Multireference covariant density functional theory for shape coexistence and isomerism in 43S

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Abstract

We extend the multireference covariant density functional theory (MR-CDFT) to describe the low-lying states of the odd-mass nucleus ^{43}S near the neutron magic number $N = 28$ with shape coexistence. The wave functions of the low-lying states are constructed as superpositions of configurations with different intrinsic shapes and K quantum numbers, projected onto good particle numbers and angular momenta. The MR-CDFT successfully reproduces the main features of the low-energy structure in ^{43}S. Our results indicate that the ground state, $3/2^-_1$, is predominantly composed of the intruder prolate one-quasiparticle (1qp) configuration $\nu 1/2^-[321]$. In contrast, the $7/2^-_1$ state is identified as a high-K isomer, primarily built on the prolate 1qp configuration $\nu 7/2^-[303]$. Additionally, the $3/2^-_2$ state is found to be an admixture dominated by an oblate configuration with $K^\pi = 1/2^-$, along with a small contribution from a prolate configuration with $K^\pi = 3/2^-$. These results demonstrate the capability of MR-CDFT to capture the intricate interplay among shape coexistence, K-mixing, and isomerism in the low-energy structure of odd-mass nuclei around $N = 28$.

Full Text

Preamble

Multireference Covariant Density Functional Theory for Shape Coexistence and Isomerism in 43S

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We extend the multireference covariant density functional theory (MR-CDFT) to describe the low-lying states of the odd-mass nucleus 43S near the neutron magic number N = 28 with shape coexistence. The wave functions of the low-lying states are constructed as superpositions of configurations with different intrinsic shapes and K quantum numbers, projected onto good particle numbers and angular momenta. The MR-CDFT successfully reproduces the main features of the low-energy structure in 43S. Our results indicate that the ground state, $3/2^-{}_1$, is predominantly composed of the intruder prolate one-quasiparticle (1qp) configuration $1/2^-[321]$. In contrast, the $7/2^-{}_1$ state is identified as a high-K isomer, primarily built on the prolate 1qp configuration $7/2^-[303]$. The $3/2^-{}_2$ state is found to be an admixture dominated by an oblate configuration with $K\pi = 1/2^-$, along with a small contribution from a prolate configuration with $K\pi = 3/2^-$. These results demonstrate the capability of MR-CDFT to capture the intricate interplay among shape coexistence, K-mixing, and isomerism in the low-energy structure of odd-mass nuclei around N = 28.

Introduction

The development of radioactive ion beam facilities [1–3] has significantly advanced nuclear physics research, enabling studies of nuclei far from the β-stability line, where the evolution of nuclear shell structure and the emergence of exotic excitation modes have garnered considerable attention [4–7].

A striking example is the evolution of the N = 28 shell gap, a magic number that arises from strong spin-orbit coupling in the single-nucleon potential [8, 9], which drives the $f_7/_2$ orbital significantly lower than the $p_3/_2$ orbital. Experimental data reveal a gradual weakening of the N = 28 shell gap in isotones lighter than 48Ca. For instance, measurements of the β-decay half-lives of 44S and 45Cl revealed deviations from shell model predictions based on spherical configurations [10], indicating the weakening of the N = 28 shell effect. Subsequent Coulomb excitation experiments observed low excitation energies of the $2^{+}{}_{1}$ states and enhanced electric quadrupole transition strengths B(E2; $0^{+}{}_{1} \rightarrow 2^{+}{}_{1}$) in 40,42,44S [11, 12]. Similar behavior has been reported in neighboring nuclei, such as 42Si [13–15] and 40Mg [16]. These observations indicate the onset of strong quadrupole collectivity in neutron-rich N = 28 isotones with proton number Z < 18, leading to the crossing of the $1/2^{-}[321]$ component of the 2 $p_{3}/_{2}$ orbital with the $7/2^{-}[303]$ component of the 1 $f_{7}/_{2}$ orbital. Consequently, several near-degenerate configurations with admixtures of $1f_{7}/_{2}$ and $2p_{3}/_{2}$ orbitals coexist at similar energies within these nuclei. In the case of 44S, two coexisting low-lying 0^{+} states have been observed [17], suggesting spherical-deformed shape coexistence. The onset of a deformed ground state in 44S is supported by quantum-number projected generator coordinate method (GCM) studies based on the Gogny force [18, 19] and collective Hamiltonian studies based on a relativistic energy density functional (EDF) [20]. These theoretical studies reveal a general trend in shape evolution: the predominant shape transitions from a γ-soft, moderately deformed configuration with β_2 [0.20, 0.30] to a strongly prolate shape with β_2 [0.35, 0.45] as the angular momentum increases up to J = 4 in the ground-state band. This rotational band coexists with a strongly prolate-deformed $0^{+}{}_{2}$ state, characterized by β_2 [0.35, 0.45]. The specific deformation parameter β_2 of the dominant configuration depends on the details of the employed EDF. A two-proton knockout reaction from 46Ar identified the $4^{+}{}_{1}$ state as an isomeric state [21], which, in combination with shell-model calculations, was suggested to exhibit strong prolate deformation. A half-life measurement revealed a hindered E2 transition with B(E2; $4^{+}{}_{1} \rightarrow 2^{+}{}_{1}$) = 0.61(19) W.u. [22], supporting the interpretation of the $4^{+}{}_{1}$ state as a K = 4 isomer. Shell-model studies further indicated that this state is predominantly characterized by the two-quasiparticle configuration $1/2^{-}[321]$ $7/2^{-}[303]$ [23].

The odd-mass neutron-rich sulfur isotope 43S exhibits a more complex low-energy structure than 44S due to the interplay between the single-particle motion of the unpaired neutron and the collective excitations of the 42S core. Mass measurements, combined with theoretical studies based on the shell model and relativistic mean-field (RMF) theory, suggested the coexistence of a prolate deformed ground state and an isomeric state in 43S [24]. Subsequent g-factor measurements [25], along with shell-model calculations and the collective Hamiltonian approach based on the Gogny force, determined the spin-parity of the isomeric state as $7/2^{-}{}_{1}$ at an excitation energy of 320.5(5) keV. These studies also established the intruder nature of the ground state with K = 1/2 [25], while initially suggesting that the $7/2^{-}{}_{1}$ isomeric state is quasispherical. However, later measurements of the spectroscopic quadrupole moment of the isomeric state yielded Qs($7/2^{-}{}_{1}$) = 23(3) efm^2 [26], significantly larger than the expected value for a single-particle state. This observation indicates a strong collective nature of the isomeric state, which is further supported by shell-model calculations [26]. The structure of 43S was investigated using antisymmetrized molecular dynamics plus GCM (AMD+GCM), which predicted a prolate-deformed ground state, a triaxially deformed $7/2^-{}_1$ state, and an oblate-deformed excited band atop the $3/2^-{}_2$ state at low excitation energy [27]. In contrast, a recent shell-model study suggested that the prolate ground-state band coexists with a triaxial band built on the $7/2^-{}_1$ isomer and an excited prolate structure associated with the $K\pi = 5/2^-$ deformed orbital [28].

Meanwhile, the angular-momentum-projected variation-after-projection (AMP+VAP) approach suggests that the ground state $3/2^-{}_1$ and the $7/2^-{}_1$ state are dominated by $K = 1/2$ and $K = 7/2$, respectively, classifying the $7/2^-{}_1$ state as a high-K isomer [23]. Experimental lifetime measurements of excited states provide the first evidence of a doublet of $(3/2^-{}_1)$ states. Together with shell-model and AMD calculations, these results suggest the possible existence of three coexisting bands built upon the $3/2^-{}_1$, $3/2^-{}_2$, and $7/2^-{}_1$ states [29]. Furthermore, Coulomb excitation experiments have shown that the intraband B(E2) values for transitions within the ground-state band $3/2^-{}_1$ and the isomeric band $7/2^-{}_1$ are large and nearly equal [30], which was also found in a study using the valence-space in-medium similarity renormalization group [31].

Over the past decades, covariant density functional theory (CDFT) has achieved remarkable success in various areas of nuclear physics [32–34]. A key advantage of CDFT is that Lorentz invariance imposes strict constraints on the number of parameters in the EDF. Moreover, the relativistic framework naturally accounts for the spin-orbit interaction, while time-odd fields are incorporated without introducing additional free parameters. This characteristic is particularly crucial for accurately describing odd-mass nuclei and rotating systems. To restore the missing quantum numbers, including particle numbers and angular momentum, in the solution of CDFT and to consider shape-mixing effects, multireference covariant density functional theory (MR-CDFT) has been developed [35–37] and successfully applied to study low-lying spectra in even-even nuclei with either triaxial or octupole shapes [38–41]. MR-CDFT has also been applied to studies of neutrinoless double-beta decay [42–45] and the low-lying states of hypernuclei [46–48].

Recently, MR-CDFT was successfully extended to describe low-lying states in odd-mass nuclei [49]. In this work, we further extend the MR-CDFT framework by mixing configurations with different quadrupole shapes and K quantum numbers, providing a complementary approach to previous studies [23, 27], with explicit consideration of triaxial deformation. The success of our framework is demonstrated through its application to the low-energy structure of 43S. It is worth noting that a similar idea has been implemented in the projected shell model (PSM) to study the effect of K-mixing on isomeric states in even-even isotopes with $N = 104$ [50], although shape mixing was not included in that study. Our extended MR-CDFT enables us to identify the dominant mechanism responsible for the formation of the isomeric state, shedding new light on the interplay among shape coexistence, K-mixing, and isomerism in the low-energy structure of odd-mass nuclei.

The article is arranged as follows. In Sec. II, we present the extended framework of MR-CDFT for odd-mass nuclei. The results of calculations for 43S are discussed in Sec. III. The conclusion of this study is summarized in Sec. IV.

II. The MR-CDFT for Odd-Mass Nuclei

The MR-CDFT theory for the low-lying states of odd-mass nuclei has been introduced in detail in Ref. [49]. Here, we present only a brief description. The wave functions of low-lying states are constructed as a mixing of configurations with different deformation parameter q and quantum number K:

$$|\Psi_{\alpha}^{J\pi}\rangle = \sum_{c} f_{\alpha}^{J\pi}(c)|NZJ\pi; c\rangle. \tag{1}$$

Here, c is a collective label for (K, q), and α distinguishes states with the same angular momentum J. The basis function with quantum numbers (NZJπ) is given by

$$|NZJ\pi; c\rangle = \hat{P}_{MK}^{J}\hat{P}^{N}\hat{P}^{Z}|\Phi^{(OA)}(q)\rangle, \tag{2}$$

where $\hat{P}_{MK}^{J}$ and $\hat{P}^{N(Z)}$ are projection operators that select components with angular momentum J and neutron (proton) number N (Z) [51].

The mean-field configurations $|\Phi^{(OA)}(q)\rangle$ for odd-mass nuclei are chosen as one-quasiparticle (1qp) states:

$$|\Phi^{(OA)}(q)\rangle = \alpha_{\kappa}^{\dagger}|\Phi(\kappa)(q)\rangle, \tag{3}$$

where $|\Phi(\kappa)\rangle$ denotes a quasiparticle vacuum state with even number parity obtained through the false quantum vacuum (FQV) scheme [49] in the single-reference (SR)-CDFT calculation starting from a relativistic EDF [34, 52]. The quasiparticle creation operator $\alpha_{\kappa}^{\dagger}$ switches the number parity to odd. The index distinguishes different quasiparticle states.

In the present study, axial symmetry is assumed. In this case, each configuration is labeled with the quantum numbers Kπ, which are determined by the Nilsson quantum number $\Omega\pi$ of the blocked orbital, i.e., Kπ = $\Omega\pi$.

The weight function $f_{\alpha}^{J\pi}$ in Eq. (1) is determined by variational principles, which lead to the following Hill-Wheeler-Griffin (HWG) equation [51, 53]:

$$\sum_{c'}\left[H_{cc'}^{NZJ\pi} - E_{\alpha}^{J\pi}N_{cc'}^{NZJ\pi}\right]f_{\alpha}^{J\pi}(c') = 0, \tag{4}$$

where the Hamiltonian kernel and norm kernel are defined by

$$\mathcal{O}_{cc'}^{NZJ\pi} = \langle NZJ\pi; c|\hat{\mathcal{O}}|NZJ\pi; c'\rangle, \tag{5}$$

with the operator $\hat{\mathcal{O}}$ representing $\hat{H}$ and $\hat{1}$, respectively. In the present study based on a covariant EDF, the mixed-density prescription is employed in the evaluation of the Hamiltonian kernel. Details on the calculation of the kernels in Eq. (5) can be found in Ref. [49].

The HWG equation (4) for a given set of quantum numbers (NZJπ) is solved in the standard way as discussed in Refs. [36, 51]. This is done by first diagonalizing the norm kernel $N^{NZJ\pi}$. A new set of basis functions is then constructed using the eigenfunctions of the norm kernel with eigenvalues larger than a prechosen cutoff value, which removes possible redundancy in the original basis. The Hamiltonian is diagonalized on this new basis. In this way, the energies $E_\alpha^{J\pi}$ of the nuclear states $|\Psi_\alpha^{J\pi}\rangle$ can be obtained.

Since the basis functions $|NZJ\pi; c\rangle$ are nonorthogonal to each other, one usually introduces the collective wave function $g_\alpha^{J\pi}(K,q)$ and the mixing weights $f_\alpha^{J\pi}(c)$ as

$$g_\alpha^{J\pi}(K,q) = \sum_{c'} (N^{-1/2})_{cc'}^{NZJ\pi} f_\alpha^{J\pi}(c'), \tag{6}$$

which fulfills the normalization condition. The distribution of $g_\alpha^{J\pi}(K,q)$ over K and q reflects the contribution of each basis function to the nuclear state $|\Psi_\alpha^{J\pi}\rangle$.

With the mixing weight $f_\alpha^{J\pi}(c)$, it is straightforward to determine the observables of nuclear low-lying states, including electric quadrupole moment Qs, magnetic dipole moment , as well as E2 and M1 transition strengths. The strength of the Eλ(Mλ) transition from the initial state $|\Psi_{\alpha_i}^{J_i\pi_i}\rangle$ to the final state $|\Psi_{\alpha_f}^{J_f\pi_f}\rangle$ is determined by

$$B(T\lambda, J_i\alpha_i\pi_i \to J_f\alpha_f\pi_f) = \frac{1}{2J_i+1}\left|\sum_{c_f,c_i} f_{\alpha_f}^{J_f\pi_f *}(c_f)\langle NZJ_f\pi_f, c_f||\hat{T}_\lambda||NZJ_i\pi_i, c_i\rangle f_{\alpha_i}^{J_i\pi_i}(c_i)\right|^2. \tag{7}$$

The configuration-dependent reduced matrix element is given by

$$\langle NZJ_f\pi_f; c_f||\hat{T}_\lambda||NZJ_i\pi_i; c_i\rangle = \delta_{\pi_f\pi_i,(-1)^\lambda}\frac{2J_f+1}{2J_i+1}\sum_{\nu M}\int d\Omega D_{MK_i}^{J_i *}(\Omega)\langle\Phi^{(OA)}(q_f)|\hat{T}_{\lambda\nu}\hat{R}(\Omega)\hat{P}^Z\hat{P}^N\hat{P}_{\pi_i}|\Phi^{(OA)}(q_i)\rangle \tag{8}$$

where $\hat{T}_{\lambda\nu}$ represents either an electric or magnetic multipole operator and $\hat{R}(\Omega)$ is the rotation operator. The detailed formulas can be found in Ref. [49].

In the calculation of the mean-field configurations, Dirac spinors for single nucleons are solved using a harmonic oscillator basis with a major shell number of $N_{\rm sh} = 10$. Pairing correlations between nucleons are treated within the BCS approximation using a density-independent δ force with a smooth cutoff [35, 54]. The PC-PK1 parameterization is employed for the relativistic EDF [52]. In the calculation of the projected kernels $\mathcal{O}^{NZJ\pi}_{cc'}$, the number of mesh points in the interval $[0, \pi]$ for the rotation angle β and the gauge angle ϕ are chosen as $N_\beta = 12$ and $N_\phi = 7$, respectively. These values are found to be sufficient to achieve convergent results for 43S.

III. Results and Discussion

Figure 1 Figure 1: see original paper presents the energies of mean-field states $|\Phi(\kappa)(q)\rangle$ from the SR-CDFT calculation based on the FQV scheme [49] as a function of the quadrupole deformation parameter $q = \beta_2$. A pronounced energy minimum appears on the prolate side with $\beta_2 \simeq 0.3$, with a second minimum on the oblate side with $\beta_2 \simeq -0.2$, suggesting that 43S may exhibit coexisting prolate and oblate shapes in its low-lying states. This phenomenon can be understood from the Nilsson diagram of neutrons in 43S, as shown in Fig. 1(b). One can see large shell gaps or low level densities on both prolate and oblate sides around the Fermi energy. Moreover, the downward $1/2^-[321]$ component of the 2 $p_3/_2$ orbital crosses with the upward $7/2^-[303]$ component of the 1 $f_7/_2$ orbital at $\beta_2 \simeq 0.22$ around the Fermi energy. This crossing leads to the population of valence neutrons from $7/2^-[303]$ to $1/2^-[321]$. This result is consistent with the AMD+GCM calculation [27]. On the oblate side, the N = 28 shell gap increases with $|\beta_2|$.

The wave functions of the mean-field states $|\Phi(\kappa)(\beta_2)\rangle$ in Fig. 1(a) do not preserve particle numbers or total angular momentum. By applying quantum-number projection operators onto the 1qp configurations with Kπ = $1/2^-$, $3/2^-$, $5/2^-$, and $7/2^-$ (cf. Eqs. (2) and (3)), one obtains the energies of symmetry-conserved 1qp states in 43S, as displayed in Fig. 2 [Figure 2: see original paper].

Figure 2(a) displays the energies of symmetry-conserving states with angular momentum J increasing from 1/2 to 9/2, projected from configurations with Kπ = $1/2^-$ as a function of the quadrupole deformation β_2. Similar to the energy curve from mean-field calculation in Fig. 1(a), all projected energy curves present two minima on the prolate and oblate sides, respectively, with $|\beta_2| \simeq 0.3$. It is interesting to note the change in energy ordering of states with different angular momenta as a function of deformation. For configurations with $\beta_2 > 0.4$, the energies of projected states with ΔJ = 1 follow the ordering ($1/2^-$, $3/2^-$, $5/2^-$, $7/2^-$, $9/2^-$), consistent with the strong-coupling limit of the particle-rotor model (PRM) [51]. In contrast, for weakly deformed configurations with

$\beta_2 < 0.3$, the $1/2^-$ state rises rapidly from the bottom as β_2 decreases toward zero. When considering only configurations from the oblate energy minima, the energy ordering becomes ($7/2^-$, $3/2^-$, $1/2^-$, $9/2^-$, $5/2^-$). After mixing configurations with different shapes but the same quantum numbers $K\pi = 1/2^-$, one obtains yrast states with the energy ordering ($3/2^-$, $1/2^-$, $5/2^-$, $7/2^-$) located mainly around $\beta_2 = 0.3$.

Figures 2(b), 2(c), and 2(d) display the energies of symmetry-conserving states with J ≥ K, projected from configurations with $K\pi = 3/2^-$, $5/2^-$, and $7/2^-$, respectively. Additionally, the two lowest energy states from shape-mixing calculations are shown. One can see that the energy level $7/2^-{}_1$ dominated by the prolate configuration with $K\pi = 7/2^-$ is the yrast state among all $J\pi = 7/2^-$ states. The low-lying states from shape-mixing calculations are plotted at their mean quadrupole deformation $\bar{\beta}_{J\pi\alpha}$, defined as

$$\bar{\beta}_{J\pi\alpha}(K\pi) = \sum_{K,\beta_2} |g_\alpha^{J\pi}(K,\beta_2)|^2 \beta_2. \tag{9}$$

Figure 3 [Figure 3: see original paper] presents the energy spectra of low-lying states in 43S from MR-CDFT calculations. Panel (b) shows results including configuration mixing with different shapes and K values, while panel (c) shows results without K mixing. Experimental data [25, 30] are displayed in panel (a). Black and blue arrows indicate B(E2) values (in units of e^2fm^4) and B(M1) values (in units of ²_N), respectively. States dominated by a prolate (oblate) configuration, with a small admixture of oblate (prolate) components, are labeled as "(Prolate)" and "(Oblate)" , respectively. The distributions of the collective wave functions $|g_\alpha^{J\pi}|^2$ for the first two states with J = 3/2, 5/2, and 7/2 are shown in panels (d, e), (f, g), and (h, i), respectively.

The main features of the measured low-lying states of 43S (cf. Fig. 3(a)) are reasonably well reproduced only in the MR-CDFT calculations that incorporate mixing of both K values and shapes with different β_2 values. Here we summarize the main findings from the MR-CDFT study based on Fig. 3. The ground state ($3/2^-{}_1$) of 43S is predominantly characterized by a prolate-deformed configuration $1/2^-[321]$ with $K\pi = 1/2^-$. In contrast, the $3/2^-{}_2$ state is dominated by an oblate configuration with $\beta_2 \simeq -0.3$ and $K\pi = 1/2^-$, with a small admixture of a prolate configuration having $K\pi = 3/2^-$. We note that in the AMD+GCM calculation [27], the $3/2^-{}_2$ state is dominated by an oblate configuration with $K\pi = 3/2^-$, followed by the $5/2^-$ and $7/2^-$ states, forming an oblate rotational band. As shown in Fig. 3(b), we predict a strong E2 transition between the $5/2^-$ and $3/2^-$ states, whereas the E2 transition from the $5/2^-$ and $7/2^-{}_2$ states to the $3/2^-{}_2$ state is much weaker. This behavior can be understood from Fig. 3(g), which shows that the $5/2^-{}_2$ state is dominated by a prolate-deformed configuration with $K\pi = 5/2^-$, in contrast to the oblate structure of the $3/2^-{}_2$ state.

The first excited state of 43S, $1/2^-{}_1$, shares a similar predominant configuration with the ground state and exhibits a strong E2 transition to the ground state. The MR-CDFT (labeled with "β_2+K mixing") predicts B(E2; $1/2^-{}_1 \rightarrow 3/2^-{}_1$) = 144 e^2fm^4, as well as a sizable M1 transition with B(M1; $1/2^-{}_1 \rightarrow 3/2^-{}_1$) = 0.45 ^{2}_N, as shown in Fig. 3(b). In the AMD+GCM [27], these values are 180 e^2fm^4 and 0.34 ^{2}_N, respectively. The B(E2; $1/2^-{}_1 \rightarrow 3/2^-{}_1$) value has not yet been measured, but experimental data are available for B(M1; $1/2^-{}_1 \rightarrow 3/2^-{}_1$) = 1.2(3) ^{2}_N [29], which is underestimated by both methods. We find that this underestimation is due to the extension of the wave function of the $3/2^-{}_1$ state into the region of large prolate deformation with $\beta_2 > 0.4$, as shown in Fig. 3(d). Moreover, we observe two ΔJ = 2 rotational bands: ($3/2^-{}_1$, $5/2^-{}_1$, $7/2^-{}_1$, $9/2^-{}_1$, $11/2^-{}_1$) and ($3/2^-{}_2$, $5/2^-{}_2$, $7/2^-{}_2$), which are connected by strong E2 transitions. The predicted B(E2; $7/2^-{}_1 \rightarrow 3/2^-{}_1$) = 59 e^2fm^4 is slightly larger than the data 46(9) e^2fm^4 [30]. All these states are predominantly characterized by the prolate-deformed configuration $1/2^-[321]$, originating from the spherical $p_3/_2$ orbital, with deformation $\beta_2 \simeq 0.3$ and Kπ = $1/2^-$, as illustrated in Fig. 1. The energy ordering of the ($3/2^-{}_1$, $5/2^-{}_1$, $7/2^-{}_1$) sequence follows the weak-coupling limit of the particle-rotor model [51], which predicts a parabolic energy pattern with a minimum at J j = 3/2.

Figure 3(h) shows that the $7/2^-{}_1$ state is dominated by the prolate-deformed configuration $7/2^-[303]$ with $\beta_2 \simeq 0.22$ and Kπ = $7/2^-$. Consequently, the decay of the $7/2^-{}_1$ state to the ground state ($3/2^-{}_1$) is strongly quenched due to ΔK = 3. Quantitatively, the predicted B(E2; $7/2^-{}_1 \rightarrow 3/2^-{}_1$) = 0.24 e^2fm^4 compares to the data 0.41 e^2fm^4 [25]. As a result, the $7/2^-{}_1$ state is classified as a high-K isomer state, consistent with previous studies [23, 28]. A comparison between Figs. 3(b) and 3(c) reveals that the excitation energy of the $7/2^-{}_1$ state decreases significantly and becomes closer to the experimental value after incorporating the K-mixing effect. In contrast, the $7/2^-{}_2$ state of oblate nature in Fig. 3(c) is pushed very high and is not shown in Fig. 3(b). As shown in Fig. 3(h), the isomeric $7/2^-{}_1$ state also contains a small admixture of an oblate configuration with Kπ = $1/2^-$. The remaining discrepancy is expected to be further reduced by including triaxial deformation effects, as suggested by the AMD+GCM calculation [27].

Table I lists the spectroscopic quadrupole moments Qs and magnetic dipole moments for 43S obtained from MR-CDFT calculations with both shape-mixing and Kπ mixing effects, in comparison with AMD+GCM calculations [27] and available data for the isomer state with Qs($7/2^-{}_1$) = 23(3) efm^2 and ($7/2^-{}_1$) = -1.110(14) _N. Overall, the results from MR-CDFT and AMD+GCM are similar, with both models reasonably reproducing the experimental data. Quantitatively, the Qs values of states in the ground-state band predicted by MR-CDFT are slightly smaller than those from AMD+GCM. Notably, the magnetic moments of the $1/2^-{}_1$ and $7/2^-{}_1$ states obtained with MR-CDFT are only about half the values predicted by AMD+GCM. A significant difference arises in the prediction for the $5/2^-{}_2$ state: while the AMD+GCM calculation indicates that this state is dominated by an oblate configuration, the MR-CDFT result suggests a prolate deformation, consistent with the latest shell-model calculations

[28]. Further experimental and theoretical benchmarks are needed to ultimately validate these findings.

IV. Summary

In this work, we have further extended the multireference covariant density functional theory (MR-CDFT) with particle-number and angular-momentum projections for odd-mass nuclei by simultaneously mixing quasiparticle configurations with different quadrupole shapes and K quantum numbers. The success of this extended framework is demonstrated through its application to the low-lying states of 43S, where the available experimental data on energy spectra, electric quadrupole and magnetic dipole transition strengths, and electromagnetic moments are reasonably well reproduced.

Our calculations reveal a pair of prolate rotational bands with $\Delta J = 2$, built on the ground-state configuration $1/2^-[321]$ ($K\pi = 1/2^-$), consistent with the weak-coupling limit of the particle-rotor model. In addition, a rotational band is found based on the configuration $7/2^-[303]$ ($K\pi = 7/2^-$), corresponding to the isomeric $7/2^-{}_1$ state. These findings are generally consistent with those from AMD+GCM and shell-model calculations, supporting the erosion of the N = 28 shell gap. We also identify a $3/2^-{}_2$ state dominated by an oblate configuration with $K\pi = 1/2^-$, where the valence neutron occupies the $1/2^-[330]$ orbital, and a $5/2^-{}_2$ state dominated by a prolate configuration with $K\pi = 5/2^-$. The latter differs from the predictions of AMD+GCM with triaxiality, which suggest an oblate shape, and thus calls for further clarification through lifetime measurements.

It is worth emphasizing that the present framework is based on axially deformed quasiparticle configurations, with triaxial effects partially incorporated through K mixing explicitly. This makes it a computationally efficient alternative to previous approaches that explicitly treat triaxiality and require full three-dimensional angular-momentum projection. The resulting efficiency enables systematic beyond-mean-field studies of shape coexistence and isomeric states in heavy deformed odd-mass nuclei, such as 229Th.

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References

[1] Y. Yano, Nucl. Instrum. Meth. B 261, 1009 (2007).
[2] T. Glasmacher, B. Sherrill, W. Nazarewicz, A. Gade, P. Mantica, J. Wei, G. Bollen, and B. Bull, Nucl. Phys. News 27, 28 (2017).
[3] Y. Ye, X. Yang, H. Sakurai, and B. Hu, Nature Rev. Phys. 7, 21 (2025).
[4] E. Caurier, G. Martinez-Pinedo, F. Nowacki, A. Poves, and A. P. Zuker, Rev. Mod. Phys. 77, 427 (2005), arXiv:nucl-th/0402046.
[5] O. Sorlin and M. G. Porquet, Prog. Part. Nucl. Phys. 61, 602 (2008), arXiv:0805.2561 [nucl-ex].
[6] T. Otsuka, A. Gade, O. Sorlin, T. Suzuki, and Y. Utsuno, Rev. Mod. Phys. 92, 015002 (2020), arXiv:1805.06501 [nucl-th].
[7] N. Tsunoda, T. Otsuka, K. Takayanagi, N. Shimizu, T. Suzuki, Y. Utsuno, S. Yoshida, and H. Ueno, Nature 587, 66 (2020).
[8] M. G. Mayer, Phys. Rev. 75, 1969 (1949).
[9] O. Haxel, J. H. D. Jensen, and H. E. Suess, Phys. Rev. 75, 1766 (1949).
[10] O. Sorlin et al., Phys. Rev. C 47, 2941 (1993).
[11] H. Scheit et al., Phys. Rev. Lett. 77, 3967 (1996).
[12] T. Glasmacher et al., Phys. Lett. B 395, 163 (1997).
[13] A. Gade et al., Phys. Rev. Lett. 122, 222501 (2019), arXiv:1905.04142 [nucl-ex].
[14] B. Bastin et al., Phys. Rev. Lett. 99, 022503 (2007), arXiv:0705.4526 [nucl-ex].
[15] S. Takeuchi et al., Phys. Rev. Lett. 109, 182501 (2012), arXiv:1207.6191 [nucl-ex].
[16] H. L. Crawford et al., Phys. Rev. Lett. 122, 052501 (2019).
[17] S. Grévy et al., The European Physical Journal A 25, 111 (2005).
[18] T. R. Rodriguez and J. L. Egido, Phys. Rev. C 84, 051307 (2011), arXiv:1109.6516 [nucl-th].
[19] J. L. Egido, M. Borrajo, and T. R. Rodríguez, Phys. Rev. Lett. 116, 052502 (2016), arXiv:1512.04232 [nucl-th].
[20] Z. P. Li, J. M. Yao, D. Vretenar, T. Niksic, H. Chen, and J. Meng, Phys. Rev. C 84, 054304 (2011), arXiv:1209.6074 [nucl-th].
[21] D. Santiago-Gonzalez et al., Phys. Rev. C 83, 061305 (2011).
[22] J. J. Parker et al., Phys. Rev. Lett. 118, 052501 (2017).
[23] Y. Utsuno, N. Shimizu, T. Otsuka, T. Yoshida, and Y. Tsunoda, Phys. Rev. Lett. 114, 032501 (2015), arXiv:1407.0444 [nucl-th].
[24] F. Sarazin et al., Phys. Rev. Lett. 84, 5062 (2000).
[25] L. Gaudefroy et al., Phys. Rev. Lett. 102, 092501 (2009).
[26] R. Chevrier et al., Phys. Rev. Lett. 108, 162501 (2012).
[27] M. Kimura, Y. Taniguchi, Y. Kanada-En’ yo, H. Horiuchi, and K. Ikeda, Phys. Rev. C 87, 011301 (2013).
[28] R. Chevrier and L. Gaudefroy, Phys. Rev. C 89, 051301 (2014).
[29] T. Mijatović et al., Phys. Rev. Lett. 121, 012501 (2018).

[30] B. Longfellow, D. Weisshaar, A. Gade, B. A. Brown, D. Bazin, K. W. Brown, B. Elman, J. Pereira, D. Rhodes, and M. Spieker, Phys. Rev. Lett. 125, 232501 (2020).
[31] Q. Yuan, J. G. Li, and W. Zuo, Phys. Rev. C 109, L041301 (2024).
[32] D. Vretenar, A. Afanasjev, G. Lalazissis, and P. Ring, Physics Reports 409, 101 (2005).
[33] J. Meng, H. Toki, S. G. Zhou, S. Q. Zhang, W. H. Long, and L. S. Geng, Prog. Part. Nucl. Phys. 57, 470 (2006), arXiv:nucl-th/0508020.
[34] J. Meng, *Relativistic Density Functional for Nuclear Structure*, Vol. 26 (World Scientific, 2016).
[35] J. M. Yao, J. Meng, P. Ring, and D. Pena Arteaga, Phys. Rev. C 79, 044312 (2009), arXiv:0903.5027 [nucl-th].
[36] J. M. Yao, J. Meng, P. Ring, and D. Vretenar, Phys. Rev. C 81, 044311 (2010), arXiv:0912.2650 [nucl-th].
[37] T. Niksic, D. Vretenar, and P. Ring, Prog. Part. Nucl. Phys. 66, 519 (2011), arXiv:1102.4193 [nucl-th].
[38] J. M. Yao, K. Hagino, Z. P. Li, J. Meng, and P. Ring, Phys. Rev. C 89, 054306 (2014), arXiv:1403.4812 [nucl-th].
[39] J. M. Yao, E. F. Zhou, and Z. P. Li, Phys. Rev. C 92, 041304 (2015), arXiv:1507.03298 [nucl-th].
[40] E. F. Zhou and J. M. Yao, Int. J. Mod. Phys. E 32, 2340011 (2023), arXiv:2309.09488 [nucl-th].
[41] X.-Y. Wu, J.-Z. Cao, K.-N. Zhao, Z.-M. Liu, J. Xiang, and E.-F. Zhou, Nucl. Sci. Tech. 35, 202 (2024).
[42] L. S. Song, J. M. Yao, P. Ring, and J. Meng, Phys. Rev. C 90, 054309 (2014).
[43] L. S. Song, J. M. Yao, P. Ring, and J. Meng, Phys. Rev. C 95, 024305 (2017).
[44] J. M. Yao, L. S. Song, K. Hagino, P. Ring, and J. Meng, Phys. Rev. C 91, 024316 (2015).
[45] J. M. Yao, J. Meng, Y. F. Niu, and P. Ring, Prog. Part. Nucl. Phys. 126, 103965 (2022), arXiv:2111.15543 [nucl-th].
[46] H. Mei, K. Hagino, and J. M. Yao, Phys. Rev. C 93, 011301 (2016).
[47] H. Xia, X. Wu, H. Mei, and J. Yao, Sci. China Phys. Mech. Astron. 62, 42011 (2019), arXiv:1811.01486 [nucl-th].
[48] H. Xia, X. Wu, H. Mei, and J. Yao, Sci. China Phys. Mech. Astron. 66, 252011 (2023), arXiv:2211.09356 [nucl-th].
[49] E. F. Zhou, X. Y. Wu, and J. M. Yao, Phys. Rev. C 109, 034305 (2024), arXiv:2311.15305 [nucl-th].
[50] F.-Q. Chen, Y. Sun, P. M. Walker, G. D. Dracoulis, Y. R. Shimizu, and J. A. Sheikh, J. Phys. G 40, 015101 (2013).
[51] P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer-Verlag, New York, 1980).
[52] P. W. Zhao, Z. P. Li, J. M. Yao, and J. Meng, Phys. Rev. C 82, 054319 (2010), arXiv:1002.1789 [nucl-th].
[53] D. L. Hill and J. A. Wheeler, Phys. Rev. 89, 1102 (1953).

[54] S. J. Krieger, P. Bonche, H. Flocard, P. Quentin, and M. S. Weiss, Nucl. Phys. A 517, 275 (1990).

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