

Theoretical Study on Negative Parity States of $^{191,193,195,197}\text{Au}$ in Particle Triaxial-Rotor Model *

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By taking the particle triaxial-rotor model with variable moment of inertia, we investigate the energy spectra, the deformation and the single particle configuration of the negative-parity states in nuclei $^{191,193,195,197}\text{Au}$ systematically. The calculated energy spectra agree well with experimental data. The obtained results indicate that the negative-parity states in $^{191,193,195,197}\text{Au}$ originate from the proton-hole $h_{11/2}$ configuration coupled to a triaxial oblate Hg core. Meanwhile the main single particle configuration of the bands 1, 2 and 3 are identified to be $|5h_{11/2} 1/2\rangle$ ($\alpha = -1/2$), $|5h_{11/2} 1/2\rangle$ ($\alpha = 1/2$) and $|5h_{9/2} 7/2\rangle$, respectively.

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Neutron-deficient odd- A gold nuclei near the $Z = 82$ shell closure have been known to exhibit general shape coexistence. Experimentally, shape coexistence has been observed in odd- A nuclei $^{173-187}\text{Au}$.^[1-6] Meanwhile, the odd- AAu nuclei provide excellent examples of low-lying states resulting from coupling of a proton-hole to the oblate Hg core states.^[7] Indeed, the first positive-parity excited states in ^{197}Au are well described with a proton-hole $d_{3/2}$ configuration coupled to the ^{198}Hg core,^[8] which gives a rise to the use of ^{197}Au as a good example for supersymmetry models.^[9] Recently, in ^{197}Au , the previously known level scheme above the ground state was extended, and the previously unknown structure of negative-parity states

above the $\frac{11}{2}^-$ isomer was established.^[10] In Ref. [10],

the $\frac{11}{2}^-$ isomer was considered to originate from the coupling of an $h_{11/2}$ proton-hole to the ^{198}Hg core, and was expected to be the head of a decoupled band. However, the nature of those recently observed rotational bands in ^{197}Au has not yet been well identified. In addition, there has been some evidence for a triaxial shape to involve significant hexadecapole component in the ground state of ^{197}Au .^[11]

On the theoretical side, the negative-parity energies of the states above the $\frac{11}{2}^-$ isomer in $^{191,193,195}\text{Au}$ calculated from particle-plus-symmetric-rotor model are in qualitative agreement with those observed ex-

perimentally. However, the fact that the calculated values are considerably higher than the experimental data indicates that there are asymmetric deformations in those nuclei.^[7] So far, no other theoretical or experimental work that confirms the above suggestions of the deformed configurations of $^{191,193,195,197}\text{Au}$ has been reported. Since the particle triaxial-rotor model^[12-14] has been known to be suitable to study the triaxial deformation and configuration mixing,^[15-17] therefore, in this Letter, we take the particle triaxial-rotor model with variable moment of inertia of the core to analyse the band structure of the negative-parity states systematically and to identify their configurations in $^{191,193,195,197}\text{Au}$.

In the particle rotor model, the Hamiltonian of an odd- A nucleus is usually written as^[12-14]

$$\hat{H} = \hat{H}_{\text{core}} + \hat{H}_{\text{s.p.}} + \hat{H}_{\text{pair}}. \quad (1)$$

In the case of triaxial deformation, the Hamiltonian of the even-even core is given by

$$\hat{H}_{\text{core}} = \sum_{i=1}^3 \frac{\hbar^2 R_i^2}{2\Im_i} = \sum_{i=1}^3 \frac{\hbar^2 (I_i - j_i)^2}{2\Im_i}, \quad (2)$$

where R , I and j are the angular momentums of the core, the nucleus and the single particle, respectively. The three rotational moments of inertia are assumed

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to be connected by a relation of hydrodynamical type

$$\mathfrak{I}_\kappa = \frac{4}{3} \mathfrak{I}_0(I) \sin^2 \left(\gamma + \frac{2\pi}{3} \kappa \right), \quad (3)$$

with

$$\mathfrak{I}_0(I) = \mathfrak{I}_0 \sqrt{1 + bI(I+1)} \quad (4)$$

being the variable moment of inertia^[18] of the core to replace the original constant \mathfrak{I}_0 to improve the calculation. In the present calculation, we take $b = 0.013$ as the same as that in Refs. [19–21].

We take $\hat{H}_{\text{s.p.}}$ to describe the Hamiltonian of the unpaired single particle. In the triaxial deformed field of the even-even core, $\hat{H}_{\text{s.p.}}$ is given by

$$\begin{aligned} \hat{H}_{\text{s.p.}} = & -\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m \omega_0^2 r_0^2 \left\{ 1 - 2\beta \left[Y_{20} \cos \gamma \right. \right. \\ & \left. \left. + \frac{1}{\sqrt{2}} (Y_{22} + Y_{2-2}) \sin \gamma \right] \right\} \\ & - \kappa \hbar \omega_0 \{ 2\mathbf{l} \cdot \mathbf{s} + \mu(l^2 - \langle l_N^2 \rangle) \}, \end{aligned} \quad (5)$$

where κ and μ are the Nilsson parameters, Y_{2q} is the rank-2 spherical harmonic function.

We taken the Hamiltonian \hat{H}_{pair} to represent the pairing correlation which can be treated in the Bardeen–Cooper–Schrieffer (BCS) formalism. The single-particle wavefunction can be expressed as

$$|\nu\rangle = \sum_{Nl,j\Omega} C_{Nl,j\Omega}^{(\nu)} |Nl,j\Omega\rangle, \quad (6)$$

where ν is the sequence number of the single-particle orbitals and $|Nl,j\Omega\rangle$ represents the corresponding Nilsson states, and $C_{Nl,j\Omega}^{(\nu)}$ is the coefficient to identify the configuration mixing. diagonalizing the single-particle Hamiltonian in the basis $|Nl,j\Omega\rangle$, we can obtain the $C_{Nl,j\Omega}^{(\nu)}$ and the single-particle eigenvalue ε_ν . The corresponding quasi-particle energy can then be determined by $E_\nu = \sqrt{(\varepsilon_\nu - \lambda)^2 + \Delta^2}$, with λ and Δ being the Fermi energy and the energy gap, respectively.

The total Hamiltonian in Eq.(1) can be diagonalized in the symmetrically strong coupling basis

$$\begin{aligned} |IKM\nu\rangle = & \sqrt{\frac{2I+1}{16\pi^2}} [D_{MK}^I \alpha_\nu^\dagger |\tilde{0}\rangle \\ & + (-1)^{I-K} D_{M-K}^I \alpha_\nu^\dagger |\tilde{0}\rangle], \end{aligned} \quad (7)$$

where α_ν^\dagger is the creation operator of the single nucleon (in the present case, proton) in the orbital $|\nu\rangle$, D_{MK}^I is the rotational matrix.

In the present calculation to investigate the properties of $^{191,193,195,197}\text{Au}$, we take the κ and μ as standard values,^[22] i.e. 0.054 and 0.690, respectively, and the pairing gap parameter as $\Delta = 12/\sqrt{A}$. To improve the agreement between the calculated results and experimental data, we introduce a Coriolis attenuation factor ξ and take the value such that we can obtain

the best agreement between the calculated and experimental energy spectra. It is found that when $\xi = 0.98$, the calculated results agree best with the experimental data of $^{191,193,195,197}\text{Au}$. In general principle, in order to describe the property more accurately and to make better agreement between the calculated and experimental data, it is necessary to involve sufficient single-particle orbitals near the Fermi surface in the calculation. Thus we take 13 orbitals near the Fermi surface to couple with the core for $^{191,193,195,197}\text{Au}$. Practical calculation shows that the Fermi levels of the negative-parity bands 1, 2, 3 (it should be noted that we denote the band labels here in order to easily compare the similar bands in different nuclei) of those nuclei lie between the 19th and 20th of the single-particle orbitals.

For the deformation parameters β and γ of the negative-parity states in $^{191,193,195,197}\text{Au}$, because of no available parameters reported, we take the values of the ground state ($\frac{3}{2}^+$ $d_{3/2}$) of ^{197}Au given in Ref. [11] as the trial initial ones to fit, i.e. $\beta = -0.15$ and $\gamma = 26.0^\circ$. Then we accomplish a series diagonalization of the total Hamiltonian with various values of β and γ to make the calculation error $\chi^2 = \frac{1}{N} \sum_j (E_j^{\text{cal}} - E_j^{\text{exp}})^2$ of the spectrum of a band smallest, where N is the number of levels in a band. In such a process, the band-head energy is fixed artificially with the definite angular momentum assigned in experiment. The best fit is, in fact, focused on the energy separations. The best fitted values of the β and γ are listed in Table 1 for nucleus ^{191}Au , ^{193}Au , ^{195}Au , ^{197}Au , respectively.

Table 1. The best fitted deformation parameters of $^{191,193,195,197}\text{Au}$.

Nucleus	Band	β	γ (degree)
^{191}Au	1	-0.165	27.3
	2	-0.165	27.3
	3	-0.162	24.5
^{193}Au	1	-0.158	26.5
	2	-0.158	26.5
	3	-0.157	23.7
^{195}Au	1	-0.156	24.8
	2	-0.156	24.8
	3	-0.155	21.7
^{197}Au	1	-0.154	24.5
	2	-0.154	24.5
	3	-0.152	20.8

The best fitted results of the energy spectra of the bands 1, 2 and 3 in $^{191,193,195,197}\text{Au}$ are illustrated in Fig. 1. It is obvious that the calculated results agree very well with the experimental data. In turn, we obtain the total wavefunctions in terms of the single-particle orbitals which, as mentioned above, is fixed by diagonalizing the single-particle Hamiltonian at each set of deformation parameters (β, γ). Since the nuclei $^{191,193,195,197}\text{Au}$ are quite similar, and the previously unknown structure of negative-parity states above the

$\frac{11}{2}^-$ isomer in ^{197}Au has recently been established, as a typical example, we analyse the band structure and the single particle configuration of ^{197}Au in detail. The obtained main components of the single-particle orbitals near the Fermi surface in terms of the Nilsson levels (in the best fitted deformation parameters) of nucleus ^{197}Au are listed in Table 2, and the total wavefunctions in terms of the single-particle orbitals are listed in Table 3.

Table 2. The main components of the single-particle levels $|\nu\rangle$ near the Fermi surface in terms of the Nilsson levels of the bands in ^{197}Au .

Band	$ \nu\rangle$	Wavefunctions in terms of $ Nlj\Omega\rangle$
1	[17]	$0.653 5h_{11/2}5/2\rangle + 0.397 5h_{11/2}7/2\rangle - 0.530 5h_{11/2}1/2\rangle$
	[18]	$0.642 5h_{11/2}3/2\rangle - 0.580 5h_{11/2}5/2\rangle + 0.349 5h_{11/2}7/2\rangle$
	[19]	$0.726 5h_{11/2}1/2\rangle - 0.561 5h_{11/2}3/2\rangle + 0.335 5h_{11/2}5/2\rangle$
	[20]	$0.971 5h_{9/2}9/2\rangle - 0.167 5h_{9/2}5/2\rangle + 0.145 5f_{5/2}5/2\rangle$
	[21]	$0.797 5h_{9/2}7/2\rangle - 0.464 5f_{7/2}7/2\rangle + 0.294 5h_{9/2}3/2\rangle$
	[17]	$0.653 5h_{11/2}5/2\rangle + 0.397 5h_{11/2}7/2\rangle - 0.530 5h_{11/2}1/2\rangle$
2	[18]	$0.642 5h_{11/2}3/2\rangle - 0.580 5h_{11/2}5/2\rangle + 0.349 5h_{11/2}7/2\rangle$
	[19]	$0.726 5h_{11/2}1/2\rangle - 0.561 5h_{11/2}3/2\rangle + 0.335 5h_{11/2}5/2\rangle$
	[20]	$0.971 5h_{9/2}9/2\rangle - 0.167 5h_{9/2}5/2\rangle + 0.145 5f_{5/2}5/2\rangle$
	[21]	$0.797 5h_{9/2}7/2\rangle - 0.464 5f_{7/2}7/2\rangle + 0.294 5h_{9/2}3/2\rangle$
	[19]	$0.741 5h_{11/2}1/2\rangle + 0.555 5h_{11/2}3/2\rangle + 0.321 5h_{11/2}5/2\rangle$
	[20]	$0.980 5h_{9/2}9/2\rangle - 0.136 5h_{9/2}5/2\rangle + 0.121 5f_{5/2}5/2\rangle$
3	[21]	$0.807 5h_{9/2}7/2\rangle - 0.502 5f_{7/2}7/2\rangle + 0.239 5h_{9/2}3/2\rangle$
	[22]	$0.617 5h_{9/2}7/2\rangle - 0.533 5f_{7/2}5/2\rangle + 0.352 5h_{9/2}1/2\rangle$
	[23]	$0.561 5h_{9/2}5/2\rangle - 0.537 5f_{7/2}7/2\rangle + 0.450 5h_{9/2}7/2\rangle$

From Table 3, we can recognize that the bands 1, 2 (i.e. the first excited state of the decoupled band) come mainly from the 19th, partially from the 18th proton-hole single particle orbitals coupling with the oblate ^{198}Hg core. As listed in Table 2, the

19th orbital contains 53% of $|5h_{11/2} 1/2\rangle$, 31% of $|5h_{11/2} 3/2\rangle$ and 11% of $|h_{11/2} 5/2\rangle$ configurations, while the 18th orbital contains 41% of $|5h_{11/2} 3/2\rangle$, 34% of $|5h_{11/2} 5/2\rangle$ and 12% of $|5h_{11/2} 7/2\rangle$ configurations. Since all the components are in $h_{11/2}$, and the largest component is $|5h_{11/2} 1/2\rangle$, the bands 1 and 2 can be assigned as the one arising from the proton-hole $h_{11/2}$ configuration $|5h_{11/2} 1/2\rangle$. Combining Fig. 1 with Table 3, and considering the principle of angular momentum coupling and the identical characteristic of the band structure, we can infer that the rotational band 1 built upon the $h_{11/2}$ configuration is an unfavourable band, and the band 2 based on the $h_{11/2}$ configuration a favoured band, i.e. bands 1 and 2 are a pair of a signature partner, which is consistent with the prediction in Ref. [10]. Similarly, combining Table 3 with Table 2, we can notice that band 3 originates mainly from the 21st single particle orbital.

Table 3. Theoretically calculated main components of the wavefunctions of bands 1, 2 and 3 in ^{197}Au in terms of the single-particle levels.

Band	I^π	Wavefunctions $ \nu K\rangle$
1	$\frac{13}{2}^-$	$0.562 19 1/2\rangle + 0.474 19 3/2\rangle + 0.325 18 3/2\rangle$
	$\frac{2}{2}^-$	$0.599 19 1/2\rangle + 0.463 19 3/2\rangle + 0.313 18 3/2\rangle$
	$\frac{11}{2}^-$	$0.642 19 1/2\rangle + 0.476 19 3/2\rangle + 0.301 18 3/2\rangle$
2	$\frac{15}{2}^-$	$0.650 19 1/2\rangle + 0.458 19 3/2\rangle + 0.325 18 3/2\rangle$
	$\frac{19}{2}^-$	$0.600 19 1/2\rangle + 0.389 18 3/2\rangle + 0.333 19 3/2\rangle$
	$\frac{7}{2}^-$	$0.890 21 7/2\rangle - 0.260 22 7/2\rangle + 0.202 22 5/2\rangle$
3	$\frac{9}{2}^-$	$0.682 21 7/2\rangle + 0.305 20 9/2\rangle + 0.300 22 5/2\rangle$
	$\frac{1}{2}^-$	$0.650 21 7/2\rangle + 0.342 20 9/2\rangle + 0.302 22 5/2\rangle$

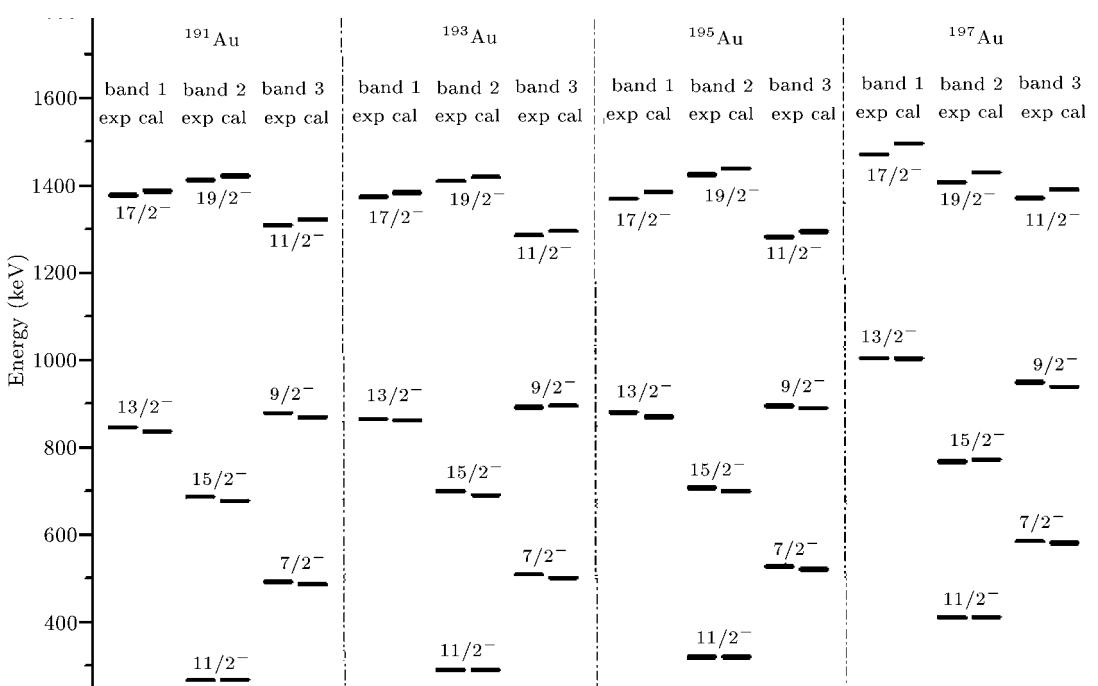


Fig. 1. Comparison of calculated energy levels of the rotational bands in $^{191,193,195,197}\text{Au}$ with the experimental data (taken from Refs. [7,10,23]).

The 21st orbital contains 64% of $|5h_{9/2} 7/2\rangle$ configuration. Thus, band 3 can be identified as the one generated by the proton-hole $h_{9/2}$ configuration $|5h_{9/2} 7/2\rangle$, which is consistent with the suggestion of $K = 7/2$ in Ref. [7], where K is the projection of I on j .

In addition, in the same way, the results similar to those in ^{197}Au are obtained for the corresponding bands in $^{191,193,195}\text{Au}$.

In summary, we have systematically calculated the energy spectra, deformation parameters and wavefunctions of the negative-parity states in nuclei $^{191,193,195,197}\text{Au}$ in the particle triaxial-rotor model with variable moment of inertia. By a least square fitting calculation, we reproduce the experimentally observed energy spectra of the bands 1, 2 and 3 in $^{191,193,195,197}\text{Au}$ quite well globally. The deformation parameters $\{\beta, \gamma\}$ of the states are then obtained. Considering both the parameters determined (especially $\beta < 0, \gamma > 0^\circ$) and the agreement between the calculated results and experimental data, we conclude that the negative-parity states in $^{191,193,195,197}\text{Au}$ originate from the proton-hole configuration coupled to a triaxial oblate Hg core. By analysing the configuration of bands 1, 2 and 3 in ^{197}Au in detail as an example, we assign the main single particle configuration of the negative-parity bands 1, 2 and 3 in $^{191,193,195,197}\text{Au}$ to be $|5h_{11/2} 1/2\rangle$ ($\alpha = -1/2$), $|5h_{11/2} 1/2\rangle$ ($\alpha = 1/2$) and $|5h_{9/2} 7/2\rangle$, respectively.

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