n_2} = \tfrac{1}{2} \sum_{n_3 n_4} \bar{v}_{n_1 n_2 n_3 n_4} \kappa_{n_3 n_4}.$$

The HFB energy (4) has the form of local energy density functional for Skyrme forces,

$$E[\rho, \tilde{\rho}] = \int d^3 r \mathcal{H}(r), \qquad (5)$$

where

$$\mathcal{H}(r) = H(r) + \tilde{H}(r)$$

is the sum of the mean field and pairing energy densities. Variation of the energy (5) with respect to ρ and $\tilde{\rho}$ of results in Skyrme HFB equations:

$$\sum_{\sigma'} \begin{pmatrix} h(r, \sigma, \sigma') & \tilde{h}(r, \sigma, \sigma') \\ \tilde{h}(r, \sigma, \sigma') & -h(r, \sigma, \sigma') \end{pmatrix} \begin{pmatrix} U(E, r\sigma') \\ V(E, r\sigma') \end{pmatrix}$$
$$= \begin{pmatrix} E + \lambda & 0 \\ 0 & E - \lambda \end{pmatrix} \begin{pmatrix} U(E, r\sigma') \\ V(E, r\sigma') \end{pmatrix} \qquad (6)$$

Where λ is chemical potential and where local fields $h(r, \sigma, \sigma')$ and $\tilde{h}(r, \sigma, \sigma')$ can be calculated in the coordinate space by using following explicit expressions:

$$h(r, \sigma, \sigma') = -\nabla M_q \nabla + U_q$$
$$+ \tfrac{1}{2i} \textstyle\sum_{ij} \left(\nabla_i \sigma_j B_{q,ij} + B_{q,ij} \nabla_i \sigma_j \right),$$

$$\tilde{h}(r, \sigma, \sigma') = V_0 \left(1 - V_1 \left(\frac{\rho}{\rho_0} \right)^{\gamma} \right) \tilde{\rho}_q, \qquad (7)$$

where

$$M_q = \frac{\hbar^2}{2m} + \frac{1}{4}t_1\left[\left(1+\tfrac{1}{2}x_1\right)\rho - \left(x_1+\tfrac{1}{2}\right)\rho_q^2\right] + \tfrac{1}{4}t_2\left[\left(1+\tfrac{1}{2}x_2\right)\rho - \left(x_2+\tfrac{1}{2}\right)\rho_q^2\right],$$

$$B_{q,ij} = -\frac{1}{4}(t_1x_1+t_2x_2)\boldsymbol{J}_{ij} + \frac{1}{4}(t_1-t_2)\boldsymbol{J}_{q,ij} + \tfrac{1}{2}W_0\textstyle\sum_{ijk}\varepsilon_{ijk}\nabla_k(\rho+\rho_q),$$

$$U_q = t_0\left[\left(1+\tfrac{1}{2}x_0\right)\rho - \left(x_0+\tfrac{1}{2}\right)\rho_q\right] + \tfrac{1}{4}t_1\left[\left(1+\tfrac{1}{2}x_1\right)(\tau-\Delta\rho) - \left(x_1+\tfrac{1}{2}\right)\left(\tau_q-\tfrac{3}{2}\Delta\rho_q\right)\right] + \tfrac{1}{4}t_2\left[\left(1+\tfrac{1}{2}x_2\right)(\tau+\Delta\rho) + \left(x_2+\tfrac{1}{2}\right)\left(\tau_q+\tfrac{1}{2}\Delta\rho_q\right)\right] + \tfrac{1}{12}t_3\rho^\alpha\left[\left(1+\tfrac{1}{2}x_3\right)(2+\alpha)\rho - 2\left(x_3+\tfrac{1}{2}\right)\rho_q + (1-x_3)\tfrac{\alpha}{\rho}\right] - \frac{\gamma V_0 V_1}{2\rho}\left(\frac{\rho}{\rho_0}\right)^\gamma\textstyle\sum_q\tilde{\rho}_q^2 - \tfrac{1}{8}(t_1x_1+t_2x_2)\textstyle\sum_{ij}\boldsymbol{J}_{ij}^2 + \tfrac{1}{8}(t_1-t_2)\textstyle\sum_{q,ij}\boldsymbol{J}_{q,ij}^2 - \tfrac{1}{2}W_0\textstyle\sum_{ijk}\epsilon_{ijk}\nabla_k\left[\boldsymbol{J}_{ij}+\boldsymbol{J}_{q,ij}\right].$$

where index q labels the neutron (q=n) or proton (q=p) densities, while densities without index q denote the sums of proton density and neutron density. $H(\boldsymbol{r})$ and $\hat{H}(\boldsymbol{r})$ depend on the particle local density $\rho(\boldsymbol{r})$, pairing local density $\tilde{\rho}(\boldsymbol{r})$, kinetic energy density $\tau(\boldsymbol{r})$ and spin-current density $\boldsymbol{J}_{ij}(\boldsymbol{r})$. Details can be found in [6-8].

Recently, Stoitsov et al. presented a code called HFBTHO for axially deformed solution of the Skyrme HFB equations [7]. Stoitsov et al. solved the HFB equations by expanding quasiparticle wave functions on a finite basis in this code; so, the quasiparticle spectrum E_k becomes discretized. Since $E_k > 0$ and $\lambda < 0$ the lower components $V_k(\boldsymbol{r}\sigma)$ are localized functions of **r**, the density matrices

$$\rho(\boldsymbol{r}\rho,\boldsymbol{r}'\sigma') = \sum_k V_k(\boldsymbol{r}\sigma)V_k^*(\boldsymbol{r}'\sigma'),$$

$$\tilde{\rho}(\boldsymbol{r}\rho,\boldsymbol{r}'\sigma') = -\sum_k V_k(\boldsymbol{r}\sigma)U_k^*(\boldsymbol{r}'\sigma'),$$

are localized. The orthogonality relation to the single-quasiparticle HFB wave functions reads

$$\int d^3\boldsymbol{r}\sum_\sigma\left[U_k^*(\boldsymbol{r}\sigma)U_{k'}(\boldsymbol{r}\sigma) + V_k^*(\boldsymbol{r}\sigma)V_{k'}(\boldsymbol{r}\sigma)\right] = \delta_{k,k'},$$

and the norms of lower components N_k given as

$$\mathrm{N_k} = \int \mathrm{d^3\,r}\sum_\sigma|\mathrm{V_k(r\sigma)}|^2,$$

and the total number of particles defined as

$$\mathrm{N} = \int \mathrm{d^3\,r\rho(r)} = \sum_\mathrm{n}\mathrm{N_k}.$$

The best solutions of Skyrme-Hartree-Fock-Bogoliubov equations are in the coordinate space for spherical nuclei, because equation (6) reduces to a set of radial differential equations. However, for deformed nuclei, the solution of a deformed HFB equation in coordinate space is difficult and time-consuming task. Stoitsov et al. used the method proposed by Vautherin [9] to adapt the code for shorter solution time. In addition to, Stoitsov et al. treated separately the mean field and the pairing field via Hartree-Fock theory with added Lipkin-Nogami pairing. In this study this code was used.

The Strontium nuclei considered here are even nuclei with mass number A=76 up to 100. All of these isotopes are open-shell nuclei both in protons and neutrons. The number of shells taken into account is 20 and 20 for the fermionic and bosonic expansion. For solution, the basis parameter β_0 used for the calculations has been taken as 0.3.

There are number of parametrization sets for prediction of the nuclear ground state properties [10-12]. The parameter set SLy4 [12] was used in the present calculation and given in Table 1.

In Fig.1, it was shown that the binding energy per nucleon for Strontium nuclei using SLy4 parameter set in the Skyrme HFB method. Also, for comparison, empirical values, predictions of the finite-range droplet model (FRDM) [14], predictions of the extended Thomas-Fermi with Strutinsky Integral (ETF-SI) model and predictions of the relativistic mean field theory with NL-SH parameter set was showed [13]. The minimum in the binding energy per nucleon is observed at the magic neutron number N=50 in the SHFB method as well as the other nuclear models.

Table 1. SLy4 parameter set of the Skyrme forces used in this study.

Parameter	Sly4
$t_0(MeVfm^3)$	-2488.9
$t_1(MeVfm^5)$	486.82
$t_2(MeVfm^5)$	-546.40
$t_3(MeVfm^4)$	13777
x_0	0.8340
x_1	-0.3440
x_2	-1.0
x_3	1.3540
$W_0(MeVfm^5)$	123
γ	1.0

The total binding energies for Sr isotopes using SHFB with SLy4 parameter set were well produced by our calculation. The maximal error is 3 MeV for total binding energy which corresponds approximately to 0.05 MeV per particle.

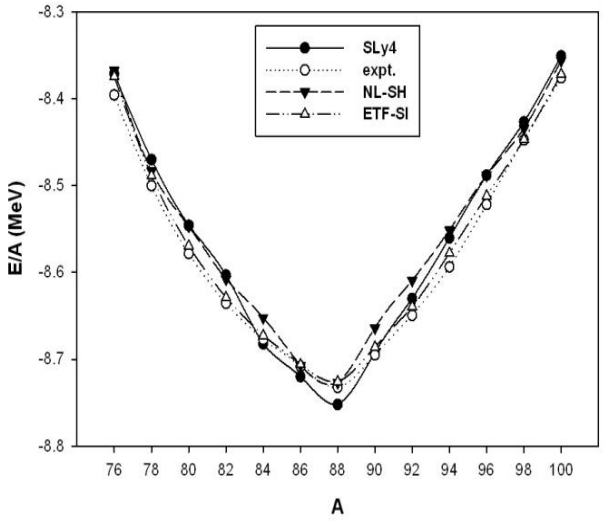

Fig.1 The binding energy per nucleon for Sr isotopes in the Skyrme HFB method with the force SLy4. The calculations from the FRDM [14], ETF-SI and relativistic mean field theory with the force NL-SH are also shown for comparison [13].

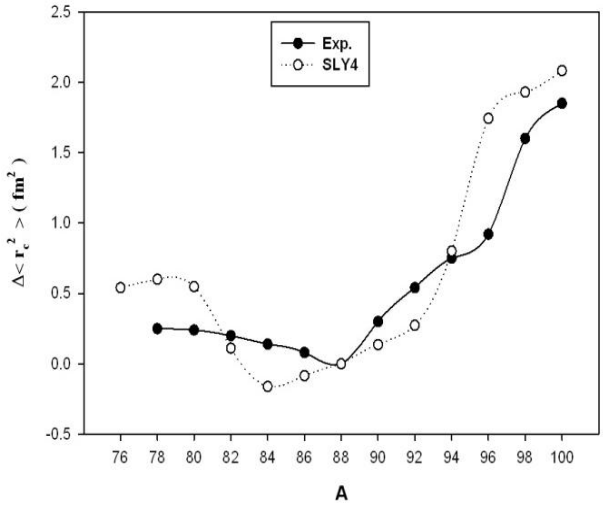

Fig.2 The isotope shifts for Sr nuclei calculated with the SLy4 parameters set. Experimental isotope shifts are also shown [15].

Isotopic shift are closely related to deformation properties and shapes. In Fig.2, the isotope shifts normalized to $< r_c^2 >_{A=88}$ for Sr isotopic chains are shown. Also, empirical data obtained from atomic laser spectroscopy [13] are shown. The predictions for isotopic shift are not totally agreement with experimental values. On the other hand, for isotopes with A>88, the agreement with empirical values is better than nuclei have A<88.

In Fig.3 values of neutron radii and rms charge radii for Sr isotopic chains are presented. General behaviour of charge radii from the lighter isotopes to the heavier ones decreases trend up to the magic isotopes. At below the magic numbers, lighter nuclei posses higher charge radii then the heavier which are closed neutron shell nucleus. This situation is agreement with kink showed in Fig.2. Adding further neutrons, the charge radii of nuclei which are heavier than the closed neutron shell starts increasing. On the other hand, also neutron radii show a kink about the neutron shell closure. However, general trend of neutron radii increases with adding neutron.

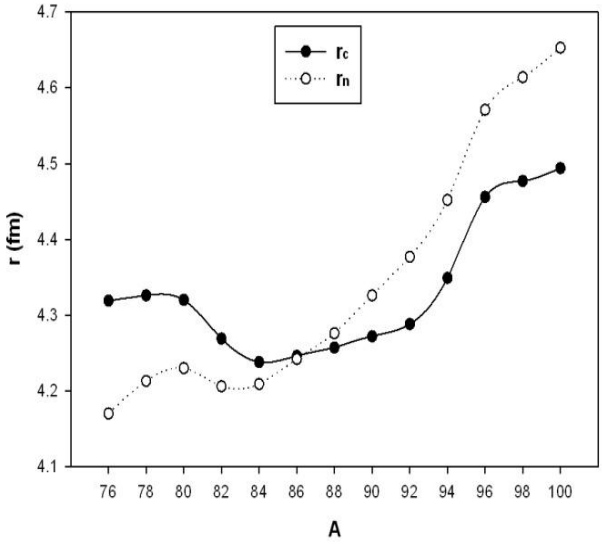

Fig. 3 The neutron and rms charge radii of Sr isotopic chains obtained in the SHFB method using Sly4 set.

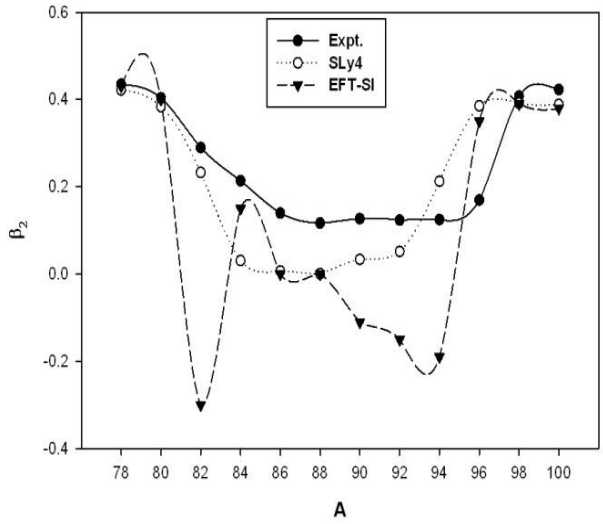

Fig.4 The quadrupole deformation β_2 for Sr isotopic chains using Sly4 parameter set. The predictions of the mass models ETF-SI and experimental values are showed for comparison.

In this work, the calculations have been performed in the Skyrme HFB method for both the prolate and oblate configurations. Results of the calculation predict deformed shapes for a large number of Sr isotopes. In Fig.4, quadrupole deformation (β_2) for the shape corresponding to the lowest energy are shown. Also predictions of finite range drop model (FRDM), predictions of ETF-SI and experimental values are shown

for comparison. As seen from the Fig.4, the predictions to the shape of Sr nuclei using axially deformed Skyrme HFB method are better than the predictions of FRDM and ETF-SI. In isotopic chain of Sr, Skyrme HFB method gives a well defined prolate shape for lighter isotopes. An addition of a few neutrons below the closed neutron shell leads to oblate shape because the shape of nuclei turn into spherical ones as nuclei approach the magic neutron number. Nuclei above this magic number (N=50) revert to the prolate shape.

In Fig.5, prolate-oblate shape coexistence of neutron-rich Sr isotopes was shown as a function of mass number. Several isotopes exhibit a second minimum beside lowest minimum. This implies shape coexistence. The prolate shape results being a few hundreds keV lower in energy than the oblate one.

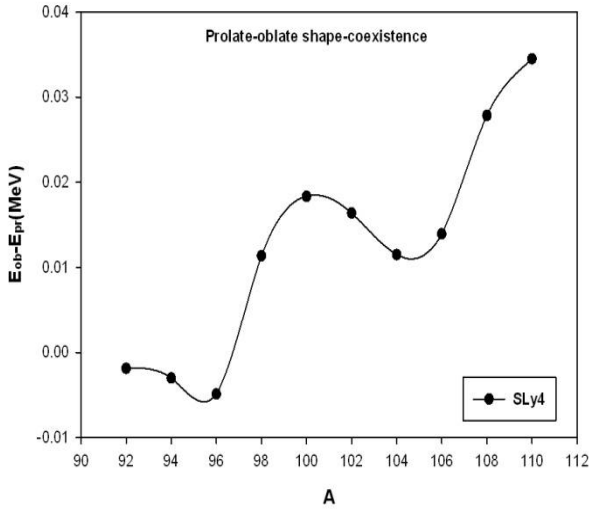

Fig.5 The prolate-oblate shape coexistence of neutron-rich Sr isotopes obtained using SHFB method.

In Table.2, calculated quadrupole values of proton, neutron and total quadrupole values for Sr nuclei are shown.

Table2.The calculated quadrupole values of Sr nuclei

	Q_p(barn)	Q_n(barn)	Q(barn)
^{74}Sr	3,579	3,127	6,707
^{76}Sr	3,718	3,567	7,286
^{78}Sr	3,693	3,739	7,433
^{80}Sr	3,442	3,513	6,935
^{82}Sr	2,070	2,176	4,246
^{84}Sr	0,249	0,328	0,577
^{86}Sr	0,062	0,076	0,138
^{88}Sr	0,006	0,006	0,012
^{90}Sr	0,270	0,435	0,704
^{92}Sr	0,405	0,721	1,126
^{94}Sr	1,908	0,932	4,840
^{96}Sr	3,752	5,702	9,454
^{98}Sr	3,844	6,119	9,964
^{100}Sr	3,873	6,347	10,220

As a result of this work, Skyrme HFB theory has been employed to obtain the ground-state properties of the isotopic chain of Sr. Region which are near the Sr nuclei are interesting because nuclei in this region have large transformations of shapes and exhibit anomalous behaviour in the isotope shifts. Using SLy4 parameters set in the Skyrme HFB method, isotopic shifts and large deformation were predicted clearly. On the other hand, Skyrme HFB method predicts prolate-oblate shape coexistence in heavy Sr nuclei. The binding energies of Sr nuclei have been described successfully in the Skyrme HFB method. The parabolic behaviour of the binding energy per nucleon was obtained well. Curve of the binding energies per nucleon are agreement with experimental curve and with the extensive mass fits of FRDM. Also, this curve is consistent with RMF theory using NL-SH parameter set. All of these reasons Skyrme HFB method provide good description of the ground state nuclear properties to isotopic chain of Sr.

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