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Nature of Isomerism in Exotic Sulfur Isotopes

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We clarify the origin of the anomalously hindered $E2$ decay from the 4_1^+ level in ^{44}S by performing a novel many-body analysis in the shell model. Within a unified picture about the occurrence of isomerism in neutron-rich sulfur isotopes, the 4_1^+ state is demonstrated to be a $K = 4$ isomer dominated by the two-quasiparticle configuration $\nu\Omega^\pi = 1/2^- \otimes \nu\Omega^\pi = 7/2^-$. The 4_1^+ state in ^{44}S is a new type of high- K isomer which has significant triaxiality.

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Among the most fundamental properties of nuclei is quadrupole collectivity, based on which the yrast $0^+, 2^+, 4^+, \dots$ states in even-even nuclei are, in general, connected with strong $E2$ matrix elements. For open-shell nuclei in particular, $B(E2)$ values between neighboring yrast states are tens to hundreds of times larger than the Weisskopf estimate [1]. Contrary to common sense, a recent experiment has reported [2] that the 4^+ state of ^{44}S located at 2.4 MeV, most likely the yrast state due to its small $E_x(4^+)$ to $E_x(2_1^+)$ ratio 1.9, has a strongly hindered $B(E2)$ value ($\lesssim 1$ W.u.) for the transition to 2_1^+ . While this quite unusual $E2$ property of the 4_1^+ state, a kind of isomer, has been described with shell-model calculations [2], its underlying nuclear structure and lowering mechanism are still unclear. While a $K = 4$ high- K isomeric state is suggested in analogy to heavy-mass nuclei [2], this hypothesis is not supported by later microscopic calculations [3,4].

Besides the 4_1^+ level in ^{44}S , plenty of exotic nuclear properties have been reported for neutron-rich sulfur isotopes. A modest $B(E2; 0_1^+ \rightarrow 2_1^+)$ value in ^{44}S [5] indicates the development of quadrupole collectivity despite the neutron magic number 28. An extraordinary low-lying isomeric 0_2^+ state in ^{44}S [6,7] might suggest a spherical-deformed shape coexistence. Similarly, an isomeric $7/2_1^-$ state in ^{43}S is also possibly an indication of shape coexistence [8,9]. Those observations have triggered state-of-the-art theoretical investigations based on the large-scale shell-model calculations [4,10–13], the beyond-mean-field approaches [3,14–16], and the antisymmetrized molecular dynamics (AMD) [17].

In this Letter, we demonstrate that the isomeric 4_1^+ state in ^{44}S occurs due to the dominance of a $K = 4$ intrinsic state by means of beyond-mean-field approximations to the shell model. We also present a unified understanding of the occurrence of the exotic isomers in neutron-rich sulfur isotopes $^{43,44}\text{S}$, thus confirming the robustness of the

present approaches and results. ^{44}S is the lightest-mass case among the high- K isomers ever identified in the $A \sim 100$, $A \sim 130$, $A \sim 180$, and $A \sim 250$ regions [18]. More surprisingly, this nucleus is triaxially deformed in contrast to the known cases having well-developed axially symmetric shapes [19].

We start with the conventional shell-model calculations for neutron-rich nuclei around $N = 28$ in the $\pi(sd)^{Z-8}\nu(pf)^{N-20}$ valence space with the SDPF-MU interaction [13]. As we will show in more detail later, the nuclear structure of the sulfur isotopes of the present interest is very well reproduced with the SDPF-MU interaction, as well as with the SDPF-U interaction [10].

While the shell-model calculation is capable of describing observables of nuclei quite quantitatively, it is not necessarily easy to draw a comprehensive picture of nuclear structure, in particular, from the intrinsic-frame point of view. Introducing an appropriate mean-field based method into the shell model is a key to solving this problem. The method to be taken should represent spin-dependent intrinsic structure to describe the abrupt change between 2_1^+ and 4_1^+ in ^{44}S and should provide high-quality many-body wave functions comparable to the full shell-model calculation. Clearly, simple mean-field calculations such as the Hartree-Fock method cannot satisfy those demands. Here we take the variation after angular-momentum projection (AM-VAP) as a beyond-mean-field method to efficiently describe spin dependence within a framework that can well define an intrinsic state.

In the AM-VAP, wave functions are determined to minimize the energy $E(I\sigma) = \langle IM\sigma | H | IM\sigma \rangle_{\text{AM-VAP}} / \langle IM\sigma | IM\sigma \rangle_{\text{AM-VAP}}$ in the form of a wave function

$$|IM\sigma\rangle_{\text{AM-VAP}} = \sum_K g_K^{IM\sigma} \hat{P}_{MK}^I |\Phi(IM\sigma)\rangle, \quad (1)$$

where $|\Phi(IM\sigma)\rangle = \prod_k (\sum_l D_{lk}^{IM\sigma} c_l^\dagger) |-\rangle$ is a general single Slater determinant parametrized by $D_{lk}^{IM\sigma}$ and can be

regarded as the intrinsic state of $|IM\sigma\rangle_{\text{AM-VAP}}$. \hat{P}_{MK}^I is the usual angular-momentum projection operator [20] with I , M , and K denoting the total angular momentum and its z components along the laboratory and intrinsic frames, respectively, and each state with a given (I, M) is labeled with σ . The mixing of K in $|IM\sigma\rangle_{\text{AM-VAP}}$ is represented by $g_K^{IM\sigma}$. $D_{lk}^{IM\sigma}$ and $g_K^{IM\sigma}$ are the variational parameters which are optimized using the conjugate gradient method [21] [see [22] for the expression of the gradient of $E(I\sigma)$]. Furthermore, we calculate the overlap probabilities between the solutions found in this procedure and the shell-model wave functions of interest in order not to miss important solutions. Those overlap probabilities also work to test the quality of the AM-VAP wave functions. Multiple AM-VAP solutions, if found, are treated as separate levels if they are nearly orthogonal.

Figure 1 shows energy levels and $B(E2)$ values in $^{43,44}\text{S}$ compared among experiments, the full shell-model calculation, and the AM-VAP calculation. The $E2$ effective charges $(e_p, e_n) = (1.35e, 0.35e)$ are taken. As presented in Fig. 1, the results of the AM-VAP calculations are very close to those of the full shell-model calculations, including a strongly hindered $B(E2; 4_1^+ \rightarrow 2_1^+)$ value in ^{44}S .

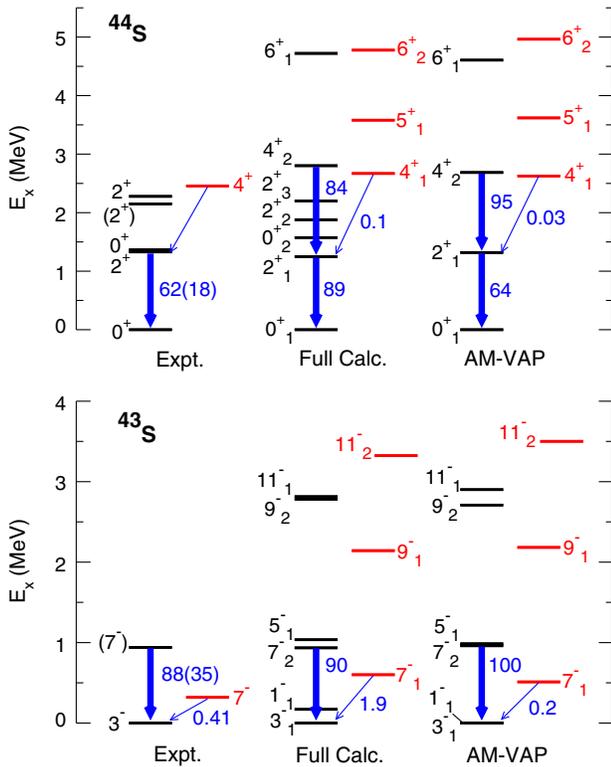


FIG. 1 (color online). Energy levels and $B(E2)$ values (in $e^2\text{fm}^4$) in $^{43,44}\text{S}$ compared among experiments (Expt.), the full shell-model calculation (Full Calc.), and the AM-VAP approximation to the shell model (AM-VAP). The spin-parity is denoted as J^π for ^{44}S and $2J^\pi$ for ^{43}S . Experimental data are taken from [2,5,6,9,23,24].

The overlap probabilities calculated between the full shell-model states and the AM-VAP states are rather close to unity: 0.92, 0.81, 0.86, 0.88, and 0.90 for the 0_1^+ , 2_1^+ , 4_1^+ , 4_2^+ , and 5_1^+ states in ^{44}S , respectively, and 0.96, 0.91, 0.85, 0.93, 0.93, 0.92, 0.93, 0.92, and 0.84 for the $1/2_1^-$, $3/2_1^-$, $5/2_1^-$, $7/2_1^-$, $7/2_2^-$, $9/2_1^-$, $9/2_2^-$, $11/2_1^-$, and $11/2_2^-$ states in ^{43}S , respectively. The 6^+ states of the AM-VAP split into the two shell-model states because of the accidental degeneracy of the 6^+ states in the shell-model calculation.

Supported by those very large overlaps, it is reasonable to deduce intrinsic properties of many-body wave functions from the corresponding AM-VAP intrinsic states, $|\Phi(IM\sigma)\rangle$ in Eq. (1). The intrinsic mass quadrupole moments Q_0 and Q_2 are given as the expectation values of the mass quadrupole operators r^2Y_{20} and r^2Y_{22} in $|\Phi(IM\sigma)\rangle$, respectively, where the axes of the intrinsic frame are determined to diagonalize the quadrupole tensor and to satisfy the order $\langle Q_{zz} \rangle \geq \langle Q_{xx} \rangle \geq \langle Q_{yy} \rangle$. It is noted that a similar method has been used to deduce shape fluctuation in exotic Ni isotopes from the Monte Carlo shell-model wave functions [25]. The quadrupole deformation parameters (β, γ) are then defined in the usual way as $\beta = f_{\text{scale}} \sqrt{5/16\pi(4\pi/3R^2A)} \sqrt{(Q_0)^2 + 2(Q_2)^2}$ and $\gamma = \arctan(\sqrt{2}Q_2/Q_0)$, with $R = 1.2A^{1/3}$ fm [26]. Here, a factor $f_{\text{scale}} = e_p/e + e_n/e$ is introduced to rescale quadrupole matrix elements between the shell-model space and the full single-particle space. Since the intrinsic axes are thus determined, the K quantum number is well defined apart from its sign. The distribution of K , which is normalized to unity, is calculated by following the method shown in Ref. [26].

The intrinsic properties of the AM-VAP states defined above are listed in Tables I and II for ^{44}S and ^{43}S , respectively. We first outline the properties of ^{44}S . The 0_1^+ , 2_1^+ , 4_2^+ , 6_1^+ sequence, connected with strong $E2$ matrix elements, is dominated by the $K=0$ state as usually conceived for the ground-state band, whereas the $K=1$ component grows with increasing spin because of the Coriolis coupling. The shape of the ground-state band evolves from triaxial to prolate. This shape evolution is

TABLE I. Distribution of $|K|$ and deformation parameters (β, γ) (γ : in deg.) in the AM-VAP states for ^{44}S .

I_σ^π	$ K $							β	γ
	0	1	2	3	4	5	6		
0_1^+	1.00							0.24	33
2_1^+	0.98	0.00	0.01					0.26	23
4_2^+	0.92	0.08	0.00	0.00	0.00			0.28	14
6_1^+	0.76	0.23	0.01	0.00	0.00	0.00	0.00	0.28	13
4_1^+	0.00	0.00	0.00	0.07	0.93			0.23	28
5_1^+	0.00	0.00	0.01	0.08	0.85	0.07		0.23	24
6_2^+	0.00	0.01	0.01	0.14	0.80	0.04	0.00	0.23	26

TABLE II. Same as Table I but for ^{43}S .

I^π_σ	$ K $						β	γ
	1/2	3/2	5/2	7/2	9/2	11/2		
$1/2^-_1$	1.00						0.27	15
$3/2^-_1$	0.98	0.02					0.25	17
$5/2^-_1$	0.97	0.03	0.00				0.27	16
$7/2^-_2$	0.96	0.04	0.00	0.00			0.25	16
$9/2^-_2$	0.96	0.04	0.00	0.00	0.00		0.28	15
$11/2^-_1$	0.91	0.09	0.00	0.00	0.00	0.00	0.25	16
$7/2^-_1$	0.00	0.01	0.01	0.98			0.22	31
$9/2^-_1$	0.00	0.01	0.04	0.95	0.01		0.23	31
$11/2^-_2$	0.00	0.01	0.01	0.08	0.03	0.87	0.25	37

very similar to the results of a beyond-mean-field calculation based on the GCM [3] and an analysis based on the quadrupole rotational invariants in the shell-model wave functions [4]. On the other hand, the $4^+_1, 5^+_1, 6^+_2$ sequence, also connected with strong $E2$ matrix elements, is missing in the beyond-mean-field study of Ref. [3], but appears in the shell model both with the SDPF-U interaction [2,4] and with the SDPF-MU interaction [13].

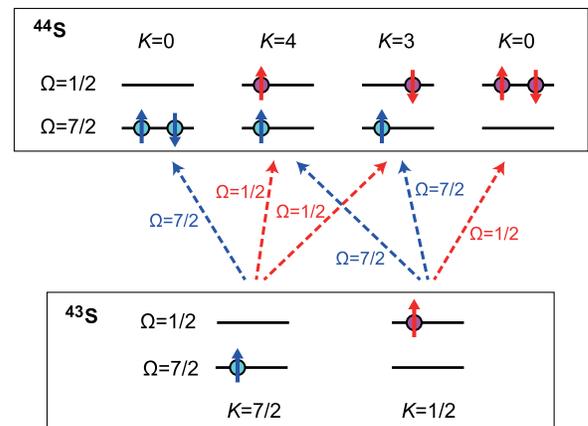
The present AM-VAP calculation demonstrates that this band is strongly dominated by the $K = 4$ state for the first time. Experimentally, while this K assignment has been suggested in [2], its basis is only the weak $E2$ transition to the 2^+_1 level because the usual shell-model calculation cannot provide K quantum numbers. In light nuclei, however, such a high- K isomer has not been known and is rather unexpected. It is commonly believed that the high- K isomerism occurs only in axially symmetric, stably deformed nuclei [19], whereas this condition is not satisfied in light nuclei. What is surprising in the present case is that the concentration of the K numbers takes place in the $K = 4$ band in spite of the significant triaxiality of the $K = 4$ states. The AM-VAP calculation shows that although the K numbers are strongly mixed in the intrinsic state $|\Phi\rangle$ of Eq. (1), the purity of K is approximately restored after diagonalizing the Hamiltonian in the K space.

Why does the $K = 4$ band emerge at such a low excitation energy in ^{44}S ? The structure of ^{43}S brings key information on this question, which we briefly examine here. The energy levels in ^{43}S are presented in Fig. 1, and their intrinsic properties are listed in Table II. The observed energy levels and the $E2$ transitions are well reproduced with the full shell-model and AM-VAP calculations. The strong $E2$ excitation to the 940 keV state [24] and the isomeric state at 320 keV [8,9], shown in Fig. 1, suggest a possible coexistence of configurations. While the ground state should be deformed on the basis of the large $B(E2; \text{g.s.} \rightarrow 940 \text{ keV})$ value, the structure of $7/2^-_1$ has been less understood. Although an early analysis [9] proposed a quasispherical state, the large quadrupole moment in this state measured later [27], $|Q| = 23(3) \text{ efm}^2$,

casts doubt on this interpretation. The AM-VAP analysis demonstrates that the ground state and the $7/2^-_1$ state are dominated by $K = 1/2$ and $K = 7/2$, respectively, and that this K forbiddenness causes the isomerism in $7/2^-_1$. Although this result is consistent with the suggestion of [17], the present calculation is the first to quantitatively provide the distribution of K . The $K = 7/2$ and $K = 1/2$ states have triaxial and nearly prolate deformations, respectively, in accordance with [4,17]. Thus, similar to the $K = 4$ band in ^{44}S , the $K = 7/2$ band in ^{43}S has an approximately good K number in spite of the development of triaxiality.

Since ^{43}S is an even-odd nucleus, the K quantum number is determined by that of the unpaired neutron Ω^π . On the basis of the above analysis, we hereafter assume a good Ω^π quantum number even in the case of non-axially symmetric deformation. As expected from the Nilsson diagram (see also Ref. [17]), the orbit of the last neutron can be $\Omega^\pi = 1/2^-$, which favors prolate deformation, or $\Omega^\pi = 7/2^-$, which favors oblate deformation. Thus, the $K = 1/2$ state favors a prolate shape because of the preference of prolate deformation for both the $\Omega^\pi = 1/2^-$ neutron and the ^{42}S core (see the potential energy surface of ^{42}S , e.g., in Ref. [13]). The $K = 7/2$ state, on the other hand, is inclined to be triaxial due to the opposite shape preference between the last neutron and the core.

Now we turn to ^{44}S . It is reasonable to fix the ^{42}S core and to take into account only the two quasiparticle degrees of freedom, $\Omega^\pi = 1/2^-$ and $7/2^-$. It is noted that the quasiparticle state is introduced, as usual, to include pairing correlation within the single-particle picture. Those two orbits are regarded to be nearly degenerate in this simple picture, similarly to the small energy difference between the $3/2^-_1$ and $7/2^-_1$ states in ^{43}S . For the two-quasiparticle system of ^{44}S , two $K = 0$ states, one $K = 3$ state, and one $K = 4$ state can be constructed by adding a neutron, as illustrated in Fig. 2. We then consider the competition of energy between different K states by decomposing the

FIG. 2 (color online). Possible low-lying neutron configurations for ^{44}S and ^{43}S .

energy of a state into the intrinsic energy and the rotational energy. Concerning the intrinsic energy, the lowest $K = 0$ zero-quasiparticle state is, in general, lower than the $K \neq 0$ two-quasiparticle states even if the relevant quasiparticle states are degenerate because the former gains additional energy due to pairing, which amounts to 2Δ , where Δ is the pairing gap. Thus, the $K = 0$ state usually dominates the yrast $0^+, 2^+, 4^+, \dots$ sequence. High- K states are, however, advantageous over the $K = 0$ state in terms of the loss of the rotational energy $E_{\text{rot}} = (\hbar^2/2\mathcal{I})(I(I+1) - K^2)$, which is smaller for high- K states. This is the standard picture for the occurrence of high- K isomers seen usually in the medium-heavy-mass or heavy-mass regions [28]. In those heavier-mass regions, the $K \neq 0$ states cannot be lower than the $K = 0$ member unless K is sufficiently large because moments of inertia are rather large. On the other hand, for lighter nuclei with relatively small moments of inertia, a state with a modest K can, in principle, intrude into the yrast $0^+, 2^+, 4^+, \dots$ sequence if a high- Ω orbit is located very close to the Fermi surface. ^{44}S is such a very rare case, but similar situations can occur in other nuclei. For nuclei around ^{44}S , two quasiparticle states are estimated to appear above $2\Delta \approx 2.5$ MeV, where the pairing gap is evaluated from one-neutron separation energies of $^{43,44,45}\text{S}$. This energy estimate accounts for the excitation energy of the measured isomeric 4^+ state. On the other hand, the 4^+ state with $K = 0$ is roughly estimated to lie around 3 MeV by assuming a normal $E_x(4^+)/E_x(2^+)$ ratio, ~ 2.5 . This is how the $K = 4$ state becomes the yrast state in ^{44}S when $\Omega^\pi = 7/2^-$ and $\Omega^\pi = 1/2^-$ are nearly degenerate.

In the beyond-mean-field approach of Ref. [3], the low-lying $K = 4$ state is missing despite many other similarities, such as shapes, to the present calculations. This is due to the restriction of time-reversal symmetry on the intrinsic states imposed in the calculation of Ref. [3]. The AM-VAP calculation, in fact, demonstrates that the time-reversal symmetry is almost completely broken for the intrinsic state of the $K = 4$ state. The overlap probabilities between $|\Phi\rangle$ of Eq. (1) and its time-reversed state $\mathcal{T}|\Phi\rangle$ are calculated to be only 0.02–0.08 for the $K = 4$ members. The breaking of time-reversal symmetry in the intrinsic state is almost solely attributed to the neutron part of the wave function.

Here we confirm that the actual shell-model wave function of 4_1^+ is indeed dominated by the above-mentioned two-quasiparticle state by calculating its spectroscopic strengths. The full shell-model calculation leads to large overlap probabilities of the 4_1^+ state with the $\mathcal{A}[\nu p_{3/2} \otimes 7/2_1^-]^{J=4}$ and $\mathcal{A}[\nu f_{7/2} \otimes 7/2_2^-]^{J=4}$ states (0.66 and 0.54, respectively), where \mathcal{A} denotes antisymmetrization and normalization. On the other hand, its overlap probabilities with $\mathcal{A}[\nu f_{7/2} \otimes 7/2_1^-]^{J=4}$ and $\mathcal{A}[\nu p_{3/2} \otimes 7/2_2^-]^{J=4}$ are much smaller (0.19 and 0.00, respectively). This is a direct consequence of the dominance of the configurations

illustrated in Fig. 2, since the $7/2_1^-$ and $7/2_2^-$ states are dominated by $K = 7/2$ and $K = 1/2$, respectively, and the $\Omega^\pi = 1/2^-$ and $\Omega^\pi = 7/2^-$ single-particle states are dominated by $p_{3/2}$ and $f_{7/2}$, respectively.

We also point out that the configurations shown in Fig. 2 account for the reason why the 0_2^+ state in ^{44}S lies extraordinarily low. In Fig. 2, two $K = 0$ states exist, having similar diagonal energies. The off-diagonal Hamiltonian matrix element between those $K = 0$ states strongly mixes them and repels the energy levels, but the excited $K = 0$ state can be rather low if the two quasiparticle states are nearly degenerate. The strong mixing between those two $K = 0$ states is supported by the shell-model result that the overlap probability of the 0_1^+ state with $\mathcal{A}[\nu f_{7/2} \otimes 7/2_1^-]^{J=0}$ (0.61) is close to the one with $\mathcal{A}[\nu p_{3/2} \otimes 3/2_1^-]^{J=0}$ (0.39). When the total spin for each $K = 0$ state increases, the state with a larger moment of inertia is relatively lowered. Here, the $K = 0$ state that occupies $\Omega^\pi = 1/2^-$ is the case because of larger, prolate deformation. This accounts for the shape evolution toward prolate deformation within the $K = 0$ band shown in Table I. It is noted that the ground state and $K = 4$ states deviate from a prolate shape because they occupy the oblate-favored $\Omega^\pi = 7/2^-$ orbit.

Finally, we note that the $K = 3$ state illustrated in Fig. 2 is also found in the shell-model and AM-VAP calculations. In the shell-model calculation, the 3_1^+ level appears very close to 4_1^+ , dominated by the $K = 3$ AM-VAP state. The $K = 3$ states are distinguishable from the $K = 4$ states by the neutron intrinsic-spin expectation value because of differences in neutron spin orientation.

In conclusion, we have clarified that the isomeric 4_1^+ state in ^{44}S observed recently [2] originates from the dominance of the $K = 4$ state by means of the AM-VAP approximation to the shell model. This result is very robust because it is understood within a unified picture about the occurrence of exotic isomeric states in $^{43,44}\text{S}$ including the $7/2_1^-$ state in ^{43}S and the 0_2^+ in ^{44}S . The $K = 4$ state is missing in the beyond-mean-field calculation [3] due to the restriction of time-reversal symmetry and may appear without it. Having extraordinary light mass and triaxial deformation, the $K = 4$ isomer in ^{44}S is distinct from previously known high- K isomers. Thus, the possibility of the occurrence of high- K isomerism is greatly extended to the whole chart of nuclides, which provides new experimental and theoretical opportunities.

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