General formalism of collective motion for any deformed system

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Based on Bohr model, I have presented a general formalism describing the collective motion for any deformed system, in which the collective Hamiltonian is expressed as vibrations in the body-fixed frame, rotation of whole system around the laboratory frame, and coupling between vibrations and rotation. Under the condition of decoupling approximation, I have derived the quantized Hamiltonian operator. Based on the operator, I have calculated the rotational spectra for some special octupole and hexadecapole deformed systems and shown their dependencies on deformation. The result indicates that the contribution of octupole or hexadecapole deformations to the lowest band is regular, while that to higher bands is dramatic. These features reflecting octupole and hexadecapole deformations are helpful in recognizing the properties of real nuclei with octupole and/or hexadecapole deformations coexisting with quadrupole deformations.

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I. INTRODUCTION

The theory of collective motion was developed a long time ago. The classical case corresponds to the quadruple deformations, which was established by Bohr in 1952 [1,2]. The Bohr Hamiltonian is very useful in describing the vibrations and rotation for quadruple deformed nuclei. Especially for the shape evolution and phase transitions [3], the Bohr Hamiltonian is a powerful tool for investigating the critical-point symmetries like E(5) [4], X(5) [5], Y(5) [6], and Z(5) [7]. More research on the collective motion by Bohr model can be found in the literature [8–10] and references therein. Several recent advances include the Bohr Hamiltonian solved with a mass- and deformation-dependent Kratzer potential [11], an approximate analytical formula for the energy spectrum for a prolate γ-rigid collective Hamiltonian with a harmonic oscillator potential corrected by a sextic term [12], and an analytical solution of the Davydov-Chaban Hamiltonian with a sextic potential for $\gamma = 30^\circ$ and its satisfactory description for the shape phase transition in Xe isotopes in comparison with experiment [13].

The Bohr Hamiltonian is applicable to nuclei with quadruple deformations. Although the quadruple deformations are the most frequently encountered in real nuclei, the higher multipolar deformations are also essential for satisfactory description of nuclear properties. The description of octupole deformations has been a long-standing problem in nuclear physics [14]. Theoretical calculations [15,16] predicted the existence of octupole stable deformations and this problem stirred considerable interest, especially in the Ce-Ba and the Rn-Th regions. The level scheme of a few moderately or weakly deformed nuclei, such as ^{64}Ge [17], ^{148}Sm [18], or ^{233,235}Ra [19] presents features that may be related to octupole instabilities and softness of the nucleus with respect to possible exotic octupole deformations. There has been evidence for the existence of stable octupole deformations in the Rn-Th region [20,21]. For example, the existence of stable octupole deformations in ^{224}Ra has been verified in a recent experiment [22]. Furthermore, in the region $N = 92,94$, octupole correlations were observed in ^{150,152}Ce isotopes [23,24].

These examples show that there exist certainly the octupole deformations and/or correlations in certain regions. For the study of collective motion involving octupole deformations, the generalization of the Bohr Hamiltonian was explored in Ref. [25]. Its application to the problem of octupole vibrations in nuclei was elaborated in the review [26]. The vibrational and rotational spectra obtained by the model reproduce well the experimental data for some rare-earth and actinide nuclei [27,28]. In Refs. [29,30], the analytic solutions of the Bohr Hamiltonian involving axially symmetric quadrupole and octupole deformations with an infinite well potential or Davidson potential were obtained, and normalized spectra and B(EL) ratios were found to agree with experimental data for ^{226}Ra and ^{226}Th. Here, B(EL) is the reduced transition rates, its definition is given by Eq. (20) in Ref. [29]. Because it is difficult to determine the intrinsic frame, the parametrizations of octupole deformations were probed in Refs. [26,31–33]. Moreover, an alternative parametrization describing nuclear quadruple and octupole deformations was introduced in Ref. [34], and the transitional nuclei ^{224,226}Ra, ^{224}Th, and X(5) nuclei ^{150}Nd, ^{152}Sm were studied with satisfactory results in comparison with experiment [35,36]. Based on this model, the stable octupole deformed nucleus ^{224}Ra was well described in Ref. [37]. More research on the octupole deformations and correlations can be found in Ref. [38] and references therein.

Besides the quadruple and octupole deformations, the hexadecapole deformations are also necessary for the understanding of equilibrium shapes and the fission process of super- and hyperdeformed nuclei [39,40]. Observations of the $\Delta I = 4$ bifurcation (also called $\Delta I = 2$ staggering) phenomenon in superdeformation bands [41–46] have aroused great enthusiasm for the study of hexadecapole deformations. Many efforts have been devoted to the subject, with possible explanations given in terms of the presence of a tetrahedral symmetry [47–50] and the absence of any tetrahedral symmetry [51–60]. The parametrization of hexadecapole deformations has been discussed in Refs. [61–63].

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In real nuclei, hexadecapole deformations always coexists with quadrupole deformations. Therefore, it is natural to take the quadrupole and hexadecapole degrees of freedom simultaneously into account [64], especially in relation to the possible appearance of intrinsic shapes with tetrahedral or octahedral symmetry. The tetrahedral and octahedral shapes have been predicted by the realistic mean-field calculations [65,66]; their experimental identification in medium- and heavy-mass nuclei is an open problem of current interest. Recently, the tetrahedral symmetry has been found in the light nucleus ^{16}O [67].

From the preceding analysis, it is evident that the quadrupole, octupole, and hexadecapole deformations have occurred in real nuclei and produced significant effects to nuclear properties. Hence, it is interesting to discuss the collective motion for any deformed system. In the paper, I present a general formalism describing the collective motion for any deformed system. First, I give the classical Hamiltonian of collective motion in a laboratory system, then transform it into a body-fixed frame to separate vibrations, rotation, and the coupling between them. Under the condition of decoupling approximation, I derive the quantized Hamiltonian operator. As examples, I calculate the rotational spectra for some special octupole and hexadecapole deformed systems and analyze the properties of rotational spectra and their dependence on deformation.

II. THE CLASSICAL THEORY OF COLLECTIVE MOTION FOR ANY DEFORMED SYSTEM

To describe the collective motion for any deformed system, one can expand the surface radius of the system as

$$R(\vartheta,\varphi) = R_0\left[1 + \sum_{lm} \alpha_{lm} Y_{lm}(\vartheta,\varphi)\right], \tag{1}$$

where α_{lm} represents the deformations deviating from the spherical shape in the laboratory frame with the relation $\alpha^*_{lm} = (-)^m \alpha_{l,-m}$ and R_0 is the equilibrium radius. When α_{lm} are regarded as variables, the Hamiltonian describing collective motion is obtained as

$$H = T + V, \tag{2}$$

where the kinetic energy is expressed as

$$T = \frac{1}{2}\sum_{lm} B_l |\dot{\alpha}_{lm}|^2, \tag{3}$$

and the potential energy takes the form

$$V = \frac{1}{2}\sum_{lm} C_l |\alpha_{lm}|^2. \tag{4}$$

Here B_l and C_l are respectively the parameters reflecting the vibrational strength and the elastic coefficient against deformation. In the Hamiltonian H, vibrations and rotation are entangled together. It is difficult to study collective motion by using this H. To separate vibrations and rotation from H, it is necessary to transform the variables in the collective Hamiltonian from the laboratory frame (K system) to a body-fixed frame (K' system) by rotation, which is defined by

$$R(\theta_i) = e^{-i\theta_2 J_3} e^{-i\theta_1 J_2} e^{-i\theta_3 J_3}, \tag{5}$$

where J_1, J_2, and J_3 are the angular momenta along the fixed coordinate axes (K system) and $\theta_i = (\theta_1,\theta_2,\theta_3)$ are the Euler angles characterizing the orientation of K' with respect to a fixed frame of reference K. Through the rotation, the variables α_{lm} in the K system can be transformed into the K' system as

$$\alpha_{lm} = \sum_{m'} D^l_{mm'} \beta_{lm'}, \tag{6}$$

where β_{lm} are the deformation variables in the body-fixed frame, and $D^l_{mm'}(\theta_i)$ are the Wigner function of θ_i. In $D^l_{mm'}(\theta_i)$, l is the angular-momentum quantum number and m and m' are the projections of angular momentum on the laboratory fixed z axis and the body-fixed z' axis, respectively:

$$D^l_{mm'}(\theta_i) = \langle lm| e^{-i\theta_2 J_3} e^{-i\theta_1 J_2} e^{-i\theta_3 J_3} |lm'\rangle. \tag{7}$$

To present the collective Hamiltonian using the variables (β_{lm},θ_i), one can calculate the time derivative of α_{lm} as

$$\dot{\alpha}_{lm} = \sum_{m'} \left[D^l_{mm'}(\theta_i)\dot{\beta}_{lm'} + \dot{D}^l_{mm'}(\theta_i)\beta_{lm'}\right], \tag{8}$$

where the time derivative of $D^l_{mm'}(\theta_i)$ is presented as

$$\dot{D}^l_{mm'}(\theta_i) = -i\sum_k D^l_{mk}(\theta_i)\langle lk|\vec{\omega}\cdot\vec{J}|lm'\rangle. \tag{9}$$

In Eq. (9),

$$\begin{aligned}
\omega_1 &= \dot{\theta}_1 \sin\theta_3 - \dot{\theta}_2 \sin\theta_1 \cos\theta_3,\\
\omega_2 &= \dot{\theta}_1 \cos\theta_3 + \dot{\theta}_2 \sin\theta_1 \sin\theta_3,\\
\omega_3 &= \dot{\theta}_3 + \dot{\theta}_2 \cos\theta_1,
\end{aligned} \tag{10}$$

are angular velocities around the axes coincide with the body (K' system). Putting $\dot{\alpha}_{lm}$ into Eq. (3), the kinetic energy splits into three parts. The first part is quadratic in $\dot{\beta}_{lm}$ and represents vibrations by which the body changes its shape, but retains its orientation. The second part, quadratic in $\dot{\theta}_i$, represents the rotation of the body without change of shape. The third part contains the mixed time derivatives $\dot{\beta}_{lm}\cdot\dot{\theta}_i$, as can be shown from simple properties of the $D^l_{mm'}$ functions and their derivatives. One can thus write

$$T = T_{\rm vib} + T_{\rm rot} + T_{\rm cou}. \tag{11}$$

In Eq. (11), the vibrational energy

$$T_{\rm vib} = \frac{1}{2}\sum_{lm} B_l |\dot{\beta}_{lm}|^2, \tag{12}$$

the rotational energy

$$T_{\rm rot} = \frac{1}{2}\sum_{i,j} \mathscr{J}_{ij}\omega_i\omega_j, \tag{13}$$

with the moments of inertia

$$\mathscr{J}_{ij} = \frac{1}{2}\sum_{lmm'} B_l \langle lm'|\{J_i, J_j\}|lm\rangle \beta_{lm}\beta^*_{lm'}, \tag{14}$$

and the coupling between vibrations and rotation

$$T_{\text{cou}} = \sum_i \omega_i \kappa_i, \tag{15}$$

with

$$\kappa_i = -\text{Im} \sum_{lmm'} B_l \langle lm'|J_i|lm\rangle \dot{\beta}_{lm} \beta^*_{lm'}. \tag{16}$$

Here the internal variables β_{lm} are of complex number. For simplicity, I introduce a set of real parameters a_{lm} and b_{lm} to describe the deformations as follows:

$$\sum_{l,m} \beta_{lm} Y_{lm}(\theta,\phi) = \sum_l a_{l0} Y_{l0}(\theta,\phi) + \sum_{l,m>0} \left[a_{lm} Y^{(+)}_{lm}(\theta,\phi) + b_{lm} Y^{(-)}_{lm}(\theta,\phi)\right]. \tag{17}$$

Here the spherical harmonics

$$Y^{(+)}_{lm}(\theta,\phi) = \frac{1}{\sqrt{2}}[Y_{lm}(\theta,\phi) + Y^*_{lm}(\theta,\phi)],$$
$$Y^{(-)}_{lm}(\theta,\phi) = \frac{1}{i\sqrt{2}}[Y_{lm}(\theta,\phi) - Y^*_{lm}(\theta,\phi)]. \tag{18}$$

From Eq. (17), one obtains

$$\beta_{l0} = a_{l0}, \quad \beta_{l,m} = \frac{a_{lm} - i b_{lm}}{\sqrt{2}}, \quad \beta_{l,-m} = (-1)^m \frac{a_{lm} + i b_{lm}}{\sqrt{2}}, \tag{19}$$

where $m = 1,2,3,\ldots,l$. Then the kinetic energy of vibrations in the body-fixed frame becomes

$$T_{\text{vib}} = \frac{1}{2}\sum_l B_l \left[\dot{a}^2_{l0} + \sum_{m>0}\left(\dot{a}^2_{lm} + \dot{b}^2_{lm}\right)\right]. \tag{20}$$

I use the relations

$$J_\pm|lm\rangle = \sqrt{(l\mp m)(l\pm m+1)}|l\, m\pm 1\rangle,$$
$$J_3|lm\rangle = m|lm\rangle, \tag{21}$$

where $J_\pm = J_1 \pm i J_2$. κ_i and $\mathscr{J}_{ij}$ are expressed as the functions of the real variables a_{lm} and b_{lm} as

$$\kappa_1 = \frac{1}{2}\sum_l B_l \Bigg\{-\sqrt{2l(l+1)}\dot{a}_{l0} b_{l1} + \sum_{m>0} o^l_m(-\dot{a}_{lm} b_{lm+1} + \dot{b}_{lm} a_{lm+1}) + \sum_{m>0} o^l_{-m}(-\dot{a}_{lm} b_{lm-1} + \dot{b}_{lm} a_{lm-1})\Bigg\}, \tag{22}$$

$$\kappa_2 = \frac{1}{2}\sum_l B_l \Bigg\{\sqrt{2l(l+1)}\dot{a}_{l0} a_{l1} + \sum_{m>0} o^l_m(\dot{a}_{lm} a_{lm+1} + \dot{b}_{lm} b_{lm+1}) - \sum_{m>0} o^l_{-m}(\dot{a}_{lm} a_{lm-1} + \dot{b}_{lm} b_{lm-1})\Bigg\}, \tag{23}$$

$$\kappa_3 = \sum_{l,m>0} B_l m(a_{lm}\dot{b}_{lm} - \dot{a}_{lm} b_{lm}), \tag{24}$$

$$\mathscr{J}_{11} = \frac{1}{4}\sum_l B_l \Bigg\{2l(l+1)a^2_{l0} + \sqrt{2l(l^2-1)(l+2)}a_{l0}a_{l2} + 2\sum_{m>0}[l(l+1)-m^2]\left(a^2_{lm}+b^2_{lm}\right) + \sum_{m>0} o^l_m o^l_{m+1}(a_{lm}a_{lm+2} + b_{lm}b_{lm+2}) + \sum_{m>0} o^l_{-m} o^l_{-m+1}(a_{lm}a_{lm-2} + b_{lm}b_{lm-2})\Bigg\}, \tag{25}$$

$$\mathscr{J}_{22} = \frac{1}{4}\sum_l B_l \Bigg\{2l(l+1)a^2_{l0} - \sqrt{2l(l^2-1)(l+2)}a_{l0}a_{l2} + 2\sum_{m>0}[l(l+1)-m^2]\left(a^2_{lm}+b^2_{lm}\right) - \sum_{m>0} o^l_m o^l_{m+1}(a_{lm}a_{lm+2} + b_{lm}b_{lm+2}) - \sum_{m>0} o^l_{-m} o^l_{-m+1}(a_{lm}a_{lm-2} + b_{lm}b_{lm-2})\Bigg\}, \tag{26}$$

$$J_{33} = \sum_{l,m>0} B_l m^2\left(a^2_{lm} + b^2_{lm}\right), \tag{27}$$

$$\mathscr{J}_{12} = \frac{1}{4}\sum_l B_l \Bigg\{\sqrt{2l(l^2-1)(l+2)}a_{l0}b_{l2} + \sum_{m>0} o^l_m o^l_{m+1}(a_{lm}b_{lm+2} - b_{lm}a_{lm+2}) - \sum_{m>0} o^l_{-m} o^l_{-m+1}(a_{lm}b_{lm-2} - b_{lm}a_{lm-2})\Bigg\}, \tag{28}$$

$$\mathscr{J}_{13} = \frac{1}{4}\sum_l B_l \Bigg\{\sqrt{2l(l+1)}a_{l0}a_{l1} + \sum_{m>0}(2m+1)o^l_m(a_{lm}a_{lm+1} + b_{lm}b_{lm+1}) + \sum_{m>0}(2m-1)o^l_{-m}(a_{lm}a_{lm-1} + b_{lm}b_{lm-1})\Bigg\}, \tag{29}$$

$$\mathscr{J}_{23} = \frac{1}{4}\sum_l B_l \Bigg\{\sqrt{2l(l+1)}a_{l0}b_{l1} + \sum_{m>0}(2m+1)o^l_m(a_{lm}b_{lm+1} - b_{lm}a_{lm+1}) - \sum_{m>0}(2m-1)o^l_{-m}(a_{lm}b_{lm-1} - b_{lm}a_{lm-1})\Bigg\}, \tag{30}$$

where

$$o^l_m = \sqrt{(l-m)(l+m+1)}, \tag{31}$$

and the moments of inertia are real symmetrical: $\mathscr{J}_{ij} = \mathscr{J}_{ji}$. These formulas have presented a general formalism describing the collective motion for any deformed system, where the collective motion is treated as vibrations in the body-fixed frame (a_{lm} and b_{lm} vibrations), rotation of whole system about the axes of laboratory system, and the coupling between vibrations and rotation.

The general formalism can be applied to describe the collective motion of a classical system with any deformation. However, it should be noticed that the variables a_{lm} and b_{lm} are not independent of each other. Three of them have been replaced by the Euler angles. How to remove the three superfluous variables is a problem. For the octupole and higher multipolar deformed systems, the problem could be solved in many ways, too many to have an obvious and natural definition of the body-fixed frame.

Some progress has been achieved for octupole deformed systems. The surface radius expressed by the parameters a_{3m} and b_{3m} was reparametrized by a set of biharmonic coordinates [26,31]. In the parametrizations, the system obeys relatively simple transformation rules under the O_h group. Similar parametrization was finished in Ref. [32], where the intrinsic frame was defined with four independent variables, which is a simple combination of a_{3m} and b_{3m}. To remove the off-diagonal elements of inertia tensor, in Ref. [33], the intrinsic frame was defined by the variables (X,Y,Z,γ). In comparison with the present formalism, there exist the following relations:

$$\begin{aligned}
\beta_{33} &= \frac{1}{\sqrt{2}}a_{33} - i\frac{1}{\sqrt{2}}b_{33} \\
&= \left(\cos\gamma - \frac{\sqrt{3}}{2}\sin\gamma\right)X + i\left(\cos\gamma + \frac{\sqrt{3}}{2}\sin\gamma\right)Y, \\
\beta_{32} &= \frac{1}{\sqrt{2}}a_{32} - i\frac{1}{\sqrt{2}}b_{32} = \frac{1}{\sqrt{2}}\sin\gamma Z, \\
\beta_{31} &= \frac{1}{\sqrt{2}}a_{31} - i\frac{1}{\sqrt{2}}b_{31} = \frac{\sqrt{5}}{2}\sin\gamma X + i\frac{\sqrt{5}}{2}\sin\gamma Y, \\
\beta_{30} &= a_{30} = \sqrt{5}\cos\gamma Z.
\end{aligned} \tag{32}$$

Namely,

$$\begin{aligned}
a_{33} &= (\sqrt{2}\cos\gamma - \sqrt{3/2}\sin\gamma)X, \\
b_{33} &= -(\sqrt{2}\cos\gamma + \sqrt{3/2}\sin\gamma)Y, \\
a_{32} &= \sin\gamma Z, \\
b_{32} &= 0, \\
a_{31} &= \sqrt{5/2}\sin\gamma X, \\
b_{31} &= -\sqrt{5/2}\sin\gamma Y, \\
a_{30} &= \sqrt{5}\cos\gamma Z.
\end{aligned} \tag{33}$$

Putting Eqs. (33) into Eqs. (25)–(30), for a pure octupole deformed system, one can obtain $J_{12} = J_{13} = J_{23} = 0$, and J_{11}, J_{22}, and J_{33} fitting the results in Ref. [33]. For example,

$$\begin{aligned}
J_{12} &= 2\sqrt{15}a_{30}b_{32} - 6a_{31}b_{31} + \sqrt{15}a_{31}b_{33} - \sqrt{15}a_{33}b_{31} \\
&= -6\left(\sqrt{\frac{5}{2}}\sin\gamma X\right)\left(-\sqrt{\frac{5}{2}}\sin\gamma Y\right) \\
&\quad + \sqrt{15}\left(\sqrt{\frac{5}{2}}\sin\gamma X\right)\left(-\sqrt{2}\cos\gamma - \sqrt{\frac{3}{2}}\sin\gamma\right)Y \\
&\quad - \sqrt{15}\left(\sqrt{2}\cos\gamma - \sqrt{\frac{3}{2}}\sin\gamma\right)X\left(-\sqrt{\frac{5}{2}}\sin\gamma Y\right) = 0.
\end{aligned} \tag{34}$$

Similarly, one can also reproduce the inertia tensor in Refs. [29,34,38] by a correct replacement of deformation parameters in the present formalism.

From these discussions, I have shown that there are simple relations between the parameters in Refs. [26,31–33] and (a_{lm},b_{lm}) in the present formalism. Hence, the results in these references [26,31–33] can be obtained by the present formalism. Particularly, the present formalism is appropriate to describe the collective motion for not only the systems defined in Refs. [26,31–33], but also those with other deformations, which is useful in investigating the atomic nuclei with some special deformations.

In real nuclei, octupole deformations always coexist with quadrupole deformations. Many studies [15,25,27–30,33–38] have been performed for the system with the coexistence of quadrupole and octupole deformations. The present formalism is convenient for describing the coexistence of quadrupole and octupole deformations. When the parameters including the coexistence of quadrupole and octupole deformations are defined properly, the Hamiltonian in Refs. [15,25,27–30,33–38] can be obtained using the present formalism.

Similarly, hexadecapole deformations always coexist with quadrupole deformations in real nuclei. Many studies have been performed for the collective motion for hexadecapole deformations coexisting with quadrupole deformations [64]. Especially for the nuclei with tetrahedral and octahedral shapes, which have been predicted by the realistic mean-field method [65,66] and verified in a recent experiment [67], the present formalism is convenient for taking the quadrupole and hexadecapole degrees of freedom simultaneously into account. When a_{lm} and b_{lm} are reparametrized according to the scheme in Refs. [65,66], the nuclei with tetrahedral and octahedral shapes can be studied by the present formalism. In addition, the pure hexadecapole deformations are also concerned. In Refs. [61–63], the parametrization of pure hexadecapole deformations has been discussed, and the surface radius of the system is represented as

$$R(\theta,\phi) = R_0\left\{1 + a_{40}Y_{40}(\theta,\phi) + \sum_{\mu>0}\left[a_{4\mu}Y_{4\mu}^{(+)}(\theta,\phi) + b_{4\mu}Y_{4\mu}^{(-)}(\theta,\phi)\right]\right\}. \tag{35}$$

Here the definitions of $Y_{\lambda\mu}^{(+)}(\theta,\phi)$ and $Y_{\lambda\mu}^{(-)}(\theta,\phi)$ are the same as those in Eqs. (18). It shows that the parameters $(a_{40},a_{4\mu},b_{4\mu},\mu = 1,2,3,4)$ are just some special sampling of (a_{lm} and b_{lm}). To make the system obey relatively simple transformation rules under the O_h group, this set of parameters $(a_{40},a_{4\mu},b_{4\mu})$ has been reparametrized with a set of biharmonic coordinates. Because there exists a simple relationship between these biharmonic coordinates and $(a_{40},a_{4\mu},b_{4\mu})$, it is easy to give out these results in Refs. [61–63] using the present formalism. The present formalism is appropriate for any deformed system including those defined in Refs. [61–63,65,66] and can be used to explore the collective motion for the system with special shape.

The preceding formalism is suitable for a classical system. To describe the collective motion of a quantum system like atomic nucleus, it is necessary to quantize the collective Hamiltonian. In the following, I derive the quantized Hamiltonian for the collective motion with any deformation.

III. QUANTIZATION OF THE CLASSICAL HAMILTONIAN

Considering that the internal variables a_{lm} and b_{lm} in the present formalism are not independent, one needs to remove three superfluous variables among a_{lm} and b_{lm} to quantify the collective Hamiltonian. For a quadruple deformed system, one can regard a_{21}, b_{21}, and b_{22} as superfluous variables. When a_{21}, b_{21}, and b_{22} are removed, $T_{\rm cou}$ disappears, Bohr Hamiltonian can be obtained conveniently by a simple quantization procedure. For any deformed system, it is difficult for us to pick out three superfluous variables to remove $T_{\rm cou}$. Even an octupole deformed system, a set of internal parameters that make $T_{\rm cou}$ disappear is not still found up to now. Here I adopt an approximate method to eliminate $T_{\rm cou}$ by freezing a part of deformation parameters. From Eqs. (22)–(24), one can see, to make $T_{\rm cou}$ disappear, there are many choices of freezing deformation parameters. In the case of freezing the least deformation parameters, the most appropriate choice of freezing deformation parameters is that $a_{l0}, a_{l2}, a_{l4}, \ldots, a_{l,l\,\text{or}\,l-1}$ are reserved and the rest are removed. Then the kinetic energy becomes

$$\begin{aligned} T &= \tfrac{1}{2}B_2\left(\dot a_{20}^2+\dot a_{22}^2\right)+\tfrac{1}{2}B_3\left(\dot a_{30}^2+\dot a_{32}^2\right)\\ &\quad+\tfrac{1}{2}B_4\left(\dot a_{40}^2+\dot a_{42}^2+\dot a_{44}^2\right)+\cdots\\ &\quad+\tfrac{1}{2}\left(\mathscr{J}_1\omega_1^2+\mathscr{J}_2\omega_2^2+\mathscr{J}_3\omega_3^2\right), \end{aligned} \tag{36}$$

with the moments of inertia

$$\begin{aligned} \mathscr{J}_1 &= \frac{1}{4}\sum_l B_l\Bigg\{2l(l+1)a_{l0}^2+\sqrt{2l(l^2-1)(l+2)}a_{l0}a_{l2}\\ &\quad+\sum_{m=2,4}^{l\,\text{or}\,l-1}\left(o_m^l o_{m+1}^l a_{lm}a_{lm+2}+o_{-m}^l o_{-m+1}^l a_{lm}a_{lm-2}\right)\\ &\quad+2\sum_{m=2,4}^{l\,\text{or}\,l-1}[l(l+1)-m^2]a_{lm}^2\Bigg\}, \end{aligned} \tag{37}$$

$$\begin{aligned} \mathscr{J}_2 &= \frac{1}{4}\sum_l B_l\Bigg\{2l(l+1)a_{l0}^2-\sqrt{2l(l^2-1)(l+2)}a_{l0}a_{l2}\\ &\quad-\sum_{m=2,4}^{l\,\text{or}\,l-1}\left(o_m^l o_{m+1}^l a_{lm}a_{l,m+2}+o_{-m}^l o_{-m+1}^l a_{lm}a_{l,m-2}\right)\\ &\quad+2\sum_{m=2,4}^{l\,\text{or}\,l-1}[l(l+1)-m^2]a_{lm}^2\Bigg\}, \end{aligned} \tag{38}$$

$$\mathscr{J}_3 = \sum_l B_l \sum_{m=2,4}^{l\,\text{or}\,l-1} m^2 a_{lm}^2. \tag{39}$$

To obtain a quantized Hamiltonian, one can write the kinetic energy as

$$T = \tfrac{1}{2}g_{ij}\dot q_i \dot q_j, \tag{40}$$

where $q_i = a_{20}, a_{22}, a_{30}, a_{32}, a_{40}, a_{42}, a_{44}, \ldots, \phi_1, \phi_2, \phi_3$. The metric matrix G is diagonal, i.e.,

$$G = [B_2 \quad B_2 \quad B_3 \quad B_3 \quad \cdots \quad \mathscr{J}_1 \quad \mathscr{J}_2 \quad \mathscr{J}_3], \tag{41}$$

and its determinant

$$g = \det G = B_2^2 B_3^2 \cdots \mathscr{J}_1\mathscr{J}_2\mathscr{J}_3. \tag{42}$$

Because G is diagonal, G^{-1} can be calculated easily. By using a usual quantized procedure, the quantized kinetic operator is obtained as

$$\begin{aligned} T &= -\frac{\hbar^2}{2}\frac{1}{\sqrt{g}}\frac{\partial}{\partial q_i}G_{ij}^{-1}\sqrt{g}\frac{\partial}{\partial q_j}\\ &= -\frac{\hbar^2}{2B_i}\frac{1}{\sqrt{\mathscr{J}_1\mathscr{J}_2\mathscr{J}_3}}\frac{\partial}{\partial q_i}\sqrt{\mathscr{J}_1\mathscr{J}_2\mathscr{J}_3}\frac{\partial}{\partial q_i}+\sum_{i=1}^{3}\frac{R_i^2}{2\mathscr{J}_i}, \end{aligned} \tag{43}$$

where $q_i = a_{20}, a_{22}, a_{30}, a_{32}, a_{40}, a_{42}, a_{44}, \ldots$, and $R_i = -i\hbar\frac{\partial}{\partial\phi_i}$ $(i = 1,2,3)$ are the components of angular momentum in the intrinsic frame. In the kinetic energy operator, the rotational part has been separated. If the only quadruple, octupole, and hexadecapole deformations are considered, with the transformations

$$\begin{aligned} a_{20} &= \beta_2\cos\gamma_2,\\ a_{22} &= \beta_2\sin\gamma_2,\\ a_{30} &= \beta_3\cos\gamma_3,\\ a_{32} &= \beta_3\sin\gamma_3,\\ a_{40} &= \beta_4\cos\gamma_4,\\ a_{42} &= \beta_4\cos\delta_4\sin\gamma_4,\\ a_{44} &= \beta_4\sin\delta_4\sin\gamma_4, \end{aligned} \tag{44}$$

the quantized kinetic operator in the curve coordinates is obtained.

For a pure quadruple deformed system, one obtains immediately

$$\begin{aligned} T_2 &= -\frac{\hbar^2}{2B_2}\left(\frac{1}{\beta_2^4}\frac{\partial}{\partial\beta_2}\beta_2^4\frac{\partial}{\partial\beta_2}+\frac{1}{\beta_2^2\sin 3\gamma_2}\frac{\partial}{\partial\gamma_2}\sin 3\gamma_2\frac{\partial}{\partial\gamma_2}\right)\\ &\quad+\sum_{i=1}^{3}\frac{R_i^2}{2\mathscr{J}_i}, \end{aligned} \tag{45}$$

with

$$\mathscr{J}_i = 4B_2\beta_2^2\sin^2\left(\gamma_2 - i\frac{2\pi}{3}\right), \quad (i = 1,2,3). \tag{46}$$

T_2 is the kinetic energy operator in Bohr Hamiltonian.

For a pure octuple deformed system, one obtains

$$T_3 = -\frac{\hbar^2}{2B_3}\left[\frac{1}{\beta_3^4}\frac{\partial}{\partial\beta_3}\beta_3^4\frac{\partial}{\partial\beta_3} + \frac{1}{\beta_3^2 w(\gamma_3)}\frac{\partial}{\partial\gamma_3}w(\gamma_3)\frac{\partial}{\partial\gamma_3}\right] + \sum_{i=1}^{3}\frac{R_i^2}{2\mathscr{J}_i}, \tag{47}$$

with

$$w(\gamma_3) = \sin\gamma_3\sqrt{9 - 21\sin^2\gamma_3 + 16\sin^4\gamma_3}, \tag{48}$$

and the moments of inertia,

$$\begin{aligned}\mathscr{J}_1 &= B_3\beta_3^2[1 + 8\sin^2(\gamma_3 + \gamma_0)],\\ \mathscr{J}_2 &= B_3\beta_3^2[1 + 8\sin^2(\gamma_3 - \gamma_0)],\\ \mathscr{J}_3 &= 4B_3\beta_3^2\sin^2\gamma_3,\end{aligned} \tag{49}$$

where $\gamma_0 = \arctan\sqrt{5/3}$.

For a pure hexadecapole deformed system, one obtains

$$\begin{aligned}T_4 = -\frac{\hbar^2}{2B_4}\bigg[&\frac{1}{\beta_4^5}\frac{\partial}{\partial\beta_4}\beta_4^5\frac{\partial}{\partial\beta_4}\\ &+\frac{1}{\beta_4^2\sin\gamma_4 w(\gamma_4,\delta_4)}\frac{\partial}{\partial\gamma_4}\sin\gamma_4 w(\gamma_4,\delta_4)\frac{\partial}{\partial\gamma_4}\\ &+\frac{1}{\beta_4^2\sin^2\gamma_4 w(\gamma_4,\delta_4)}\frac{\partial}{\partial\delta_4}w(\gamma_4,\delta_4)\frac{\partial}{\partial\delta_4}\bigg] + \sum_{i=1}^{3}\frac{R_i^2}{2\mathscr{J}_i},\end{aligned} \tag{50}$$

with

$$w(\gamma_4,\delta_4) = \sqrt{\mathscr{J}_1'\mathscr{J}_2'\mathscr{J}_3'}, \tag{51}$$

and the moments of inertia

$$\mathscr{J}_i = B_4\beta_4^2\mathscr{J}_i', \quad (i = 1,2,3). \tag{52}$$

Here

$$\begin{aligned}\mathscr{J}_1' &= 10 + 3\sqrt{5}\cos\delta_4\sin 2\gamma_4\\ &\quad+(3\cos 2\delta_4 + \sqrt{7}\sin 2\delta_4 - 5)\sin^2\gamma_4,\\ \mathscr{J}_2' &= 10 - 3\sqrt{5}\cos\delta_4\sin 2\gamma_4\\ &\quad+(3\cos 2\delta_4 + \sqrt{7}\sin 2\delta_4 - 5)\sin^2\gamma_4,\\ \mathscr{J}_3' &= (\cos^2\delta_4 + 4\sin^2\delta_4)\sin^2\gamma_4.\end{aligned} \tag{53}$$

From Eq. (45), one can notice that the fourth power of β_2 appears in the first term of the kinetic energy. The same case also appears in Eq. (47) for β_3. Different from Eqs. (45) and (47), the fifth power of β_4 appears in the first term of the kinetic energy. This is because the power of $\beta_i (i = 2,3,4)$ appearing in the first term of the kinetic energy depends on the number of degrees of freedom. For T_2 and T_3, only two deformation variables (a_{20},a_{22}) and (a_{30},a_{32}) are taken into account, while for T_4, three deformation variables (a_{40},a_{42},a_{44}) are taken into account.

IV. THE ROTATIONAL SPECTRA FOR SOME SPECIAL DEFORMED SYSTEMS

In the preceding section, I have derived the quantized kinetic operator for multipolar deformed systems, including the quadruple, octupole, and hexadecapole deformed systems. When the potential against deformation is included, the quantized Hamiltonian operator describing multipolar deformed system is obtained. The Hamiltonian can be used to study the collective motion of a quantum system with multipolar deformations. As the Hamiltonian is complicated, here I do not discuss in detail the solution of the general Hamiltonian. Following Davydov's assumption, I regard the deformation variables as parameters and investigate the rotation of multipolar deformed systems, which is very interesting in studying the rotational spectra in atomic nuclei.

To obtain the rotational spectra for some special deformed systems, one can introduce the axially symmetrical spheroidal wave functions

$$|IK\pm\rangle = \sqrt{\frac{2I+1}{16\pi^2(1+\delta_{K0})}}\left[D_{MK}^I \pm (-1)^I D_{M,-K}^I\right] \tag{54}$$

as bases in calculating the energy spectra of rotational Hamiltonian. As $P|IK\pm\rangle = \pm|IK\pm\rangle$, where P is parity operator, I choose $|IK,+\rangle$ as bases for the positive-parity states, and $|IK,-\rangle$ as bases for the negative-parity states.

By using Eqs. (5), (7), and (21), one obtains the equations

$$\begin{aligned}R_1^2|IK\pm\rangle &= \tfrac{1}{2}[I(I+1)-K^2]|IK\pm\rangle + \tfrac{1}{4}o_K^I o_{K+1}^I|I,K+2\pm\rangle\\ &\quad+\tfrac{1}{4}o_{K-1}^I o_{K-2}^I|I,K-2\pm\rangle,\end{aligned} \tag{55}$$

$$\begin{aligned}R_2^2|IK\pm\rangle &= \tfrac{1}{2}[I(I+1)-K^2]|IK\pm\rangle - \tfrac{1}{4}o_K^I o_{K+1}^I|I,K+2\pm\rangle\\ &\quad-\tfrac{1}{4}o_{K-1}^I o_{K-2}^I|I,K-2\pm\rangle,\end{aligned} \tag{56}$$

$$R_3^2|IK\pm\rangle = K^2|IK\pm\rangle, \tag{57}$$

where R_1, R_2, and R_3 are the rotational operators around the first, second, and third axis in the body-fixed frame, respectively. The expression of o_K^I is the same as o_m^l in Eq. (31). With the relations, the matrix elements of the rotational operator are obtained as

$$\begin{aligned}\langle IK'|&\sum_{i=1}^{3}\frac{R_i^2}{2\mathscr{J}_i}|IK\rangle\\ &= \frac{1}{4}\left(\frac{1}{\mathscr{J}_1} + \frac{1}{\mathscr{J}_2}\right)I(I+1)\delta_{K'K}\\ &\quad+\frac{1}{2}\left(\frac{1}{\mathscr{J}_3} - \frac{1}{2\mathscr{J}_1} - \frac{1}{2\mathscr{J}_2}\right)K^2\delta_{K'K}\\ &\quad+\frac{1}{8}\left(\frac{1}{\mathscr{J}_1} - \frac{1}{\mathscr{J}_2}\right)\sqrt{1+\delta_{K0}}\,o_K^I o_{K+1}^I\delta_{K'K+2}\\ &\quad+\frac{1}{8}\left(\frac{1}{\mathscr{J}_1} - \frac{1}{\mathscr{J}_2}\right)\sqrt{1+\delta_{K'0}}\,o_{K-1}^I o_{K-2}^I\delta_{K'K-2}.\end{aligned} \tag{58}$$

By using Eq. (58), one can study the collective rotation for the system with the deformations $a_{l0},a_{l2},a_{l4},\dots,a_{l,l\,or\,l-1}$.

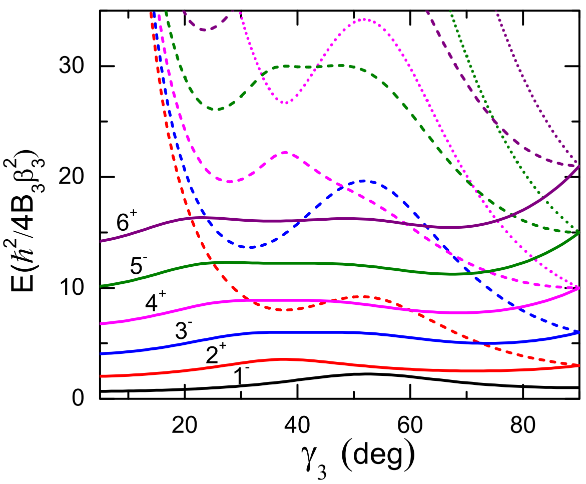

FIG. 1. (Color online) Evolution of rotational spectra to γ_3 for an octupole deformed system. Here the solid, dashed, and dotted lines with the same color represent, respectively, the first, second, and third energy levels for these states with the same angular momentum and parity.

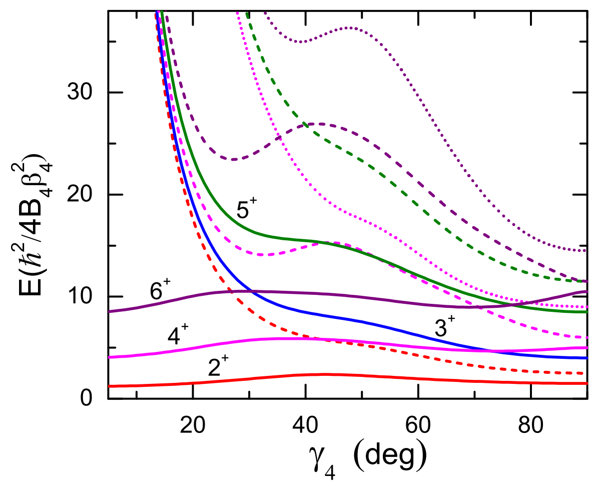

FIG. 2. (Color online) Evolution of rotational spectra to γ_4 for a hexadecapole deformed system (δ is fixed to 0°). Here, the solid, dash, and dot lines with the same color represent respectively the first, second, and third energy levels for these states with the same angular momentum and parity.

Here I do not focus on the full spectrum of a deformed nucleus with dominant quadrupole deformation. I am only concerned about rotational spectra for the system with pure octupole or hexadecapole deformations. Although octupole or hexadecapole deformations always coexist with quadrupole deformations in real nuclei, these studies can provide some information on rotational spectra for octupole and hexadecapole deformed systems, for which the properties of atomic nuclei with octupole or hexadecapole deformations coexisting with quadrupole deformations are helpful to know.

Considering that the most interesting rotational spectra are those with the lowest K, I have calculated the rotational spectra with the lowest K for the octupole and hexadecapole deformed systems. In Fig. 1, I have shown the variation of rotational spectra with γ_3 for an octupole deformed system. For simplicity, I take the 2^+ state as an example to analyze the relationship between the level energy and γ_3 deformation. For the 2^+ state, there are two levels. The first (lowest) 2^+ level is denoted by red solid line and the second 2^+ level by red dash line. With the change of γ_3, the first 2^+ level varies slowly. In the vicinity of $\gamma_3 = 0°$, the first 2^+ level appears to be a little decreasing with the decreasing γ_3, while that appears to increase a little with the increasing γ_3 closing to $\gamma_3 = 90°$. In the range of $\gamma_3 = 20°$ and $70°$, the energy of the first 2^+ level is nearly a constant. The same phenomena also appear in the first 3^+ level, the first 4^+ level, the first 5^+ level, and the first 6^+ level. For all these levels with the same angular momentum and parity, the lowest level is insensitive to γ_3. Different from these lowest levels, the second and third levels in every angular momentum and parity go to infinity, with γ_3 going to zero. With the increasing of γ_3, the second and third levels appear as valleys, i.e., metastable states, which may be the isomers of γ_3 deformation. When $\gamma_3 = \gamma_0$, the second and/or third levels appear as peaks, i.e., γ_3 unstable states. When $\gamma_3 = 90°$, a_{30} disappears, only a_{32} deformation exists in the nuclei, the shape of this system possesses T_d symmetry, and the rotational Hamiltonian is then reduced to a spherical top, so the rotational levels with the same angular momentum are degenerate. In a word, the contribution of the octupole term to the spectrum is smooth for the lowest band, while it becomes irregular for higher bands. In real nuclei, this contribution from the octupole term will be added to the dominant quadrupole contribution; thus, it will most probably result in some small deviations from the quadrupole spectrum. However, the character of octupole spectrum can reflect the information on the properties of real nuclei with octupole deformations coexisting with the quadrupole deformations.

Besides the octupole deformed system, I have also calculated the rotational spectra for a hexadecapole deformed system. In Fig. 2, I demonstrate the evolution of rotational spectra to γ_4 with δ_4 fixed to 0, i.e., with only a_{40} and a_{42} deformations under consideration. Over the range of γ_4, the lowest levels of even angular-momentum states are almost independent of γ_4. Only in the vicinity of $\gamma_4 = 0°$ and $\gamma_4 = 90°$ do these levels appear to be a little decreasing or increasing with γ_4. However, for these levels corresponding to the odd and higher even angular momentum states, their energies are sensitive to γ_4. Similar to that of octupole deformation, these levels go to infinity when γ_4 goes to 0°. With the increasing of γ_4, these levels drop quickly, but not monotonously, and appear as a valley: metastable state, which may be the isomer of γ_4 deformation; and peak, unstable state. When γ_4 is added to 90°, a_{40} disappears, all the rotational levels become relatively low, which implies that it is relatively easy to detect a_{42} deformation in real nuclei.

When δ_4 is fixed to 45°, the rotational spectra varying with γ_4 is displayed in Fig. 3. Except for the lowest levels of 2^+ and 4^+ states, the other levels depend remarkably on γ_4. Only in the vicinity of $\gamma_4 = 0°$, the lowest levels of even angular-momentum states keep a good structure of rotational spectra, while the other levels go to infinity. With the increasing of γ_4, these levels corresponding to the odd and higher even angular momentum states change dramatically. In the region around

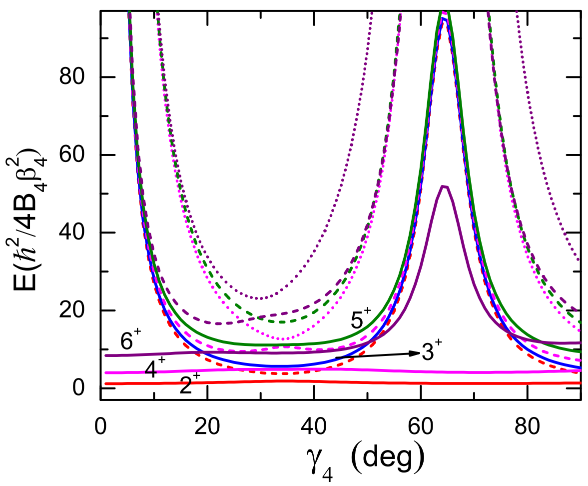

FIG. 3. (Color online) The same as Fig. 2, but δ_4 is fixed to 45°.

$\gamma_4 = 30^\circ$ and $\gamma_4 = 90^\circ$, all the levels are relatively low. In the other region, except for the lowest levels of 2^+ and 4^+, the other levels are too high, so it is difficult to detect these levels in real nuclei. Furthermore, a sharp peak appears in these levels, which corresponds to the γ_4 unstable state. As the peak is too high, it is impossible to detect the γ_4 unstable state in real nuclei, which is different from that in Fig. 2.

In Fig. 4, I show the variation of rotational spectra with γ_4 for $\delta_4 = 90^\circ$. In the case where only a_{40} and a_{44} deformations are concerned, the shape of system possesses D_{4h} symmetry and the corresponding moments of inertia $\mathscr{J}_1 = \mathscr{J}_2$. From Fig. 4, one can see that there exists a critical point of γ_4 deformation ($\gamma_4^c \approx 40.2^\circ$). In the point $\mathscr{J}_1 = \mathscr{J}_2 = \mathscr{J}_3$, the rotational Hamiltonian is reduced to a spherical top and the rotational levels with the same angular momentum degenerate. When $\gamma_4 < \gamma_4^c$, the lowest levels of even angular-momentum states form a good rotational spectrum although the energies of these levels increase with the increasing γ_4. However for the odd angular-momentum states, their energies go to infinity when γ_4 goes to 0. The same case also appears in the second and third levels of even angular-momentum states. This means that it is difficult to detect the rotational states with odd angular-momentum or the excited states with even angular momentum in the vicinity of $\gamma_4 = 0^\circ$. When $\gamma_4 > \gamma_4^c$, the energies of all the levels increase with the increasing γ_4, which shows that it is more unstable for the nuclei with a larger γ_4 deformation.

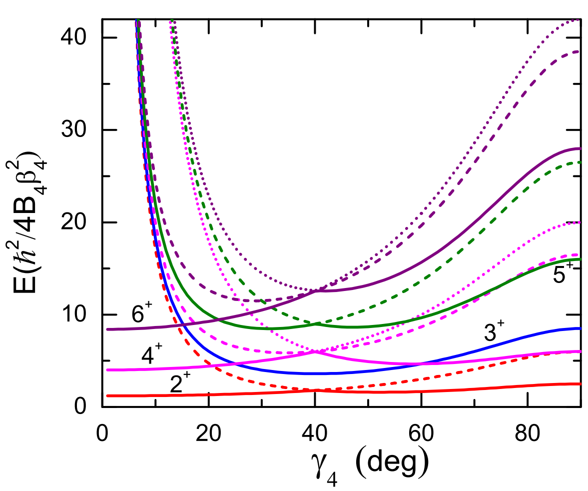

FIG. 4. (Color online) The same as Fig. 2, but δ_4 is fixed to 90°.

Over Figs. 2–4, one can see that the contributions of hexadecapole deformations to the lowest band are regular, while those to higher bands are irregular. In real nuclei, these contributions from hexadecapole deformations will be added to those from the dominant quadrupole deformations and will bring a bit of deviations from the energy spectrum of quadrupole deformations. However, the feature reflecting hexadecapole deformations will be reserved, which is useful to know the properties of real nuclei with hexadecapole deformations coexisting with the quadrupole deformations.

V. CONCLUSIONS

Based on the Bohr model, I have presented a general formalism describing the collective motion for any deformed system in which the collective Hamiltonian is expressed as vibrations in the body-fixed frame, rotation of whole system around the laboratory frame, and coupling between vibrations and rotation. Under the condition of decoupling approximation, I have derived the quantized Hamiltonian operator. Based on the operator, I have calculated the rotational energy for some special octupole and hexadecapole deformed systems and shown their dependencies on deformation. In the octupole deformed nuclei, for these states with the same angular momentum and parity, the lowest level is insensitive to γ_3, and all the lowest levels form a regular rotational spectrum. Different from the lowest levels, the higher levels depend remarkably on γ_3. In the vicinity of $\gamma_3 = 0^\circ$, these higher levels go to infinity. With the increasing of γ_3, these levels drop quickly, but not monotonously. There appear to be peaks (unstable state) and valleys (metastable state) in these levels over the range of γ_3. These metastable states may form the isomers of γ_3 deformation. A similar case also appears in the hexadecapole deformed system with $\delta_4 = 0^\circ$. The lowest levels of even angular-momentum states are almost independent of γ_4 and form a regular rotational band. For the odd and higher even angular-momentum states, the corresponding levels are sensitive to γ_4. They go to infinity closing to $\gamma_4 = 0^\circ$ and decline fast with the increasing γ_4. Similarly, there appear γ_4 unstable and metastable states in the range of γ_4. For the hexadecapole deformations with δ_4 fixed to 45° and 90°, the lowest levels of even angular momentum states form regular rotational spectra in the vicinity of $\gamma_4 = 0^\circ$. With the increasing of γ_4, these levels for the odd and higher even angular-momentum states change dramatically. These show that the octupole and/or hexadecapole contributions to the lowest band are regular, while those to higher bands are dramatic. In real nuclei, these contributions will be added to a dominant quadrupole contribution and produce some small influences on the energy spectrum of quadrupole deformations. Nevertheless, these features reflecting octupole and hexadecapole deformations are helpful in understanding the properties of real nuclei with octupole and/or hexadecapole coexisting with the quadrupole deformations.

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