Systematics of nuclear ground-state properties of Sr isotopes by covariant density functional theory

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Systematics of nuclear ground state properties in Sr-isotope by covariant density functional theory

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The hyperfine structure and isotope shifts of Sr-isotopes, both even-even and odd-even nuclei, are studied in the covariant density functional theory (DFT) with the new parameter set DD-PC1. Pairing correlation is treated by using the Bogoliubov with a separable form of the pairing interaction. Spin-parity, charge radii, two-neutron separation energies, and pairing energies of ground states are calculated and compared with experimental data. We find a shape transition at $N \approx 60$ in charge radii and spin-parity, which are consistent to each other, and generally agree with experiments. Although the nuclear masses are not very sensitive to these shape changes, odd-even mass different and pairing effect are very important to study the shape transition and shape coexistence phenomena in Sr-isotopes.

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With new generations of radioactive beam facilities in many countries around the world, experimental and theoretical studies on the properties of the nuclear shape evolution as the number of neutron changes is nowadays one of the most active and fruitful research in nuclear physics. In recent decades, several measurements on isotopes with $Z = 36 - 40$ [1–5] have found a sudden shape transition at $N \approx 60$, but the nature of this transition remains disputed. On the theoretical side, both phenomenological models [6, 7] and microscopical models [8–11] have been used to study these isotopes. Most of these models can identify the shape evolution around $N \approx 60$ correspond to the competition between the prolate and oblate minimum, the ground states depend on the details of calculations. One of the major goals of the current manuscript is to try to understand to how the uncertainties in the extrapolation of the pairing strength towards shape coexistence.

Strontium isotope, with 38 protons, belong to the Z=40 sub-shell closure which have a rapid variation of nuclear ground state properties as a function of the neutron number towards both sides of the line of β-stability [5, 12]. The charge radius decreases smoothly form the neutron-deficient side $N \approx Z = 38$ to the neutron shell closure $N = 50$, then an almost linear increase is followed by a strong discontinuity at $N = 59 - 60$. It means that the ground states of Sr-isotopes with N ranging around the magic number $N = 50$ are weakly deformed, but they undergo two shape transition from nearly spherical to well deformed deformation at both neutron deficient and rich side.

At present, covariant Density Functional Theory (DFT) based on the mean-field theory provides a very reasonable concept for a universal description of nuclei all over the periodic table [13, 14]. Relativistic models incorporate Lorentz invariance, connecting in a consistent way the spin and spatial degrees of freedom of the nucleus, and provide thus a relatively simple phenomenological description for many nuclear properties using only a few phenomenological parameters. In this framework, there are several popular parameter sets, including NL3 [15], PK1 [16] for the nonlinear RMF model, DD-ME2 [17], PKDD [16] for density-dependent RMF model, DD-PC1 [18], PC-PK1 [19] for the point-coupling RMF model. Among these parameter sets, the DD-PC1 was proposed very recently by additional fitting to the masses of 64 axially deformed nuclei. Comparing with the available data, DD-PC1 provide a very good agreement to the properties of spherical and deformed medium-heavy and heavy nuclei, including binding energies, charge radii, deformation parameters, neutron skin thickness, and excitation energies of giant multipole resonances.

In most calculations of DFT, the pairings have often been taken into account in a very phenomenological way in the BCS model with the monopole pairing force, adjusted to the experimental odd-even mass differences. In many cases, however, this approach presents only a poor approximation. The physics of weakly bound nuclei, in particular, necessitates a unified and self-consistent treatment of mean-field and pairing correlations. This has led to the formulation and development of the relativistic Hartree-Bogoliubov (RHB) model, which represents a relativistic extension of the conventional Hartree- Fock-Bogoliubov framework. In most applications of the RHB model simple phenomenological pairing forces such as the monopole force taking into account pairing correlations only in the $J = 0$ channel or density dependent δ interaction(DDDI) [20–22] where additional simplifying assumptions have to be introduced as for instance a pairing window. Gogny forces [23–25] with finite range are considered to provide the best phenomenological description of pairing correlations in nuclei. However, because of their numerical complexity, they are applied only by a rather limited number of groups in the literature.

Recently, we have introduced a separable form of the pairing force for RHB calculations in finite nuclei [26–30]. The force is separable in momentum space, and is determined by two parameters that are adjusted to reproduce the pairing gap of the Gogny force in symmetric nuclear matter. Using the Talmi-Moshinsky techniques [31–33], it can be represented as a series of separable terms in a harmonic oscillator basis. Although different from the Gogny force, the corresponding effective pairing interaction has been shown to reproduce with high accuracy pairing gaps and energies calculated with the original Gogny force, both in spherical and deformed nuclei. In particular, this approach retains the basic advantage of the finite-range Gogny force, and the numerical calculation is much simpler. Therefore, in this work, we study the ground states properties of Sr-isotope in the framework of the self-consistent RHB approximation based on the DD-PC1 parameter set together with the separable pairing force.

In the framework of covariant DFT, the energy functional of RHB model depends not only on the density matrix $\hat{\rho}$ and the meson fields ϕ_m, but in addition also on the pairing tensor:

$$E_{RHB}[\hat{\rho},\phi_m,\hat{\kappa}] = E_{RMF}[\hat{\rho},\phi_m] + E_{pair}[\hat{\kappa}] \qquad (1)$$

where $E_{RMF}[\hat{\rho},\phi_m]$ is the RMF-functional based on the density dependent point-coupling interaction DD-PC1 [18], and the pairing energy $E_{pair}[\hat{\kappa}]$ is given by

$$E_{pair}[\hat{\kappa}] = \frac{1}{4}Tr[\hat{\kappa}^* V^{pp}\hat{\kappa}] \qquad (2)$$

V^{pp} denotes the two-body pairing interaction. Here we use the separable form of the pairing force

$$\langle k|V^{^1S_0}_{\rm sep}|k'\rangle = -Gp(k)p(k') \qquad (3)$$

A simple Gaussian ansatz $p(k) = e^{-a^2k^2}$ is assumed. In ref. [28] the two parameters G and a have been fitted to the density dependence of the gap $\Delta(k_F)$ of Gogny D1S [34] in nuclear matter. The obtained values for the parameters are $G = 728$ MeVfm^3 and $a = 0.644$ fm.

The odd-A nuclei can be considered as an even-even core plus an unpaired nucleon (or quasiparticle). Using the equal filling approximation (EFA) [35, 36], the unpaired nucleon is treated in an equal footing with its time-reversed state by sitting half a nucleon in a given orbital and the other half in the time-reversed partner. For the axially deformed nuclei, the spin is simply the projection of the angular momentum along the symmetry axis for the last occupied proton or neutron level, when this level is occupied by a single nucleon. For the spherical nuclei with degenerate levels, the nuclear spin is defined as the maximum value of j_z, which is $|j|$.

The mean-square charge radius is calculated as [37, 38]:

$$r_c^2 = \frac{1}{Z}\int r^2 d^3 n_p(r) + r_p^2 + \frac{N}{Z}r_n^2 - r_{c.m.}^2, \qquad (4)$$

where $n_p(r)$ is the point-proton density and $r_p^2 = 0.63$ fm^2 and $r_n^2 = -0.12$ fm^2 are the rms proton and neutron charge radii, respectively. The center-of-mass correction is computed as $r_{c.m.}^2 = 3\hbar/2m\omega A$ fm^2, with $\omega = 1.85 + 35.5/A^{1/3}$ MeV. We show in Fig.1 the comparison of calculated and experimental charge radii, plotted as $\delta\langle r_c^2\rangle^{50,N} = \langle r_c^2\rangle^N - \langle r_c^2\rangle^{50}$.

A	N	Exp.[40]	spherical	oblate	prolate
83	45	7/2+(9/2+)	$g_{9/2}$		
85	47	9/2+	$g_{9/2}$		
87	49	9/2+	$g_{9/2}$		
89	51	5/2+	$d_{5/2}$		
91	53	5/2+	$d_{5/2}$		
93	55	5/2+	$d_{5/2}$	$3+[402]$	$3+[422]$
95	57	1/2+		$1+[400]$	$3-[541]$
97	59	1/2+		$1+[400]$	$9+[404]$
99	61	3/2+			$3+[411]$
101	63	5/2-			$5-[532]$
103	65				$5+[413]$

TABLE I: Experimental spin-parity assignments [40] compared with RHB-EFA results for one-quasiparticle states in odd-A Sr-isotopes.

The potential energy surface (PES) in the plane of deformation variables is obtained by imposing a quadratic constraint on the mass quadrupole moments

$$\langle H\rangle + C_{20}(Q_{20} - q_{20})^2 \qquad (5)$$

Where $\langle H\rangle$ is the total energy, and q_{20} is a constrained value of the quadrupole moments, and C_{20} is the corresponding stiffness constant [39]. The quadrupole Q_{20} moments for neutrons and protons are calculated using the expressions

$$Q_{20} = \langle 2r^2 P_2(cos\theta)\rangle_{n,p} = \langle 2z^2 - x^2 - y^2\rangle \qquad (6)$$

The conventional deformation parameter β is obtained from the calculated quadrupole moments through

$$Q_{20} = \sqrt{\frac{16\pi}{5}}\frac{3}{4\pi}AR_0^2\beta \qquad (7)$$

with $R_0 = 1.2A^{1/3}$ (fm).

In this letter, we also calculate the 3-point neutron pairing energy (Δ_n^3) and two-neutron separation energy (S_{2n}) of the Sr-isotope, which can be easily obtained from the binding energies (BE),

$$\Delta_n^3(N,Z) = \frac{1}{2}(BE(N-1,Z) - 2BE(N,Z) + BE(N+1,Z) \qquad (8)$$

$$S_{2n}(N,Z) = BE(N-2,Z) - BE(N,Z) \qquad (9)$$

The ground state properties of Sr-isotope from N=44 to N=66 with both even-even and even-odd nuclei have been calculated with RHB theory with DD-PC1 [18] and the separable pairing force [27].

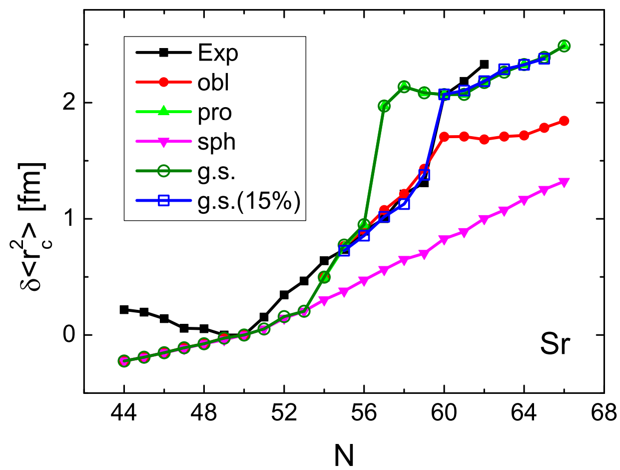

FIG. 1: (Color on line) Calculated $\delta\langle r_c^2\rangle$ in Sr isotopes compared to experimental data from Ref. [41]. Results for oblate, prolate and spherical minima are displayed with different symbols (see legend). Open circles and squares correspond to ground-state results with different pairing strength.

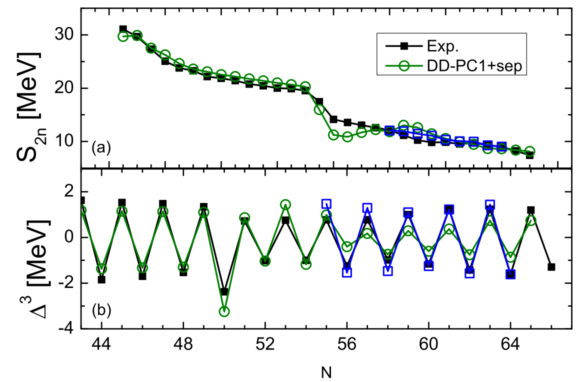

FIG. 2: (Color on line) Calculated S_{2n} (a) and Δ^3 (b) compared to experimental data from Ref. [42]. The open squares are the results of S_{2n} and Δ^3 with larger pairing strength.

The experimental spin-parity assignments in odd-A Sr-isotopes [40] are shown in the second column of Tablet.I. They are compared to the one-quasiparticle states calculated by the RHB-EFA. In our calculations, Sr isotopes evolve from spherical shapes in $^{83-91}$Sr around $N = 50$ with the spherical $g_{9/2}$ and $d_{5/2}$ shells involved, to slightly deformed shapes in ^{93}Sr, and finally to shape coexistence in $^{95-103}$Sr. In the lighter isotopes the two spherical shells give the same ground states as the experimental. For slightly deformed nuclei, the experimental ground states are 5/2+ in ^{93}Sr. In ^{93}Sr, the potential energy surface (PES) is very flat. Although the oblate minimum ($\beta \approx -0.2$) with $3+[402]$ is slightly deeper, the spherical minimum with $d_{5/2}$ is very close and it consistences with the measurement. For the $N \geq 57$ Sr-isotopes, these are two minimums for oblate and prolate shape. The competition between these two minimums are very sensitive to the calculations. In our work, the oblate ground state in ^{95,97}Sr is $1+[400]$, and the prolate ground state is $3-[541]$ and $9+[404]$ respectively. Comparing with the measurements, these two nuclei should be oblate deformed. But our results prefer the prolate ground state, since $N = 58$ is a sub-shell structure in prolate side for our calculation. For the higher isotopes, the prolate ground state with $3+[411]$ in ^{99}Sr and $5-[532]$ in ^{101,103}Sr are agreement with the experiment.

Fig.1 displays the evolution of the nuclear charge radii in Sr isotopes, where the experimental [41] and the calculated charge radii corresponding to the oblate, prolate and spherical including both even-even and odd-A isotopes are plotted as functions of neutron number. The charge radii decrease until the shell closure at $N = 50$. After that, an almost linear increase is followed by a strong discontinuity at $N = 59-60$.

For $44 \leq N \leq 55$, our calculation predict that these nuclei are soft against deformation. The softness, or the width of the PES around $\beta = 0$, increase as one departs from the shell closure at $N = 50$. Thus, the actual charge radius of our calculation will slightly increases and very closes to the experimental data if we take account the contributions of deformed configuration for the ground state.

For neutron rich ($N \geq 56$) nuclei, the axial symmetric calculation provides two minimum in both the prolate and the oblate region. The binding energy differences between the lowest oblate and prolate minima is less than 1 MeV for these nuclei. We indicate a sudden rising of charge radius from $N = 56$ to $N = 57$, which corresponds to the transition from the oblate $\beta = -0.2$ (^{94}Sr) to the prolate shape $\beta = 0.5$ (^{95}Sr). As we see from fig.1 the jump of experiment is observed between $N = 59-60$. However, we do not think this discrepancy is significant since it is related to the subtle competition between prolate and oblate shapes.

In fig.2 we can see the results of two neutron separation energy S_{2n} and 3-points neutron pairing energy Δ^3 are shown as a function of the neutron number for both even and odd. In general, we reproduce the experimental data reasonably well, which is taken from the mass table [42]. Between $N = 52$ and $N = 54$, the S_{2n} energies are underestimated by the calculations, which are also found by ref. [10]. In our calculations a change in the tendency is observed from $N = 56$ to $N = 57$, and the 3-points neutron pairing energies from $N = 56$ to $N = 59$ are slightly smaller than the experimental data.

In general, our calculations for Sr-isotope follow the measurements very well expect the nuclei around $N = 58$. Since the effective mass of DD-PC1 is a little small, a sub-shell structure has been found in prolate ground state of the nuclei around $N = 58$ for our calculations. This spe-

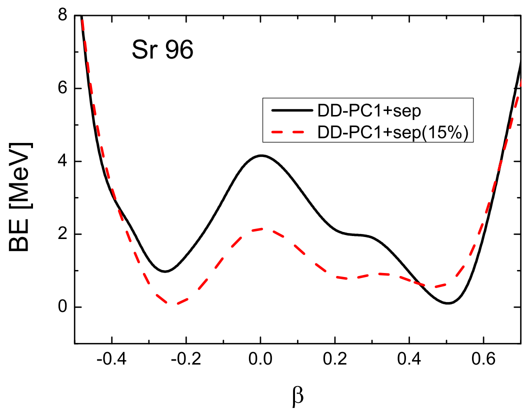

FIG. 3: (Color on line) The potential energy surfaces in ^{96}Sr obtained in different pairing schemes (see legend) with DD-PC1 parameterization of the RMF Lagrangian.

N	β	BE	$\delta\langle r_c^2\rangle$	BE(15%)	$\delta\langle r_c^2\rangle$(15%)	$\delta\langle r_c^2\rangle$(exp)
57	obl	-810.320	1.075	-811.911	1.018	1.003
	pro	-811.294	1.971	-811.192	1.693	
58	obl	-816.909	1.214	-818.917	1.128	1.213
	pro	-817.764	2.137	-818.385	1.965	
59	obl	-821.918	1.431	-822.975	1.378	1.312
	pro	-822.750	2.086	-822.906	2.071	

TABLE II: The binding energy and charge radii of nuclei around $N = 58$ subshell with different pairing interaction.

cial structure makes $N = 58$ as a 'magic' number at the prolate side, and become more stable than other minimums. However, the experiment spin-parity and charge radii have shown us that the oblate minimum of these nuclei are the real ground state. The basic idea to solve this problem is to use another parameter set with large effective mass, such as Skyrme(SkM*) or Gogny D1S interaction, which we will discuss in the future.

Seen from Fig.2(b), the calculated Δ^3 is smaller than the experimental data after $N = 55$. So here we slightly increase the pairing strength (15%) to fit the experimental results (open square line in Fig.2 (b)) and study how the pairing effect on shape coexistence. As we can see from Fig.1 and Fig.2, the calculated $\delta\langle r_c^2\rangle$ and two neutron separation energy with larger pairing are much closer to the experimental results, especially for the nuclei around $N = 58$. In Fig.3 we display the potential energy surfaces of ^{96}Sr obtained from self-consistent RHB calculation based on the parameter set DD-PC1 using the separable pairing with 100%(black) and 115%(red) strength in the pairing channel. And we find the ground state of ^{96}Sr jump from the prolate to oblate. In table.II, we compare the ground state properties of the nuclei around $N = 58$ with different pairing strength. Compare with the experimental $\delta\langle r_c^2\rangle$ and spin-parity results in Sec. III.A, the oblate minimum should be the ground state for these three nuclei. The separable pairing interaction is introduced by reproducing the pairing properties of Gogny D1S in nuclear matter. And we have proved that the separable pairing interaction can give the same pairing properties as Gogny D1S in both spherical and deformed nuclei [26–30]. Compare the experimental Δ^3, Gogny D1S is obviously too small for these nuclei. And the same problem happens in the HFB calculation with Gogny D1S, they cannot reproduce the experimental for these three nuclei too [43]. In this manuscript, by increasing a litter bit of the pairing strength, we not only reproduce the experimental Δ^3, but other ground states of nuclei around $N = 58$, such as: charge radii, two neutron separation energy and spin-parity properties of the odd-A nuclei.

In summary we have studied the ground states properties of Sr-isotopes in the neutron-rich side. We have analyzed various sensitive nuclear observables, such as charge radii, two-neutron separation energy, neutron pairing energy and the spin-parity of the ground states in a search for signatures of shape transitions. We have found that the charge radii and the spin-parity are very sensitive to the shape changes. In addition, although the pairing can not change the level density, the effect is very important, and should be treated very carefully.

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