Covariant description of shape evolution and shape coexistence in neutron-rich nuclei at $N \approx 60$

J. Xiang, Z. P. Li, Z. X. Li

School of Physical Science and Technology, Southwest University, Chongqing 400715, China

J. M. Yao

School of Physical Science and Technology, Southwest University, Chongqing, 400715 China

Physique Nucléaire Théorique, Université Libre de Bruxelles, C.P. 229, B-1050 Bruxelles, Belgium

J. Meng

State Key Laboratory of Nuclear Physics and Technology, School of Physics, Peking University, Beijing 100871, China

School of Physics and Nuclear Energy Engineering, Beihang University, Beijing 100191, China

Abstract

The shape evolution and shape coexistence phenomena in neutron-rich nuclei at $N \approx 60$, including Kr, Sr, Zr, and Mo isotopes, are studied in the covariant density functional theory (DFT) with the new parameter set PC-PK1. Pairing correlations are treated using the BCS approximation with a separable pairing force. Sharp rising in the charge radii of Sr and Zr isotopes at $N = 60$ is observed and shown to be related to the rapid changing in nuclear shapes. The shape evolution is moderate in neighboring Kr and Mo isotopes. Similar as the results of previous Hartree-Fock-Bogoliubov (HFB) calculations with the Gogny force, triaxiality is observed in Mo isotopes and shown to be essential to reproduce quantitatively the corresponding charge radii. In addition, the coexistence of prolate and oblate shapes is found in both $^{98}\text{Sr}$ and $^{100}\text{Zr}$. The observed oblate and prolate minima are related to the low single-particle energy level density around the Fermi surfaces of neutron and proton respectively. Furthermore, the 5-dimensional (5D) col-
lective Hamiltonian determined by the calculations of the PC-PK1 energy functional is solved for $^{98}$Sr and $^{100}$Zr. The resultant excitation energy of $0^+_2$ state and E0 transition strength $\rho^2(E0; 0^+_2 \rightarrow 0^+_1)$ are in rather good agreement with the data. It is found that the lower barrier height separating the two competing minima along the $\gamma$ deformation in $^{100}$Zr gives rise to the larger $\rho^2(E0; 0^+_2 \rightarrow 0^+_1)$ than that in $^{98}$Sr.

**Keywords:**
Covariant density functional, shape evolution and shape coexistence, charge radii, neutron-rich Kr, Sr, Zr, Mo isotopes

1. **Introduction**

In recent decades, the evolution of nuclear shapes along isotopic and isotonic chains in neutron-rich nuclei at $N \approx 60$ has attracted many attentions. The sudden onset of quadrupole deformation in neutron-rich Sr and Zr isotopes at the neutron number $N = 60$ is of particular interest. Such a rapid shape evolution has been deduced from the abrupt changing of lifetimes of $2^+_1$ states $[1, 2]$ as well as the quadrupole moments of rotational bands $[3]$. Besides, the excitation energies of $2^+_1$ states $[4]$, two-neutron separation energies $[5]$, and mean-square charge radii $[6]$ exhibit a dramatic change between $N = 58$ and 60 in Sr and Zr isotopes. Very recently, the systematic of the $2^+_1$ states in Kr isotopes has been extended up to $N = 60$ $[7]$, at which nucleus, the energy of the first excited state drops down suddenly by $\sim 400$ keV. It indicates that the shape transition is also rather abrupt in Kr isotopes. However, the measured charge radii was shown to be increasing moderately with the neutron number at $N = 60$ $[8]$.

Essential to the understanding of this dramatic shape evolution is the coexistence of different shapes in the two lowest $0^+$ states. Shape coexistence phenomena at low energy in Sr and Zr isotopes around $N = 60$ have been shown in many experimental measurements. In Ref. $[9]$, Jung et al. discovered two low-lying $0^+$ states in $^{96}$Sr at 1229 and 1465 keV respectively. Later on, an extremely strong electric monopole transition of $\rho^2(E0) = 0.18$ was observed between the first two $0^+$ states $[10, 11]$. The analysis of $B(E2)$ and $\rho^2(E0)$ values for both $^{98}$Sr and $^{100}$Zr by Mach et al. indicates that these two nuclei have very similar structures $[12]$. Schussler et al. discovered a very low-lying $0^+$ state at 215.5 keV in $^{98}$Sr. The transition probabilities, the reduced E0 matrix element and the observed level structure suggest the
coexistence of a quadrupole deformed ground state and a spherical excited 0+ state in ⁹⁸Sr [13]. To clarify such a picture of shape coexistence, an experiment to measure the spectroscopic quadrupole moment of the 2⁺₁ state has been proposed [14].

On the theoretical side, the shape evolution around N = 60 has been studied extensively with various theoretical models, including the phenomenological models [15, 16, 17, 18, 19, 20, 21, 22], the interacting boson model [23], the modern shell model [24] and the self-consistent mean-field models with the Skyrme force [25, 26, 27], the Gogny force [28, 29, 30] as well as the effective relativistic Lagrangian [31]. Most of these models have shown the increasing of deformations up to N = 60 and indeed found the competing prolate and oblate minima. However, the subtle balance between these two minima depends on the details of calculations.

In recent years, nuclear covariant DFT has achieved great success in the description of ground state properties of both spherical and deformed nuclei all over the nuclear chart [32, 33, 34, 35]. In particular, the covariant DFT theory with a point-coupling interaction has recently attracted more and more attention [36]. It shows great advantages in the extension for nuclear low-lying excited states by using projection techniques [37], generator coordinate methods [38, 39, 40] and collective Hamiltonian [41]. In this framework, there are several popular parameter sets, including PC-F1 [42], DD-PC1 [43], and PC-PK1 [44]. Among these parameter sets, the PC-PK1 was proposed very recently by fitting to observables of 60 selected spherical nuclei, including the binding energies, charge radii, and empirical pairing gaps. The success of PC-PK1 has been illustrated in the description of infinite nuclear matter and finite nuclei for both ground-state and low-lying excited states. Furthermore, the PC-PK1 provides a good description for the isospin dependence of binding energy along either isotopic or isotonic chain.

Recently, a separable pairing force with two universal parameters has been introduced, which was adjusted to reproduce the pairing properties of the Gogny force D1S in nuclear matter [45]. The separable pairing force has been shown to be successful in the description of nuclear matter [45], spherical and deformed nuclei [46, 47, 48, 49]. Therefore, in this work, we would like to use the PC-PK1 parameter set together with the separable force to perform a systematic calculation for the neutron-rich Kr, Sr, Zr, and Mo isotopes. The shape evolution and shape coexistence in this region will be examined.

The theoretical framework for the relativistic point-coupling model with
the separable pairing force is described in Sec. 2. The shape evolution in neutron-rich Kr, Sr, Zr, and Mo isotopes at \( N \approx 60 \) and shape coexistence phenomena in \(^{98}\text{Sr}\) and \(^{100}\text{Zr}\) will be discussed in Sec. 3. Finally, a summary is given in Sec. 4.

2. The model

In the covariant DFT with point-coupling interaction, the energy functional has the following form \([42, 44]\),

\[
E_{\text{RMF}} = \sum_k \int dr \ v_k^2 \bar{\psi}_k(r) (-i \gamma \cdot \nabla + m) \psi_k(r)
\]

\[
+ \int dr \left( \frac{\alpha_S}{2} \rho_S^2 + \frac{\beta_S}{3} \rho_S^3 + \frac{\gamma_S}{4} \rho_S^4 + \frac{\delta_S}{2} \rho_S \Delta \rho_S 
\right.
\]

\[
+ \frac{\alpha_V}{2} j_{\mu} j^\mu + \gamma_V \left( j_{\mu} j^\mu \right)^2 + \frac{\delta_V}{2} j_{\mu} \Delta j^\mu
\]

\[
+ \frac{\alpha_{TV}}{2} j_{TV} \cdot \nabla (j_{TV})_{\mu} + \frac{\delta_{TV}}{2} j_{TV} \Delta (j_{TV})_{\mu} 
\]

\[
+ \frac{1}{4} F_{\mu\nu} F^{\mu\nu} - F_0^{\mu} \partial_0 A_{\mu} + e \frac{1 - \tau_3}{2} j_{\mu} A^\mu \right),
\]

(1)

where \( e \) is the charge unit for protons and it vanishes for neutrons. The energy functional \( (1) \) contains 9 coupling constants \( \alpha_S, \alpha_V, \alpha_{TV}, \beta_S, \gamma_S, \gamma_V, \delta_S, \delta_V \) and \( \delta_{TV} \). The subscripts indicate the symmetry of the couplings: \( S \) stands for scalar, \( V \) for vector, and \( T \) for isovector, while the symbol refer to the additional distinctions: \( \alpha \) refers to four-fermion term, \( \delta \) to derivative couplings, and \( \beta \) and \( \gamma \) to the third- and fourth-order terms, respectively.

The local densities and currents in the energy functional \( (1) \) are determined by,

\[
\rho_S(r) = \sum_k v_k^2 \bar{\psi}_k(r) \psi_k(r), \tag{2}
\]

\[
j^\mu(r) = \sum_k v_k^2 \bar{\psi}_k(r) \gamma^\mu \psi_k(r), \tag{3}
\]

\[
\bar{\gamma}^\mu j_{TV}(r) = \sum_k v_k^2 \bar{\psi}_k(r) \bar{\gamma}^\mu \psi_k(r). \tag{4}
\]
Minimizing the energy functional (1) with respect to $\psi_k$, one obtains the Dirac equation for the single nucleons

$$[\gamma_\mu (i\partial^\mu - V^\mu) - (m + S)]\psi_k = 0.$$  \hspace{1cm} (5)

The single-particle effective Hamiltonian contains local scalar $S(r)$ and vector $V^\mu(r)$ potentials,

$$S(r) = \Sigma_S,$$

$$V^\mu(r) = \Sigma^\mu + \vec{\tau} \cdot \vec{\Sigma}_{TV}^\mu,$$  \hspace{1cm} (6)

where the nucleon isoscalar-scalar $\Sigma_S$, isoscalar-vector $\Sigma^\mu$ and isovector-vector $\vec{\Sigma}_{TV}^\mu$ self-energies are given in terms of the various densities and currents,

$$\Sigma_S = \alpha_S \rho_S + \beta_S \rho_S^2 + \gamma_S \rho_S^3 + \delta_S \rho_S,$$

$$\Sigma^\mu = \alpha_V j_V^\mu + \gamma_V (j_V^\mu)^3 + \delta_V \delta j_V^\mu + eA^\mu,$$

$$\vec{\Sigma}_{TV}^\mu = \alpha_{TV} j_{TV}^\mu + \delta_{TV} \delta j_{TV}^\mu.$$  \hspace{1cm} (7)

For a system with time reversal invariance, the space-like components of the currents and the vector potential vanish. Furthermore, one can assume that the nucleon single-particle states do not mix isospin, that is, the single-particle states are eigenstates of $\tau_3$. Therefore only the third component of isovector potentials $\vec{\Sigma}_{TV}^\mu$ survives. The Coulomb field $A_0$ is determined by Poisson’s equation.

Pairing correlations between nucleons are treated using the BCS approximation with a pairing force separable in momentum space, i.e., $\langle k | V^1 S_0 | k' \rangle = -G p(k)p(k')$, introduced in Ref. [45] with a Gaussian ansatz $p(k) = e^{-a^2 k^2}$. The two parameters $G$ and $a$ have been adjusted to reproduce the pairing properties of the Gogny force D1S in nuclear matter. The obtained values for the parameters are $G = -728$ MeV·fm$^3$ and $a = 0.644$ fm.

In the coordinate space, the separable pairing force takes the following form,

$$V(r_1, r_2, r_1', r_2') = G\delta (R - R') P(r) P(r') \frac{1}{2} (1 - P^\sigma),$$  \hspace{1cm} (10)

where $R = \frac{1}{2} (r_1 + r_2)$ and $r = r_1 - r_2$ are the center-of-mass and the relative coordinates respectively. $P(r)$ is the Fourier transform of $p(k)$,

$$P(r) = \frac{1}{(4\pi a^2)^{3/2}} e^{-r^2/4a^2}.$$  \hspace{1cm} (11)
The pairing force has finite range, and it can preserve translational invariance due to the presence of the factor $\delta(R - R')$. Even though $\delta(R - R')$ implies that this force is not completely separable in coordinate space, the corresponding antisymmetrized $pp$ matrix elements can be represented as a sum of a finite number of separable terms in the basis of a three-dimensional (3D) harmonic oscillator (HO):

$$
\langle \alpha \bar{\beta} | V | \gamma \bar{\delta} \rangle = G \sum_{N_x=0}^{N_0} \sum_{N_y=0}^{N_0} \sum_{N_z=0}^{N_0} (V_{\alpha \bar{\beta}}^{N_x N_y N_z})^* V_{\gamma \bar{\delta}}^{N_x N_y N_z}, \quad (12)
$$

where $N_x$, $N_y$, and $N_z$ are the quantum numbers of the corresponding one-dimensional (1D) HO in the center-of-mass frame. The summations over $N_x$, $N_y$, and $N_z$ are restricted to finite terms with cutoffs $N_0^x$, $N_0^y$, and $N_0^z$ respectively. The convergence with respect of the cutoffs has to be checked in calculations. $V_{\alpha \bar{\beta}}^{N_x N_y N_z}$ represents the single-particle matrix element in the 3D HO basis. In this case, the pairing field can be written as a sum of a finite number of separable terms

$$
\Delta_{\alpha \bar{\beta}} = G \sum_{N_x=0}^{N_0} \sum_{N_y=0}^{N_0} \sum_{N_z=0}^{N_0} (V_{\alpha \bar{\beta}}^{N_x N_y N_z})^* P_{N_x N_y N_z}, \quad (13)
$$

with the coefficients

$$
P_{N_x N_y N_z} = \sum_{\gamma \delta > 0} V_{\gamma \bar{\delta}}^{N_x N_y N_z} \kappa_{\gamma \delta}, \quad (14)
$$

where $\kappa_{\gamma \delta}$ is the matrix element of pairing tensor. The expression of $V_{\gamma \bar{\delta}}^{N_x N_y N_z}$ has been derived in Ref. [48].

In the BCS approximation, the pairing gap $\Delta_k$ for each single-particle state $\psi_k$ is finally determined as follows,

$$
\Delta_k = \sum_{\alpha \bar{\beta}} \Delta_{\alpha \bar{\beta}} F_{k \alpha} F_{k \bar{\beta}}, \quad (15)
$$

where $F_{k \alpha}$ is the expansion coefficient for the large component in Dirac spinor $\psi_k$ on the 3D HO basis. The resultant pairing energy is given by

$$
E_{\text{pair}} = G \sum_{N_x=0}^{N_0} \sum_{N_y=0}^{N_0} \sum_{N_z=0}^{N_0} (P_{N_x N_y N_z})^* P_{N_x N_y N_z}. \quad (16)
$$
The center-of-mass correction to the energy is considered microscopically
with both the direct and exchange terms,
\[ E_{\text{c.m.}} = -\frac{\langle \hat{P}_{\text{c.m.}}^2 \rangle}{2mA}, \]  
(17)
where \( m \) is the mass of nucleons. \( A \) is mass number and \( \hat{P}_{\text{cm}} = \sum_i^A \hat{p}_i \) is the
total momentum in the c.m. frame.

The total nuclear energy is determined by
\[ E_{\text{tot}} = E_{\text{RMF}} + E_{\text{pair}} + E_{\text{c.m.}} \]  
(18)
The potential energy surface (PES) in the plane of deformation va riables is
obtained by imposing a quadratic constraint on the mass quadrupole mo-
ments
\[ \langle H \rangle + \sum_{\mu=0,2} C_{2\mu} (\langle \hat{Q}_{2\mu} \rangle - q_{2\mu})^2 \]  
(19)
where \( \langle H \rangle \) is the total energy, and \( \langle \hat{Q}_{2\mu} \rangle \) denotes the expectation value of
the mass quadrupole operator:
\[ \hat{Q}_{20} = 2z^2 - x^2 - y^2 \]  
(20)
\[ \hat{Q}_{22} = x^2 - y^2 \]  
(21)
Here \( q_{2\mu} \) is the constrained value of the quadrupole moments, and \( C_{2\mu} \) the
corresponding stiffness constant \[50\].

3. Results and discussion
The new parametrization PC-PK1 \[44\] and the separable pairing force \[45\] are adopted in the particle-hole channel and the particle-particle channel respectively. Parity, \( D_2 \) symmetry, and time-reversal invariance are imposed. The Dirac equation is solved by expanding in the basis of eigenfunctions of a 3DHO in Cartesian coordinate with 12 major shells, which are found to be sufficient to obtain a reasonably converged mean-field PES.

3.1. Shape evolution in neutron-rich Sr isotopes
Figure 1 displays the PESs of even-even \(^{88-104}\text{Sr}\) in \(\beta-\gamma\) plane, normalized to the total energy of absolute minimum. The energy difference between
Figure 1: (Color online) The potential energy surfaces of the even-even $^{88-106}$Sr isotopes in the $\beta$-$\gamma$ plane from the constrained relativistic mean-field (RMF) plus BCS calculations. All energies are normalized with respect to the total energy of the absolute minimum. The energy difference between neighboring contour lines is 0.5 MeV.
neighboring contour lines is 0.5 MeV. The PESs in Fig. 1 show a clear picture for the evolution of shapes in $^{88-104}$Sr. Starting from a well spherical shape of $^{88}$Sr, the spherical (global) minima in $^{90,92}$Sr become soft against the distortion towards oblate shape. In the mean-time, the prolate (second) minimum comes down. When the neutron number increases from $N = 56$ to $N = 60$, the global minimum is shifted to the oblate side with large deformation. Meanwhile, the prolate minimum becomes deep and competing with the oblate minimum at $N = 60$. A triaxial barrier with the height $\sim 2.22$ MeV separates these two competing minima in $^{98}$Sr. Beyond the $N = 60$, the structure of the energy maps is stable, that is, a soft oblate minimum against the distortion towards spherical shape coexists with a well prolate one.

The evolution of the nuclear charge radii in neutron-rich Sr isotopes can be seen in Fig. 2 where the calculated charge radii corresponding to the spherical, prolate, and oblate local minima in the PESs of even-even $^{88-104}$Sr (c.f. Fig. 1) are plotted as functions of neutron number. For $N \geq 54$, the charge radii of spherical shapes are given as well for comparison. It is shown that the charge radii of the spherical and prolate shapes increase smoothly in the similar slop with the neutron number. The difference in the two charge

Figure 2: (Color online) The evolution of the nuclear charge radii in Sr isotopes. The calculated values corresponding to the spherical (up triangles), prolate (circles), and oblate (down triangles) local minima in the PESs (Fig. 1) are plotted as functions of neutron number. The squares with error bars denote the experimental data [51].
radii is about 0.12 fm, originating from the effect of prolate deformation. Moreover, it means that the deformation of prolate minimum is nearly the same when the neutron number increases from $N = 60$ to $N = 68$. On the contrary, the charge radius corresponding to the oblate minimum changes rapidly with the neutron number. In particular, a sudden rising of charge radius from $N = 58$ to $N = 60$ and a sudden dropping from $N = 60$ to $N = 62$ are due to the increasing and decreasing of the oblate deformation from $\beta = -0.25$ to $\beta = -0.35$ and back to $\beta = -0.2$. Moreover, it is shown in Fig. 2 that the charge radii of prolate and oblate minima in $^{98}$Sr are similar due to the similar size of quadrupole deformation. Comparing with the available data for charge radii, one can draw a shape evolution picture for the ground states of even-even $^{88-100}$Sr, namely, from spherical shape ($^{88}$Sr) to more oblate shape ($^{94}$Sr), oblate and prolate coexistence ($^{98}$Sr) and finally more prolate shape ($^{100}$Sr).

3.2. Shape evolution in neutron-rich Kr, Zr, and Mo isotopes

The PESs of neutron-rich Kr, Zr, and Mo isotopes are shown in Figs. 3-5, respectively. In comparison with the shape evolution picture of Sr isotopes, the main difference is found in the evolution of prolate minimum in Kr isotopes, where the PESs are much softer and the prolate minima are not well developed.

The shape evolution picture of Zr isotopes is very similar as that in Sr isotopes, except the barrier height separating the prolate and oblate minima. In contrary with the case in Sr isotopes, the prolate and oblate minima are always connected through triaxial distortion with near-zero barrier height, in particular, for $^{100}$Zr with shape coexistence phenomenon.

For Mo isotopes, the shape evolution picture is similar as that in Zr isotopes. The evident difference is the occurrence of triaxial minima in the Mo isotopes with neutron number from $N = 58$ to $N = 68$.

Very recently, a global study of nuclear low-lying states based on the non-relativistic Hartree-Fock-Bogoliubov framework with the Gogny force have been done. The corresponding potential energy surfaces and other observables are given in Ref. [29]. Based on the same framework, Rodriguez-Guzmán et al. have examined in detail the shapes evolution of nuclear ground-state in neutron-rich Sr, Zr, and Mo isotopes, including both even-even and odd-A nuclei [30]. The trend of shape evolution is similar as our result based on the covariant density functional. However, the transition at
Figure 3: (Color online) Same as the Fig. but for the isotopes $^{86-104}\text{Kr}$. 

11
Figure 4: (Color online) Same as the Fig. 3 but for the isotopes $^{90-108}$Zr.
Figure 5: (Color online) Same as the Fig. 1 but for the isotopes $^{92-110}$Mo.
$N = 60$ in our calculations is a little slower along the isotopic chain, and more rapid along the isotonic chain for the $N = 60$ isotones.

The charge radii of Kr, Zr, and Mo isotopes are plotted in Figs. 6-8, respectively. The sharp transition is also observed in Zr isotopes, which also indicates the rapid change in the nuclear shapes. On the contrary, the charge radii in Kr and Mo isotopes increase smoothly with the neutron number. Similar as the calculation results of the Gogny force in Ref. [30], the triaxiality is shown to be essential to reproduce qualitatively the charge radii in Mo isotopes.

3.3. Covariant density functional based 5D collective Hamiltonian analysis of shape coexistence in $^{98}$Sr and $^{100}$Zr

The coexistence of prolate and oblate shapes observed in $^{98}$Sr and $^{100}$Zr will be studied in more detail with the 5D collective Hamiltonian determined by the constrained self-consistent RMF plus BCS calculations. The details about the covariant density functional based 5D collective Hamiltonian can be found in Ref. [48].

In Fig. 9 we plot the total energies as functions of axial deformation $\beta$ for $^{98}$Sr and $^{100}$Zr. The inset displays the PEC corresponding to the projections on the $\gamma$ deformation, that is, the minimum for each $\gamma$ deformation on the PES in the $\beta$-$\gamma$ plane (c.f. Figs. 1 and 4). In both nuclei, the coexisting
Figure 7: (Color online) Same as the Fig.2 but for Zr isotopes.

Figure 8: (Color online) Same as the Fig.2 but for Mo isotopes.
Figure 9: (Color online) The total energies of $^{98}$Sr and $^{100}$Zr as functions of axial deformation $\beta$. All energies are normalized with respect to the total energy of the absolute minimum. The inset displays the PEC corresponding to the projections on the $\gamma$ deformation, that is, the minimum for each $\gamma$ on the PES in the $\beta$-$\gamma$ plane.

Prolate and oblate minima with very closed binding energies are observed, which are separated by certain barriers. In $^{98}$Sr, the spherical barrier height is $\sim 3.4$ MeV. After considering the $\gamma$ degree of freedom, this barrier height is lowered down to $2.2$ MeV. In $^{100}$Zr, the barrier height is much smaller with the size $\sim 0.5$ MeV if the $\gamma$ deformation is considered.

Table 1: The calculated excitation energies (in MeV) of $0^+_2$ states and E0 transition strengths $\rho^2(E0; 0^+_2 \rightarrow 0^+_1) \times 10^3$ in $^{98}$Sr and $^{100}$Zr, in comparison with the corresponding data [52, 53].

|        | $^{98}$Sr |        | $^{100}$Zr |        |
|--------|----------|--------|------------|--------|
|        | Cal. | Exp. | Cal. | Exp.            |
| E(0^+_2)(MeV) | 0.216 | 0.215 | 0.468 | 0.331          |
| $\rho^2(E0; 0^+_2 \rightarrow 0^+_1) \times 10^3$ | 116.841 | 51(5) | 150.321 | 108(19)         |

The excitation energy of the $0^+_2$ state and the E0 transition strength $\rho^2(E0; 0^+_2 \rightarrow 0^+_1)$ between the $0^+_2$ and $0^+_1$ states are two key quantities in the
study of shape coexistence,

\[ \rho^2(E_0; 0^+_2 \rightarrow 0^+_1) = \left| \frac{\langle 0^+_2 | \sum_k e_k r^2_k | 0^+_1 \rangle}{e R_0^2} \right|^2, \]  

(22)

where \( R_0 \simeq 1.2A^{1/3} \) fm. The \( \rho^2(E_0; 0^+_2 \rightarrow 0^+_1) \) is related to the change in the root mean-square charge radius of the nucleus between the \( 0^+_1 \) and \( 0^+_2 \) states, and therefore carries important information about the change in deformation and the overlap of the wave functions.

In Tab. 1, we list the calculated excitation energies of \( 0^+_2 \) states and \( E_0 \) transition strengths \( \rho^2(E_0; 0^+_2 \rightarrow 0^+_1) \) in \(^{98}\)Sr and \(^{100}\)Zr from the solution of 5D collective Hamiltonian based on the energy functional PC-PK1 plus the separable pairing force. The experimental data [52, 53] are also shown for comparison. The existence of very low-lying \( 0^+_2 \) state is often used as a strong signal for the shape coexistence. As expected, the calculated excitation energies of \( 0^+_2 \) states in both nuclei are predicted in very low values, that is, 0.216 MeV for \(^{98}\)Sr and 0.468 MeV for \(^{100}\)Zr, which are also very close to the data. Although the experimental \( E_0 \) transition strengths \( \rho^2(E_0; 0^+_2 \rightarrow 0^+_1) \) are overestimated by the collective Hamiltonian based on PC-PK1 functional, they are all typically large, again confirming the shape coexistence phenomena in these two \( N = 60 \) isotones.

The mixing between the \( 0^+_1 \) and \( 0^+_2 \) states can be further understood from the distribution of the wave functions of the \( 0^+_1 \) and \( 0^+_2 \) states. Figure 10 displays the probability density distribution of \( 0^+_1 \) and \( 0^+_2 \) states in \( \beta-\gamma \) plane for \(^{98}\)Sr and \(^{100}\)Zr. Due to the high triaxial barrier (c.f. Fig. 1), two peaks corresponding to the coexisting prolate and oblate shapes are observed in both \( 0^+_1 \) and \( 0^+_2 \) states in \(^{98}\)Sr. However, in \(^{100}\)Zr, the probability density of the \( 0^+_1 \) state is almost uniformly distributed along the \( \gamma \) deformation, connecting the prolate and oblate shapes. Since there is one node in the probability distribution of \( 0^+_2 \) state, the resultant \( \rho^2(E_0; 0^+_2 \rightarrow 0^+_1) \) is the consequence of cancelation from the probability distributions of prolate and oblate parts. This cancelation is larger in \(^{98}\)Sr than that in \(^{100}\)Zr. As a result, the obtained \( \rho^2(E_0; 0^+_2 \rightarrow 0^+_1) \) in \(^{98}\)Sr is much smaller than the value in \(^{100}\)Zr, as shown in Tab. 1.

The observed shape coexistence phenomenon can be understood from the distribution of single-nucleon levels. In Fig. 11, we plot the neutron and proton single-particle energy levels in \(^{98}\)Sr as functions of the axial deformation parameter \( \beta \). The thick dotted curves denote the position of the corresponding Fermi levels. It is shown that the neutron Fermi level goes across the
Figure 10: (Color online) Probability density distribution in the $\beta$-$\gamma$ plane for the $0^+_1$ and $0^+_2$ states of $^{98}$Sr and $^{100}$Zr.

Figure 11: (Color online) Neutron and proton single-particle levels for $^{98}$Sr as functions of the axial deformation parameter $\beta$. The thick dotted curves denote the corresponding Fermi levels.
deformation region of low level density with $-0.4 \leq \beta \leq -0.15$, giving rise to the oblate minimum. On the other hand, the proton Fermi level locates in the middle of the energy gap around $\beta \sim 0.45$, which gives rise to the prolate minimum in $^{98}$Sr.

4. Summary

In summary, the triaxial relativistic mean-field plus BCS model with a point-coupling interaction in the particle-hole channel and a separable pairing force in the particle-particle channel has been established and applied to study the shape evolution and shape coexistence phenomena in neutron-rich $A \sim 100$ nuclei, including Kr, Sr, Zr, and Mo isotopes using the newly parameterized PC-PK1 energy functional. The evolution of potential energy surfaces and charge radii with the neutron number in each isotopes have been presented. Sharp rising in the charge radii of Sr and Zr isotopes at $N = 60$ has been observed and shown to be related to the rapid changing in the nuclear shape. This dramatic evolution of charge radii is smoothed out in Mo isotopes due to the occurrence of triaxial minimum, which is similar as the results of Hartree-Fock-Bogoliubov calculations with the Gogny force. In particular, the triaxiality has been shown to be essential to reproduce quantitatively the charge radii of Mo isotopes.

The coexistence of prolate and oblate shapes has been observed in $^{98}$Sr and $^{100}$Zr. However, the barrier height separating the coexisting minima along the $\gamma$ deformation in $^{100}$Zr has been shown much lower than that in $^{98}$Sr. The observed oblate minimum and prolate minimum are related to the low single-particle energy level density around the Fermi surfaces of neutron and proton respectively. Furthermore, the 5D collective Hamiltonian determined by the calculations of the PC-PK1 energy functional has been constructed and solved for $^{98}$Sr and $^{100}$Zr. The resultant excitation energy of $0^+_2$ state and $E0$ transition strength $\rho^2(E0; 0^+_2 \rightarrow 0^+_1)$ are in rather good agreement with the data. It has been found that the lower barrier height in $^{100}$Zr gives rise to the larger $\rho^2(E0; 0^+_2 \rightarrow 0^+_1)$ than that in $^{98}$Sr.

Acknowledgments

JMY would like to thank Peter Ring and Yuan Tian for helpful discussions and acknowledge a postdoctoral fellowship from the F.R.S.-FNRS (Belgium). This work was partly supported by the Major State Basic Research
Developing Program 2007 CB815000, the National Science Foundation of China under Grants No. 10947013 and No. 10975008, the Fundamental Research Funds for the Central Universities (XDJK2010B007), and the Southwest University Initial Research Foundation Grant to Doctor (SWU109011 and SWU110039).

References

[1] H. Mach et al., Nucl. Phys. A523 (1991) 197.
[2] C. Goodin et al., Nucl. Phys. A787 (2007) 231.
[3] W. Urban et al., Nucl. Phys. A689 (2001) 605.
[4] National Nuclear Data Center, Brookhaven National Laboratory, http://www.nndc.bnl.gov/.
[5] U. Hager et al., Phys. Rev. Lett. 96 (2006) 042504.
[6] F. C. Charlwood et al., Phys. Lett. B674 (2009) 23.
[7] N. Marginean et al., Phys. Rev. C80 (2009) 021301(R).
[8] M. Keim, E. Arnold, W. Borchers et al., Nucl. Phys. A586 (1995) 219.
[9] G. Jung et al., Phys. Rev. C22 (1980) 252.
[10] K. Kawade et al., Z. Phys. A 304 (1982) 293.
[11] G. Lhersonneau et al., Phys. Rev. C49 (1994) 1379.
[12] H. Mach et al., Phys. Lett. B230 (1989) 21.
[13] F. Schussler, J. A. Pinston, B. Monnand and A. Moussa, Nucl. Phys. A339 (1980) 415.
[14] E. Clément et al., CERN-INTC-2010-009/INTC-P-216-ADD-108/01/ 2010.
[15] P. Federman and S. Pittel, Phys. Lett. B77 (1978) 29.
[16] A. Kumar and M. R. Gunye, Phys. Rev. C32 (1985) 2116.
[17] D. Galeriu, D. Bucurescu, and M. Ivaqcu, J. Phys. G12 (1986) 329.
[18] S. Michiaki and A. Akito, Nucl. Phys. A515 (1990) 77.
[19] P. Möler, J. R. Nix, W. D. Myers, and W. J. Swiatecki, At. Data Nucl. Data Tables 59 (1995) 185.
[20] J. Skalski, S. Mizutori, and W. Nazarewicz, Nucl. Phys. A617 (1997) 282.
[21] F. R. Xu, P.M. Walker, and R. Wyss, Phys. Rev. C65 (2002) 021303(R).
[22] S. Verma, P. Ahmad Dar, and R. Devi, Phys. Rev. C77 (2008) 024308.
[23] J. García-Ramos, K. Heyde, R. Fossion, V. Hellemans, and S. De Baerdemacker, Eur. Phys. J. A26 (2005) 221.
[24] K. Sieja, F. Nowacki, K. Langanke, and G. Martínez-Pinedo, Phys. Rev. C79 (2009) 064310.
[25] P. Bonche, H. Flocard, P. H. Heenen, S. J. Krieger, M. S. Weiss, Nucl. Phys. A443 (1985) 39.
[26] J. Skalski, P.-H. Heenen, and P. Bonche, Nucl. Phys. A559 (1993) 221.
[27] M. Bender, G. F. Bertsch, P.-H. Heenen, Phys. Rev. C73 (2006) 034322; Phys. Rev. C78 (2008) 054312.
[28] J.-P. Delaroche, M. Girod, J. Libert et al., Phys. Rev. C81 014303 (2010).
[29] S. Hilaire and M. Girod, [http://www-phynu.cea.fr/science_en_ligne/carte_potentiels_microscopiques/carte_potentiel_nucleaire.htm](http://www-phynu.cea.fr/science_en_ligne/carte_potentiels_microscopiques/carte_potentiel_nucleaire.htm).
[30] R. Rodríguez-Guzmán, P. Sarriquen, L. M. Robledo and S. Perez-Martin, Phys. Lett. B691 (2010) 202.
[31] G. A. Lalazissis, S. Raman, P. Ring, At. Data Nucl. Data Tables 71 (1999) 1.
[32] P. G. Reinhard, Rep. Prog. Phys. 52 (1989) 439.
[33] P. Ring, Prog. Part. Nucl. Phys. 37 (1996) 193.
[34] D. Vretenar, A. V. Afanasjev, G. A. Lalazissis, and P. Ring, Phys. Rep. 409 (2005) 101.

[35] J. Meng, H. Toki, S.-G. Zhou, S.-Q. Zhang, W.-H. Long, and L.-S. Geng, Prog. Part. Nucl. Phys. 57 (2006) 470.

[36] T. Nikšić, D. Vretenar and P. Ring, Prog. Part. Nucl. Phys. 66 (2011) 519.

[37] J. M. Yao, J. Meng, P. Ring, and D. Pena Arteaga, Phys. Rev. C79 (2009) 044312.

[38] T. Nikšić, D. Vretenar, and P. Ring, Phys. Rev. C74 (2006) 064309.

[39] J. M. Yao, J. Meng, P. Ring, and D. Vretenar, Phys. Rev. C81 (2010) 044311.

[40] J. M. Yao, H. Mei, H. Chen, J. Meng, P. Ring, and D. Vretenar, Phys. Rev. C83 (2011) 014308.

[41] T. Nikšić, Z. P. Li, D. Vretenar, L. Prochniak, J. Meng, and P. Ring, Phys. Rev. C79 (2009) 034303.

[42] T. Bürvenich, D. G. Madland, J. A. Maruhn, and P.-G. Reinhard, Phys. Rev. C65, 044308 (2002).

[43] T. Nikšić, D. Vretenar, and P. Ring, Phys. Rev. C78 (2008) 034318.

[44] P. W. Zhao, Z. P. Li, J. M. Yao, and J. Meng, Phys. Rev. C82 (2010) 054319.

[45] Y. Tian and Z. Y. Ma, and P. Ring, Phys. Lett. B676 (2009) 44.

[46] Y. Tian, and Z. Y. Ma, and P. Ring, Phys. Rev. C79 (2009) 064301.

[47] Y. Tian, and Z. Y. Ma, and P. Ring, Phys. Rev. C80 (2009) 024313.

[48] T. Nikšić, P. Ring, D. Vretenar, Y. Tian, and Z. Y. Ma, Phys. Rev. C81 (2010) 054318.

[49] Z. P. Li, T. Nikšić, D. Vretenar, P. Ring, and J. Meng, Phys. Rev. C81 (2010) 064321.
[50] P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer, Heidelberg, 1980).

[51] I. Angeli, At. Data Nucl. Data Tables **87** (2004) 185.

[52] T. Kibédi and R. H. Spear, At. Data Nucl. Data Tables **89** (2005) 77.

[53] [http://ie.lbl.gov/TOI2003/GammaSearch.asp](http://ie.lbl.gov/TOI2003/GammaSearch.asp)