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Shape Coexistence in Odd-Z Isotopes from Fluorine to Potassium

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Abstract: The shape of a nucleus is one of its fundamental properties. We conduct a systematic investigation of shape coexistence in odd-Z nuclei from fluorine to potassium using the deformed relativistic Hartree–Bogoliubov theory in continuum. First, we present a simple argument regarding the energy differences between degenerate vacua, which can serve as a criterion for identifying candidates for shape coexistence. We then predict isotopes that exhibit shape coexistence.

Keywords: relativistic density functional theory; shape coexistence; potential energy curve

1. Introduction

A nucleus, composed of nucleons that can be thought of as quantum marbles, is a fascinating entity exhibiting a variety of characteristics due to the quantum nature of its constituents. Understanding how nucleons combine to form a nucleus with exotic features is a crucial problem that has garnered significant attention in recent years, especially with the advent of new rare isotope beam facilities that enable the production of more exotic nuclei. Ultimately, we must explore how the shell and collective properties of a nucleus emerge from fundamental theories such as quantum chromodynamics. The shape of a nucleus is one of its most fundamental properties; some nuclei display exotic characteristics such as pear shapes, bubble structures, and shape coexistence. The investigation of these exotic nuclear features provides invaluable insights into the complex nature of nuclear forces that govern the formation and structure of atomic nuclei. By exploring how neutrons and protons arrange themselves within these unusual shapes, one can gain a deeper understanding of the underlying nuclear forces and quantum mechanical effects at play.

Shape coexistence is a noteworthy exotic property of nuclei [1–6]. A nucleus can display different shapes with only a small energy difference compared to its total binding energy. Nuclei that exhibit shape coexistence have multiple minima in their potential energy curve. Shape coexistence is closely linked to the island of inversion [7,8] because the change in the ordering of nuclear shells in an island of inversion can result in the emergence of multiple nuclear shapes. Islands of inversion have been studied by a variety of methods, e.g., large-scale shell model calculations [9] and ab initio calculations [10].

In density functional theory, shape coexistence is closely linked to the existence of degenerate vacua. This raises the following question: how small is "small" in the context of degenerate vacua? We can roughly estimate this small energy difference using the uncertainty principle. Taking $\Delta x \cdot \Delta p \approx \hbar/2$ with a nuclear diameter $\Delta x \approx 2.5A^{1/3}$ fm, we can estimate the energy uncertainty as $\Delta E \approx (\Delta p)^2/2m \approx 3.3/A^{2/3}$ MeV $\approx$ 100–300 keV

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for most nuclei. Therefore, in the context of density functional theory, we can consider an energy difference of a few hundred keV to be "small".

The main motivation for the present theoretical survey of potential candidates for phase coexistence is the possibility to study the phenomenon in stable and exotic light nuclei in new RI facilities, and especially RAON in South Korea [11]. In a previous work [12], we focused on even$-Z$ candidates in the region from oxygen to calcium. At present, we expand our study to odd$-Z$ isotopes in the same region, from fluorine (F) to potassium (K). As in that earlier study, we use the deformed relativistic Hartree–Bogoliubov theory in continuum (DRHBc) and the PC-PK1 density functional [13]. This approach allows us to investigate the properties of both exotic and stable nuclei by self-consistently incorporating axial deformation, pairing correlations, and continuum effects [14–20]. We refer to ref. [21] for a review of shape coexistence in odd-mass nuclei and refs. [22,23] for some recent studies on shape coexistence.

2. Deformed Relativistic Hartree–Bogoliubov Theory in Continuum

The Lagrangian density of DRHBc is given by [13,19,24]:

$$\begin{aligned}\mathcal{L} &= \bar{\psi}\left(i\gamma_\mu\partial^\mu - m\right)\psi - \frac{1}{2}\alpha_S(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V\left(\bar{\psi}\gamma_\mu\psi\right)(\bar{\psi}\gamma^\mu\psi)\\ &\quad -\frac{1}{2}\alpha_{TV}\left(\bar{\psi}\vec{\tau}\gamma_\mu\psi\right)(\bar{\psi}\vec{\tau}\gamma^\mu\psi) - \frac{1}{3}\beta_S(\bar{\psi}\psi)^3 - \frac{1}{4}\gamma_S(\bar{\psi}\psi)^4 - \frac{1}{4}\gamma_V\left[\left(\bar{\psi}\gamma_\mu\psi\right)(\bar{\psi}\gamma^\mu\psi)\right]^2\\ &\quad -\frac{1}{2}\delta_S\partial_\nu(\bar{\psi}\psi)\partial^\nu(\bar{\psi}\psi) - \frac{1}{2}\delta_V\partial_\nu\left(\bar{\psi}\gamma_\mu\psi\right)\partial^\nu(\bar{\psi}\gamma^\mu\psi)\\ &\quad -\frac{1}{2}\delta_{TV}\partial_\nu\left(\bar{\psi}\vec{\tau}\gamma_\mu\psi\right)\partial^\nu\left(\bar{\psi}\vec{\tau}\gamma_\mu\psi\right) - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} - e\frac{1-\tau_3}{2}\bar{\psi}\gamma^\mu\psi A_\mu, \end{aligned} \tag{1}$$

where m represents the nucleon mass and α_S, α_V, and α_{TV} denote the coupling constants for four-fermion contact interactions. The terms involving β_S, γ_S, and γ_V account for density-dependent effects, while those with δ_S, δ_V, and δ_{TV} reflect finite-range effects. Additionally, A_μ and $F_{\mu\nu}$ correspond to the four-vector potential and the electromagnetic field strength tensor, respectively. The subscripts S, V, and TV stand for scalar, vector, and isovector, respectively.

By applying the mean-field approximation to the Lagrangian density in Equation (1) and performing the Legendre transformation, we derive the mean-field Hamiltonian density. Using the variational method on this Hamiltonian density, we then arrive at the relativistic Hartree–Bogoliubov equation [25].

$$\begin{pmatrix} h_D - \lambda & \Delta \\ -\Delta^* & -h_D^* + \lambda \end{pmatrix}\begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}. \tag{2}$$

Here, E_k denotes the quasiparticle energy, and U_k and V_k are the quasiparticle wave functions, with λ denoting the Fermi energy. The Dirac Hamiltonian h_D is given by

$$h_D(\boldsymbol{r}) = \boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta(M + S(\boldsymbol{r})) + V(\boldsymbol{r}), \tag{3}$$

and the scalar $S(\boldsymbol{r})$ and vector $V(\boldsymbol{r})$ potentials can be expressed as

$$S(\boldsymbol{r}) = \alpha_S\rho_S + \beta_S\rho_S^2 + \gamma_S\rho_S^3 + \delta_S\Delta\rho_S, \tag{4}$$

$$V(\boldsymbol{r}) = \alpha_V\rho_V + \gamma_V\rho_V^3 + \delta_V\Delta\rho_V + eA_0 + \alpha_{TV}\tau_3\rho_{TV} + \delta_{TV}\tau_3\Delta\rho_{TV}. \tag{5}$$

The local densities $\rho_S(\boldsymbol{r})$, $\rho_V(\boldsymbol{r})$, and $\rho_{TV}(\boldsymbol{r})$ can be expressed in terms of the quasiparticle wave functions as follows:

$$\rho_S(\boldsymbol{r}) = \sum_{k>0} \bar{V}_k(\boldsymbol{r}) V_k(\boldsymbol{r}), \tag{6}$$

$$\rho_V(\boldsymbol{r}) = \sum_{k>0} V_k^{\dagger}(\boldsymbol{r}) V_k(\boldsymbol{r}), \tag{7}$$

$$\rho_{TV}(\boldsymbol{r}) = \sum_{k>0} V_k^{\dagger}(\boldsymbol{r}) \tau_3 V_k(\boldsymbol{r}). \tag{8}$$

In principle, we can derive the pairing potential for the particle–particle channel from the Lagrangian density in Equation (1), but for simplicity, we adopt the following form:

$$\Delta_{kk'}(\boldsymbol{r}, \boldsymbol{r}') = -\sum_{\tilde{k}\tilde{k}'} V^{pp}_{kk',\tilde{k}\tilde{k}'}(\boldsymbol{r}, \boldsymbol{r}') \kappa_{\tilde{k}\tilde{k}'}(\boldsymbol{r}, \boldsymbol{r}'), \tag{9}$$

where the pairing tensor is defined by $\kappa = V^* U^T$. For V^{pp}, we use the density-dependent zero-range pairing interaction

$$V^{pp}(\boldsymbol{r}, \boldsymbol{r}') = \frac{V_0}{2}(1 - P^{\sigma})\delta(\boldsymbol{r} - \boldsymbol{r}')\left(1 - \frac{\rho(\boldsymbol{r})}{\rho_{sat}}\right), \tag{10}$$

where ρ_{sat} is the nuclear saturation density. The total energy of a nucleus can be expressed as

$$\begin{aligned} E_{\text{tot}} &= \sum_{k>0} (\lambda_\tau - E_k) v_k^2 - E_{\text{pair}} + E_{\text{c.m.}} - \int \mathrm{d}^3\mathbf{r} \Bigg[\frac{1}{2}\alpha_S \rho_S^2 \\ &+ \frac{1}{2}\alpha_V \rho_V^2 + \frac{1}{2}\alpha_{TV} \rho_{TV}^2 + \frac{2}{3}\beta_S \rho_S^3 + \frac{3}{4}\gamma_S \rho_S^4 + \frac{3}{4}\gamma_V \rho_V^4 \\ &+ \frac{1}{2}(\delta_S \rho_S \Delta\rho_S + \delta_V \rho_V \Delta\rho_V + \delta_{TV} \rho_3 \Delta\rho_3 + \rho_p e A^0) \Bigg], \end{aligned} \tag{11}$$

where $E_{\text{c.m.}}$ denotes the center of mass correction energy. The zero-range pairing force results in a local pairing field $\Delta(\boldsymbol{r})$ with the associated pairing energy energy expressed as follows:

$$E_{\text{pair}} = -\frac{1}{2}\int \mathrm{d}^3\boldsymbol{r} \kappa(\boldsymbol{r}) \Delta(\boldsymbol{r}). \tag{12}$$

To investigate exotic nuclear properties, it is essential to self-consistently incorporate both continuum and deformation effects, as well as pairing. We expand the wave functions using the Dirac Wood–Saxon basis to account for continuum effects. To address axial deformation while maintaining spatial reflection symmetry, we expand the potentials ($S(\boldsymbol{r})$ and $V(\boldsymbol{r})$) and densities ($\rho_S(\boldsymbol{r})$, $\rho_V(\boldsymbol{r})$, and $\rho_{TV}(\boldsymbol{r})$) in terms of Legendre polynomials. For more details on DRHBc, we refer to [17,19].

By performing constrained calculations for different degrees of quadrupole deformation, we can obtain not only the lowest energy solution for a given nucleus, but also identify other possible local minima in the potential energy curves. The existence of two near-degenerate vacua will lead to two perturbative ground states 1 and 2. Neither of them is the exact ground state. The ground state is given by the symmetric or the antisymmetric linear combination of the perturbative ground states.

3. Results

In this section, we present the candidate isotopes exhibiting shape coexistence for fluorine (F, $Z = 9$), sodium (Na, $Z = 11$), aluminium (Al, $Z = 13$), phosphorus (P, $Z = 15$), chlorine (Cl, $Z = 17$), and potassium (K, $Z = 19$).

To identify candidate isotopes that exhibit shape coexistence, we examine the potential energy curve (PEC) of each isotope as a function of the quadrupole deformation parameter (β_2). We search for isotopes with near-degenerate minima. Examples of PECs for potential candidates, namely ^{23}F, ^{31}Al, ^{38}Cl, and ^{42}K, are shown in Figure 1. The PECs are compared with existing results obtained with the Hartree–Fock–Bogoliubov approach using the Gogny D1S functional, which are available at [26] and found qualitatively similar.

Based on our rough estimates using the uncertainty principle outlined in the Introduction, we find that the energy difference ΔE for shape coexistence is typically on the order of a few hundreds keV, as also shown in ref. [27]. In this work, since we are studying light nuclei, which generally have lower total energies compared to medium- or heavy-mass nuclei, we adopt the criterion of 300 keV for shape coexistence.

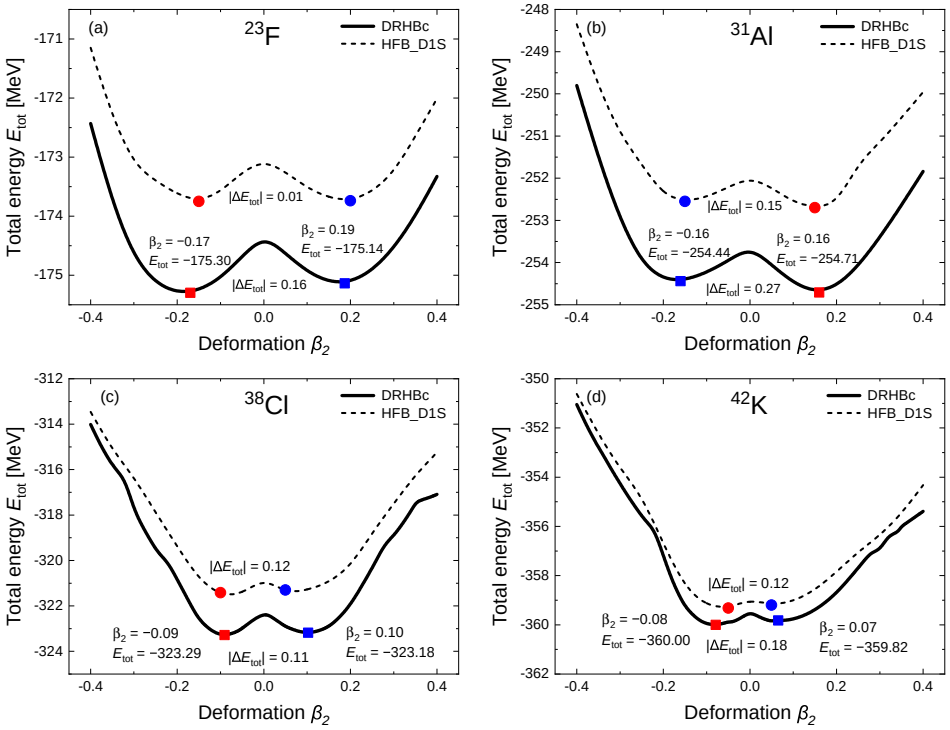


Figure 1. Potential energy curves for selected isotopes (**a**) ^{23}F, (**b**) ^{31}Al, (**c**) ^{38}Cl, and (**d**) ^{42}K as a function of the quadrupole deformation parameter (β_2). Results of the present DRHBc calculations (solid line) are shown in comparison with those of HFB calculations (dash line) with the Gogny D1S effective interaction [26]. The square and the circle represent local minima of DRHBc and HFB calculations, respectively.

In Table 1, we list all forty-six odd-Z isotopes in the range $Z = 9$ to $Z = 19$ that are found to have two minima with an energy difference ΔE smaller than 300 keV. Expanding the ΔE criterion to below 500 keV leads to twenty-four additional candidates for shape coexistence, which are not listed in Table 1, but are indicated in Figure 2.

Figure 2 shows all odd-Z nuclei from F to K which are predicted particle-bound using the DRHBc theory with the PC-PK1 functional. The candidates for shape coexistence in odd-Z isotopes are highlighted in red text within the yellow boxes ($\Delta E \leq 300$ keV) and cyan boxes ($\Delta E \leq 500$ keV). In addition, the candidates based on results with the Gogny D1S functional, available at [26], are shown with red circles. The regions of candidates predicted with the two approaches and functionals are similar, which is not surprising given that they both are mean-field approaches. Experiments on nuclei where there are deviations could offer valuable insights for further theoretical developments.

Table 1. The odd-Z isotopes we found in the range $Z = 9$ to $Z = 19$ that have two minima with an energy difference ΔE smaller than 300 keV.

Isotopes	β_2	ΔE (MeV)	Isotopes	β_2	ΔE (MeV)
^{16}F	−0.12, 0.20	0.09	^{31}Cl	−0.17, 0.09	0.27
^{17}F	−0.08, 0.10	0.03	^{32}Cl	−0.10, 0.08	0.12
^{23}F	−0.17, 0.19	0.16	^{33}Cl	−0.07, 0.06	0.08
^{24}F	−0.13, 0.13	0.13	^{38}Cl	−0.09, 0.10	0.11
^{25}F	−0.08, 0.09	0.04	^{39}Cl	−0.09, 0.12	0.05
^{26}F	−0.12, 0.13	0.02	^{44}Cl	−0.22, 0.27	0.17
^{27}F	−0.08, 0.10	0.02	^{50}Cl	−0.25, 0.06	0.23
^{28}F	−0.09, 0.09	0.02	^{51}Cl	−0.21, 0.10	0.21
^{25}Na	−0.26, 0.31	0.12	^{55}Cl	−0.10, 0.08	0.27
^{30}Na	−0.08, 0.10	0.10	^{56}Cl	−0.06, 0.06	0.06
^{27}Al	−0.27, 0.18	0.18	^{33}K	−0.09, 0.06	0.12
^{28}Al	−0.19, 0.16	0.21	^{34}K	−0.06, 0.05	0.07
^{31}Al	−0.16, 0.16	0.27	^{35}K	−0.05, 0.05	0.04
^{32}Al	−0.11, 0.11	0.25	^{37}K	−0.08, 0.04	0.21
^{33}Al	−0.04, 0.06	0.12	^{38}K	−0.07, 0.05	0.23
^{41}Al	−0.36, 0.34	0.24	^{40}K	−0.07, 0.06	0.23
^{45}Al	−0.26, 0.19	0.29	^{41}K	−0.06, 0.04	0.09
^{28}P	−0.20, 0.16	0.20	^{42}K	−0.08, 0.07	0.18
^{32}P	−0.10, 0.08	0.15	^{43}K	−0.10, 0.06	0.28
^{34}P	−0.06, 0.05	0.08	^{50}K	−0.10, 0.07	0.20
^{36}P	−0.07, 0.10	0.02	^{51}K	−0.08, 0.04	0.10
^{47}P	−0.25, 0.13	0.13	^{52}K	−0.05, 0.03	0.03
^{50}P	−0.05, 0.08	0.07	^{53}K	−0.07, 0.03	0.20

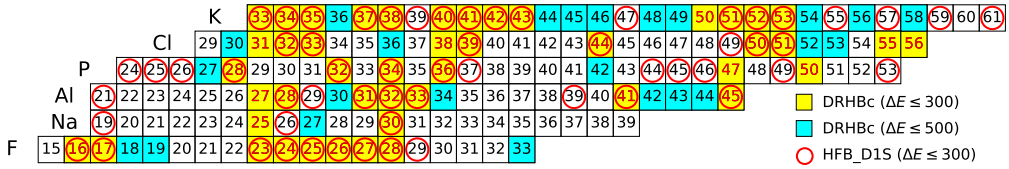


Figure 2. Summary of nuclei exhibiting shape coexistence in odd-Z isotopes from F to K. The shape coexistence candidates are highlighted in red text within yellow boxes ($\Delta E \leq 300$ keV). The x-axis represents the mass number of the isotopes. The cyan boxes represent 24 additional candidates based on the 500 keV criterion. Only odd-Z isotopes are shown for clarity.

It is worth noting that the dual-shell mechanism, used to predict regions of the nuclear chart where shape coexistence might occur, was introduced in refs. [28,29]. The studies showed that nuclei with proton or neutron numbers in the ranges 7–8, 17–20, 34–40, 59–70, 96–112, and 146–168 are potential candidates for shape coexistence. Let us take Cl isotopes as an example to compare our results with the prediction in refs. [28,29]. In our study, using the 500 MeV criterion, we identify 14 candidate isotopes, 7 of which align with the results from refs. [28,29].

4. Summary

We identified odd-Z isotopes from fluorine to potassium which are predicted to show shape coexistence within the DRHBc framework. Based on the uncertainty principle, we estimated that the energy difference ΔE between degenerate minima on the potential energy curve for shape coexistence has to be of the order of a few hundred keV. In this work, we adopted a criterion of 300 keV (500 keV) for shape coexistence in light nuclei and identified 46 (70) candidate isotopes from fluorine to potassium.

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