Explore nuclear multiple chirality in $A \sim 60$ mass region within covariant density functional theory

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Abstract

The nuclear multiple chirality in $A \sim 60$ mass region is explored by the adiabatic and configuration-fixed constrained covariant density functional theory for cobalt isotopes. The potential-energy curves and triaxiality parameters $\gamma$ as functions of the deformation parameter $\beta$ in $^{54,56,57,58,59,60}$Co are obtained. It is found that there are high-$j$ particle(s) and hole(s) configurations with prominent triaxially deformed shapes in these isotopes. This points towards that the existence of chirality or multiple chirality in $A \sim 60$ mass region are highly anticipated.

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The study of rotational motion has been at the forefront of nuclear structure physics for many decades. In particular, the chiral rotation that originally predicted in 1997 [1] is an exotic rotational phenomenon in triaxially deformed nucleus with high-$j$ valence particle(s) and high-$j$ valence hole(s). Subsequently, the prediction of multiple chiral doublets (M$\chi$D) [2] provides more and more impetus for this research area.

Experimentally, the chiral doublet bands were first observed in $N = 75$ isotones [3] in 2001. From then on, the manifestations of chirality have been extensively confirmed in the mass regions of $A \sim 80, 100, 130,$ and $190$ [4–9]. More than 50 chiral candidates spread over 46 nuclei have been reported in these four mass regions so far. For details, see very recent data tables of chiral doublets bands [10]. On the aspect of M$\chi$D, the first experimental evidence was reported in $^{133}$Ce [11]. Subsequently, a novel type of M$\chi$D with identical configuration, predicted in Refs. [12–14], was observed in $^{103}$Rh [15]. Later on, the M$\chi$D with octupole correlations has been identified in $^{78}$Br [16]. Very recently, M$\chi$D were further reported in the even-even nucleus in $^{136}$Nd [17, 18] and in the $A \sim 190$ mass region in $^{195}$Tl [19].

Theoretically, the chiral symmetry breaking was firstly predicted in the particle-rotor model (PRM) and tilted axis cranking (TAC) approach [1]. Later on, numerous efforts were devoted to the development of PRM [17, 18, 20–28] and TAC methods [29–31] to describe chiral rotation in atomic nuclei. Meanwhile, the TAC plus random-phase approximation (RPA) [32], the collective Hamiltonian method [33, 34], the interacting boson-fermion-fermion model [35], and the angular momentum projection (AMP) method [36–39] were also developed to study chiral doublet bands and yielded lots of successes.

The covariant density functional theory (CDFT) takes Lorentz symmetry into account in a self-consistent way and has received wide attention due to its successful descriptions for a large number of nuclear phenomena [40–44]. Especially for nuclear rotation, the cranking CDFT was first used to investigate the superdeformed bands [45]. Subsequently, the tilted axis cranking CDFT [46–48] has successfully provided the fully self-consistent and microscopic investigation for magnetic [46–50] and antimagnetic rotations [51–53]. Recently, the three-dimensional cranking CDFT was established [54] and applied for the chiral bands in $^{106}$Rh [54] and $^{136}$Nd [55]. Based on constrained triaxial CDFT calculations, M$\chi$D phenomenon, namely more than one pair of chiral doublet bands in one single nucleus, was suggested for $^{106}$Rh in 2006 [2]. Later on, the existence of M$\chi$D phenomenon was also
suggested in $^{104,105,106,108,110}$Rh, $^{107}$Ag, $^{125,129,131}$Cs based on the triaxial deformations of the local minima and the corresponding high–j particle(s) and hole(s) configurations that obtained by constrained CDFT calculations.

As mentioned above, lots of bands with chiral rotation have been identified in the $A \geq 80$ mass regions. It is natural to examine the existence of chirality in the nuclear system with lighter mass. As a first try, we pay attentions on the $A \sim 60$ mass region and select the cobalt isotopes as possible candidates in this paper. Following the same procedures outlined in Refs. [2, 56], the possible configurations as well as their deformation parameters in the cobalt isotopes $^{54,56,57,58,59,60}$Co will be examined by the adiabatic and configuration-fixed constrained triaxial CDFT. The reason for the choice of Co isotopes is that the proton number of Co is odd with the proton already playing a role of high-$j$ ($f_{7/2}$) hole according to the Nilsson diagram [62, 63]. To establish the chiral doublet bands, one needs only search for the case that neutron plays a role of high-$j$ particle. This makes the chiral configuration become more energy favor, and easier been populated in the experiment.

The detailed formalism and numerical techniques of the adiabatic and configuration-fixed constrained CDFT calculation adopted in this work can be seen in Refs. [2, 56] and references therein. In the calculations, the point-coupling density functional PC-PK1 [61] is employed, while the pairing correlations are neglected for simplicity. The Dirac equation is solved in a set of three dimensional harmonic oscillator basis. By increasing the number of major shells from 12 to 14, the total energy changes less than 0.1% for the ground state of $^{54}$Co. Therefore, a basis of 12 major oscillator shells is adopted. In order to obtain the triaxiality of the local minima on the potential energy curve, the constrained calculations with $\langle \hat{Q}_{20}^2 + 2 \hat{Q}_{22}^2 \rangle$, i.e., the $\beta^2$, are carried out. During the $\beta^2$-constrained calculations, triaxial deformation is automatically obtained by minimizing the energy. In order to understand configurations easily, following Ref. [47], the wave functions in the Cartesian basis $\langle n_x n_y n_z m_s \rangle$ are transformed to a spherical basis with the quantum number $\langle nljm \rangle$.

Based on adiabatic constrained CDFT calculations, the occupation for the configuration of the ground states together with the deformation parameters $(\beta, \gamma)$ in nuclei $^{54–60}$Co are obtained. In Fig. 1, we show the single-particle energy levels of protons (left column) and neutrons (right column) near the Fermi surface for the ground state in nuclei $^{54–60}$Co. For the ground state, we solve the Dirac equation by filling in each step of the iteration.
FIG. 1: (Color online) Single-proton (left column) and single-neutron (right column) Routhians near the Fermi surface in $^{54-60}$Co for the ground state.

the proton and neutron levels according to their energies from the bottom of the well. As shown in Fig. 1, for the proton single-particle energy levels, there is always a hole sitting on the top of the $f_{7/2}$ shell in the ground states of the nuclei $^{54-60}$Co due to the lack of a proton with respect to the $Z = 28$ full shell. For the neutron single-particle energy levels, there is also a hole sitting on the top of the $f_{7/2}$ shell in $^{54}$Co, since its neutron number is identical as the proton number. With the increase of neutron number, the $f_{7/2}$ shell is filled and the neutron is filled gradually onto the $(fp)$ shell above $N = 28$. Meanwhile, the deformation parameter $\beta$ increases gradually from 0.12 at $^{54}$Co to 0.20 at $^{60}$Co, and also the shape changes from prolate at $^{54,56,57}$Co to triaxial at $^{58,59,60}$Co. Therefore, for these ground states, the proton has already played a role of high-$j$ hole, but there is not high-$j$ particle involved. To search for the possible high-$j$ particle-hole configurations that suitable establish chiral doublet bands, one can excite the neutron from the $(fp)$ shell to the lowest $g_{9/2}$ orbital. Such kind of the one-particle-one-hole neutron excitation leads to the valence nucleon configuration with the form of $\pi f_{7/2}^{-1} \otimes \nu [g_{9/2}^1 (fp)^n]$. 
FIG. 2: (Color online) The potential-energy curves in adiabatic (open circles) and configuration-fixed (solid lines) constrained triaxial CDFT calculation with PC-PK1 for $^{54-60}$Co. The local minima in the energy surfaces for fixed configuration are represented as stars and labeled respectively as A, B, C and D.

The potential-energy curves for $^{54,56,57,58,59,60}$Co calculated by adiabatic and configuration-fixed constrained CDFT are presented as open circles and black solid lines in Fig. 2, respectively. In comparison with the irregularities of energy curve in adiabatic constrained calculations, continuous and smooth energy curves for each configuration are yielded by the configuration-fixed constrained calculations. The obvious local minima are represented by stars and labeled by letters of the alphabet.

Two minima observed in each potential energy curve in Fig. 2, which do not have suitable high-$j$ particle-hole configurations for chirality, are labeled A and B. Here, state A represents the ground state, with prolate shape for $^{54,56,57}$Co and triaxial deformation for $^{58,59,60}$Co. The corresponding valence nucleon configuration is $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ for the ground state of $^{54}$Co and $\pi f_{7/2}^{-1} \otimes \nu(fp)^n$ ($n = 1, 2, 3, 4, 5$) for those of $^{56,57,58,59,60}$Co. The states B in $^{56,58,59,60}$Co do not have large enough triaxial deformation parameter. Although states B of $^{54}$Co and $^{57}$Co have remarkable triaxial deformation, they do not have proper high-$j$ particle-hole configurations. Hence, the states A and B are excluded in our waiting list for the chiral candidate.

By keeping always one neutron at the bottom of the $g_{9/2}$ shell and the other neutrons
FIG. 3: (Color online) The triaxiality parameter $\gamma$ (in degrees) as a function of the deformation parameter $\beta$ in adiabatic (open circles) and configuration-fixed (solid lines) constrained triaxial CDFT calculations based on the PC-PK1 interaction for $^{54-60}$Co. The local minima in the energy curves for fixed configurations are indicated by stars and labeled as A, B, C and D in accordance with the increasing of energy respectively. The shaded area represents the triaxiality parameter $\gamma$ favorable for nuclear chirality.

filling in the orbitals according to their energies, low-lying particle-hole excitation states, labeled C in Fig. 2, are obtained. The corresponding configurations are $\pi f_{7/2}^{-1} \otimes \nu [f_{7/2}^{-2} g_{9/2}^{1/2}]$ with the two $f_{7/2}$ neutrons paired for $^{54}$Co, and $\pi f_{7/2}^{-1} \otimes \nu [g_{9/2}^{1/2} (fp)^n]$ ($n = 0, 1, 2, 3, 4$) for $^{56,57,58,59,60}$Co. Similarly, the configurations $\pi f_{7/2}^{-1} \otimes \nu [g_{9/2}^{1/2} (fp)^n]$ ($n = 0, 1, 2, 3$) of $^{57,58,59,60}$Co are connected with a two-particle-two-hole neutron excitation from the $(fp)$ shell to the two lowest $g_{9/2}$ orbitals ($\nu g_{9/2}, m_x = +9/2; \nu g_{9/2}, m_x = +7/2$) (states D in Figs. 2(c)-(f)). It should be noted that the mirror configuration $\pi [f_{7/2}^{-2} g_{9/2}^{1/2}] \otimes \nu f_{7/2}^{-1}$ (state D) of state C in $^{54}$Co is obtained by keeping always one proton at the bottom of the $g_{9/2}$ shell, and the other nucleon filling the orbitals according to their energies. In the subsequent calculations with the fixed configurations of C and D, the occupations of the valence nucleons are traced by the configuration-fixed constrained calculations [2].

The obtained results are presented as blue solid lines in Figs. 2(a)-(f). In Fig. 2(a), we find that the potential energy curve with configuration C is similar to that with configuration D for $^{54}$Co. Both minima C and D in $^{54}$Co have deformation parameters $\beta$ and $\gamma$ suitable
for chirality, which are $C(\beta = 0.259, \gamma = 18.2^\circ)$ and $D(\beta = 0.259, \gamma = 17.3^\circ)$. In addition to the states $C$ and $D$ in $^{54}$Co, there are also several excited local minima with prominent triaxial deformations in $^{56,57,58,59,60}$Co. These triaxial local minima are state $C(\beta = 0.180, \gamma = 41.5^\circ)$ for $^{56}$Co, states $C(\beta = 0.199, \gamma = 24.0^\circ)$ and $D(\beta = 0.250, \gamma = 36.0^\circ)$ for $^{57}$Co, state $D(\beta = 0.251, \gamma = 15.5^\circ)$ for $^{58}$Co, state $C(\beta = 0.249, \gamma = 21.2^\circ)$ for $^{59}$Co, states $C(\beta = 0.279, \gamma = 27.0^\circ)$ and $D(\beta = 0.301, \gamma = 15.1^\circ)$ for $^{60}$Co. All these states have triaxial deformations as well as high-$j$ particle-hole configurations that suitable for establishing chiral rotation. Therefore, the existences of chiral doublets or $M_{\chi}D$ can be expected in $^{54,56,57,58,59,60}$Co.

It is worth mentioning that in Ref. [64], a dipole band with the configuration $\pi f_{7/2}^{-1} \otimes \nu[g_{9/2}(fp)^1]$ was already observed in $^{57}$Co. It is built on the $I = 13/2^+$ state with bandhead excitation energy 5.539 MeV [64]. In the CDFT calculation, the excitation energy of the configuration is 5.790 MeV, which agree reasonably with the experimental value. With the configuration and the corresponding deformation parameters ($\beta = 0.199, \gamma = 24^\circ$), the PRM [11, 15, 18, 27] calculation is performed and the obtained energy spectra in comparison with the experimental data (cascade 1 in Ref. [64]) is shown in Fig. 4. In the calculation, the moments of inertia are taken as $J_k = J_0 \sin^2(\gamma - 2k\pi/3)$ with $J_0 = 6.0 \ h^2/\text{MeV}$ and the Coriolis attenuation factor is taken as $\xi = 0.9$. It can be seen that the calculated results can reproduce reasonably the experimental yrast band, except for the data point at $I = 10.5\hbar$ (which was tentative assigned in Ref. [64]). The energy difference between the

FIG. 4: (Color online) The calculated energy spectra by particle rotor model in comparison with the experimental data in Ref. [64]. More details can be seen in the text.
calculated partner bands is about 400 keV. This value could correspond to the picture of chiral vibration motion in the low spin region of chiral doublets. Hence, it is encouraged to further search for the partner band in this nucleus from experiment.

**TABLE I: Energies (in MeV), deformation parameters $\beta$ and $\gamma$ (in degree), as well as the corresponding configurations (both valence nucleon and unpaired nucleon) of the local minima in $^{54-60}$Co obtained by the configuration-fixed constrained triaxial CDFT calculations.**

| State | Valence-cfg. | Unpaired-cfg. | Energy  | $\beta$ | $\gamma$ |
|-------|--------------|---------------|---------|---------|----------|
| $^{54}$Co | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -462.07 | 0.123 | 0.0° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -460.34 | 0.231 | 26.2° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -453.68 | 0.259 | 18.2° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -453.97 | 0.259 | 17.3° |
| $^{56}$Co | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -485.95 | 0.124 | 0.0° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -489.17 | 0.301 | 41.5° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -496.32 | 0.178 | 0.0° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -495.00 | 0.281 | 24.0° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -490.53 | 0.199 | 24.0° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -484.50 | 0.250 | 36.0° |
| $^{58}$Co | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -504.94 | 0.197 | 14.3° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -503.77 | 0.269 | 5.5° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -501.56 | 0.249 | 6.5° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -494.91 | 0.251 | 15.5° |
| $^{59}$Co | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -514.36 | 0.202 | 22.9° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -513.15 | 0.281 | 12.5° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -510.63 | 0.249 | 21.2° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -506.61 | 0.281 | 0.0° |
| $^{60}$Co | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -522.46 | 0.199 | 11.5° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -521.46 | 0.270 | 5.0° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -520.39 | 0.279 | 27.0° |
|        | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | $\pi f_{7/2}^{-1} \otimes \nu f_{7/2}^{-1}$ | -515.71 | 0.301 | 15.1° |

The triaxial deformation parameter $\gamma$ of $^{54,56,57,58,59,60}$Co as functions of deformation $\beta$ in adiabatic and configuration-fixed constrained CDFT calculations are presented as open circles and solid lines in Fig. 3, respectively. In each panel, the stars labeled by letter of alphabet correspond to the deformation of the local minima in Fig. 2, and the yellow area represents favorable triaxial deformation for chirality. In the $\beta$-$\gamma$ curves calculated
FIG. 5: (Color online) The ratio $Z/N$ of proton number and neutron number of Co isotopes are compared with those of reported chiral nuclei and $\chi D$ nuclei in the $A \sim 80, 100, 130, \text{and } 190$ mass regions. The data are from Ref. [10] and references therein.

by the adiabatic constrained calculations, the jumps marked by the dashed-lines represent energy-favorable configurations change. In contrast, the smooth $\beta$-$\gamma$ curves for the given configurations are obtained by the configuration-fixed constrained calculations. It should be noted that triaxiality in $^{54,56,57,58,59,60}\text{Co}$ favorable for nuclear chirality appears roughly at $\beta = 0.1 \sim 0.3$.

The energies, deformation parameters $\beta$ and $\gamma$ as well as the corresponding valence nucleon and unpaired nucleon configurations for the local minima in $^{54,56,57,58,59,60}\text{Co}$, obtained by the configuration-fixed constrained triaxial CDFT calculations, are summarized in Table I. Although there are no high-$j$ neutron particles for the ground state in $^{54,56,57,58,59,60}\text{Co}$, we find that the high-$j$ particle and hole configurations are available by single-particle excitations, such as for the triaxially deformed local minima C and D in $^{54}\text{Co}$, C in $^{56}\text{Co}$, C and D in $^{57}\text{Co}$, D in $^{58}\text{Co}$, C in $^{59}\text{Co}$, and C and D in $^{60}\text{Co}$. Therefore, all of these nuclei could possibly exhibit chiral rotation characters based on the above mentioned configurations. In particular, in $^{54}\text{Co}$, $^{57}\text{Co}$ and $^{60}\text{Co}$, there are two triaxially deformed states with high-$j$ particle and hole configurations. Further experimental efforts to search for $\chi D$ in these cobalt isotopes are highly encouraged.

In Fig. 5, the ratio $Z/N$ of proton number and neutron number of Co isotopes are compared with those of reported chiral nuclei and $\chi D$ nuclei in the $A \sim 80, 100, 130, \text{and } 190$ mass regions. The data are from Ref. [10] and references therein. It can be found that
the $Z/N$ ratios of the reported chiral and $M_{\chi D}$ nuclei in the $A \sim 80, 100, 130$, and $190$ mass regions locate around the region from 0.65 to 0.85. For the Co isotopes, the ratio is from $\sim 0.80$ in $^{60}\text{Co}$ to 1.00 in $^{54}\text{Co}$. This is a unique feature in the Co isotopes, and provides the possibility that existence of $M_{\chi D}$ with mirror configuration as in $^{54}\text{Co}$. If the $M_{\chi D}$ was successfully identified in the experiment, it provides a promising example to investigate the neutron proton interactions in the chiral doublet bands.

In summary, the possible existence of chiral or multiple chiral doublets ($M_{\chi D}$) in cobalt isotopes are investigated by the adiabatic and configuration-fixed constrained CDFT approaches. The potential-energy curves and triaxial deformation parameters $\gamma$ as functions of the deformation parameter $\beta$ in $^{54,56,57,58,59,60}\text{Co}$ are obtained. Serval local energy minima with prominent triaxial deformations are found in these cobalt isotopes. According to the transformed quantum numbers $\langle nljm \rangle$, the configurations of these triaxially deformed minima are specified. It is found that the configurations $\pi f_{7/2}^{-1} \otimes \nu[g_{9/2}^{m}(fp)^{n}]$ ($m = 1$ or 2) are available for the triaxially deformed local minima in all of these isotopes. For $^{54}\text{Co}$, there are mirror configurations with $\pi[f_{7/2}^{-2}g_{9/2}^{1}] \otimes f_{7/2}^{-1}$ and $\pi f_{7/2}^{-1} \otimes [f_{7/2}^{-2}g_{9/2}^{1}]$, and both states are of the triaxiality. Based on the triaxial deformation and the corresponding high-$j$ particle and hole configurations, there could exist chiral rotation characters in $^{54,56,57,58,59,60}\text{Co}$ and $M_{\chi D}$ in $^{54,57,60}\text{Co}$. Hence, the present investigation provides not only the prediction of chirality and $M_{\chi D}$ in $A \sim 60$ mass region, but also presents an experimental opportunity for the observation of chirality in this mass region.

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