General formalism of collective motion for any deformed system

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Based on Bohr model, we 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, we have derived the quantized Hamiltonian operator. Based on the operator, we 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 to recognize 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 has been developed a long time ago. The classical case corresponds to the quadruple deformations, which was established by Bohr in 1952 [1, 2]. Bohr Hamiltonian is very useful in describing the vibrations and rotation for quadruple deformed nuclei. Especially for the shape evolution and phase transitions [3], Bohr Hamiltonian is a powerful tool to investigate the critical-point symmetries like E(5) [4], X(5) [5], Y(5) [6], and Z(5) [7]. More researches on the collective motion by Bohr model can be found in the literatures [8–10] and references therein. Several recent progresses include 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 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].

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 [13, 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 recent experiment [22]. Furthermore, in the region $N = 92, 94$, octupole correlations were observed in $^{150,152}$Ce isotopes [23, 24].

These 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 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 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. As there is the difficult to determine the intrinsic frame, the parameterizations of octupole deformations were probed in Refs. [26, 31–33]. Moreover, an alternative parameterizations describing nuclear quadrupole 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 researches on the octupole deformations and correlations can be found in Ref. [38] and references therein.

Besides of 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]. The observations of $\Delta I = 4$ bifurcation (also called $\Delta I = 2$ staggering) staggering phenomenon in superdeformation bands [41, 42] have aroused great enthusiasm for 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 \[ \text{[67] [68] [69]} \], and the absence of any tetrahedral symmetry \[ \text{[54] [55] [56]} \]. The parametrization of hexadecapole deformations has been discussed in Refs. \[ \text{[61] [62]} \].

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 \[ \text{[64]} \], 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 terms of the presence of a tetrahedral symmetry \[ \text{[47]–[50]} \], 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 \[ \text{[67]} \].

From the preceding analysis, we know 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, we present a general formalism describing the collective motion for any deformed system. Firstly, we give the classical Hamiltonian of collective motion in 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, we derive out the quantized Hamiltonian operator. As examples, we 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, we expand the surface radius of the system as

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

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

\[
H = T + V,
\]

where the kinetic energy is expressed as

\[
T = \frac{1}{2} \sum_{lm} B_l |\dot{\alpha}_{lm}|^2,
\]

and the potential energy takes the form

\[
V = \frac{1}{2} \sum_{lm} C_l |\alpha_{lm}|^2.
\]

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 \( H \). In order to separate vibrations and rotation from \( H \), it is necessary to transform the variables in the collective Hamiltonian from Laboratory frame (\( K \)-system) to body-fixed frame (\( K' \)-system) by rotation, which is defined by

\[
R(\theta_i) = e^{-i\theta_3 J_3} e^{-i\theta_2 J_2} e^{-i\theta_1 J_1},
\]

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 \( \alpha_{lm} \) in \( K \)-system can be transformed into \( K' \)-system as

\[
\alpha_{lm} = \sum_{lm'} D_{mm'}^{l'} \beta_{lm'},
\]

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

\[
D_{mm'}^{l'}(\theta_i) = \langle lm | e^{-i\theta_3 J_3} e^{-i\theta_2 J_2} e^{-i\theta_1 J_1} | l'm' \rangle.
\]

In order to present the collective Hamiltonian using the variables \( \beta_{lm}, \theta_i \), we calculate the time derivative of \( \alpha_{lm} \) as

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

where the time derivative of \( D_{mm'}^{l'}(\theta_i) \) is presented as

\[
\dot{D}_{mm'}^{l'}(\theta_i) = -i \sum_k D_{mk}^{l'}(\theta_i) \langle k | \vec{\omega} \cdot \vec{J} | l'm' \rangle.
\]

In Eq. (3),

\[
\begin{align*}
\omega_1 &= \dot{\theta}_1 \sin \theta_3 - \dot{\theta}_2 \sin \theta_1 \cos \theta_3, \\
\omega_2 &= \dot{\theta}_1 \cos \theta_3 + \dot{\theta}_2 \sin \theta_1 \sin \theta_3, \\
\omega_3 &= \dot{\theta}_3 + \dot{\theta}_2 \cos \theta_1,
\end{align*}
\]

are angular velocities around the axes coincide with the body \( (K') \)-system. Putting \( \dot{\beta}_{lm} \) 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 $D_{m\nu}^t$-functions and their derivatives. We thus write

$$T = T_{\text{vib}} + T_{\text{rot}} + T_{\text{cou}}.$$  \hfill (11)

In Eq. (11), the vibrational energy

$$T_{\text{vib}} = \frac{1}{2} \sum_{lm} B_l \left| \dot{\beta}_{lm} \right|^2,$$  \hfill (12)

the rotational energy

$$T_{\text{rot}} = \frac{1}{2} \sum_{ij} \mathcal{J}_{ij} \omega_i \omega_j,$$  \hfill (13)

with the moments of inertia

$$\mathcal{J}_{ij} = \frac{1}{2} \sum_{lm} B_l \left| \langle lm' | \{ J_i, J_j \} \vert lm \rangle \right| \beta_{lm}^* \beta_{lm'}^*.$$  \hfill (14)

and the coupling between vibrations and rotation

$$T_{\text{cou}} = \sum_l \omega_l \kappa_l,$$  \hfill (15)

with

$$\kappa_l = -\text{Im} \sum_{lm} B_l \langle lm' | J_i \vert lm \rangle \beta_{lm}^* \beta_{lm'}^*.$$  \hfill (16)

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

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

Here, the spherical harmonics

$$Y_{lm}^+(\theta, \phi) = \frac{1}{\sqrt{2}} \left[ Y_{lm} (\theta, \phi) + Y_{lm}^* (\theta, \phi) \right],$$

$$Y_{lm}^-(\theta, \phi) = \frac{1}{i \sqrt{2}} \left[ Y_{lm} (\theta, \phi) - Y_{lm}^* (\theta, \phi) \right].$$  \hfill (18)

From Eq. (17), we obtain

$$\beta_{l0} = a_{l0}, \beta_{l,m} = \frac{a_{lm} + ib_{lm}}{\sqrt{2}}, \beta_{l,-m} = (-1)^m \frac{a_{lm} - ib_{lm}}{\sqrt{2}},$$  \hfill (19)

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

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

By using the relations

$$J_{\pm \pm} (lm) = \sqrt{(l+m)(l+m+1)} |lm\rangle \langle lm|,$$

$$J_{ij} (lm) = m |lm\rangle \langle lm|.$$  \hfill (21)

Here $J_{\pm} = J_1 \pm i J_2$. $\kappa_l$ and $\mathcal{J}_{ij}$ are expressed as the functions of the real variables $a_{lm}$ and $b_{lm}$ as follows

$$\kappa_1 = \frac{1}{2} \sum_l B_l \left\{ -\sqrt{2l (l+1)} \ddot{a}_{l0} a_{l1} + \sum_{m > 0} \dot{a}_{lm} b_{lm+1} + \dot{b}_{lm} a_{lm+1} \right\},$$

$$\kappa_2 = \frac{1}{2} \sum_l B_l \left\{ \sqrt{2l (l+1)} \ddot{a}_{l0} a_{l1} + \sum_{m > 0} \ddot{a}_{lm} a_{lm+1} + \ddot{b}_{lm} b_{lm+1} \right\} - \sum_{m > 0} \ddot{a}_{lm} a_{lm-1} + \ddot{b}_{lm} b_{lm-1} \right\},$$

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

$$\mathcal{J}_{11} = \frac{1}{4} \sum_l B_l \left\{ 2l (l+1) \ddot{a}_{l0}^2 + \sqrt{2l(l^2-1)(l+2)} a_{l0} a_{l2} + 2 \sum_{m > 0} [l (l+1) - m^2] \left( a_{lm}^2 + b_{lm}^2 \right) + \sum_{m > 0} \dot{a}_{lm}^2 + \dot{b}_{lm}^2 \right\} + \sum_{m > 0} \ddot{a}_{lm} a_{lm+2} + \ddot{b}_{lm} b_{lm+2} + \sum_{m > 0} \ddot{a}_{lm} a_{lm-2} + \ddot{b}_{lm} b_{lm-2} \right\},$$

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

$$J_{33} = \sum_{l,m > 0} B_l m^2 \left( a_{lm}^2 + b_{lm}^2 \right).$$  \hfill (27)
\[ J_{ij} = \frac{1}{4} \sum_l B_l \left\{ \sqrt{2l(l+1)} a_{l0} b_{l2}^i \right. \\
+ \sum_{m>0} a_{m}^i a_{m+1}^j (a_{lm} b_{lm+2} - b_{lm} a_{lm+2}) \\
- \left. \sum_{m>0} a_{m}^j a_{m+1}^i (a_{lm} b_{lm-2} - b_{lm} a_{lm-2}) \right\} \]

\[ J_{12} = \frac{1}{4} \sum_l B_l \left\{ \sqrt{2l(l+1)} a_{l0} a_{l1} \right. \\
+ \sum_{m>0} (2m+1) a_{m}^i a_{m+1}^j (a_{lm} a_{lm+1} + b_{lm} b_{lm+1}) \\
- \left. \sum_{m>0} (2m-1) a_{m}^j a_{m+1}^i (a_{lm} b_{lm-1} + b_{lm} a_{lm-1}) \right\} \]

\[ J_{23} = \frac{1}{4} \sum_l B_l \left\{ \sqrt{2l(l+1)} b_{l0} b_{l1} \right. \\
+ \sum_{m>0} (2m+1) a_{m}^i a_{m+1}^j (a_{lm} b_{lm+1} - b_{lm} a_{lm+1}) \\
- \left. \sum_{m>0} (2m-1) a_{m}^j a_{m+1}^i (a_{lm} b_{lm-1} - b_{lm} a_{lm-1}) \right\} \]

where

\[ a_{m}^i = \sqrt{(l-m)(l+m+1)}, \]

and the moments of inertia are real symmetrical: \( J_{ij} = J_{ji} \). 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 each other. Three of them have been replaced by the Euler angles. How to remove off three superfluous variables is a trouble 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 progresses have been achieved for octupole deformed system. The surface radius expressed by the parameters \( a_{3m} \) and \( b_{3m} \) was re-parameterized by a set of biharmonic coordinates \( a_{3m} \) and \( b_{3m} \). In the parameterizations, 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 \( b_{3m} \). In order to remove off the off-diagonal elements of inertia tensor, in Ref. [33], the intrinsic frame was defined by the variables (\( X, Y, Z, \gamma \)).

In comparison with the present formalism, there exist the following relations:

\[ \beta_{33} = \frac{1}{\sqrt{2}} a_{33} - i \frac{1}{\sqrt{2}} b_{33} \]
\[ = \left( \cos \gamma - \sqrt{\frac{3}{2}} \sin \gamma \right) X + i \left( \cos \gamma + \sqrt{\frac{3}{2}} \sin \gamma \right) Y, \]

\[ \beta_{32} = \frac{1}{\sqrt{2}} a_{32} - i \frac{1}{\sqrt{2}} b_{32} = \frac{1}{\sqrt{2}} \sin \gamma \cdot Z, \]

\[ \beta_{31} = \frac{1}{\sqrt{2}} a_{31} - i \frac{1}{\sqrt{2}} b_{31} = \frac{\sqrt{5}}{2} \sin \gamma \cdot X + i \frac{\sqrt{5}}{2} \sin \gamma \cdot Y, \]

\[ \beta_{30} = a_{30} = \sqrt{5} \cos \gamma \cdot Z. \]

Namely,

\[ a_{33} = \left( \sqrt{2} \cos \gamma - \sqrt{3/2} \sin \gamma \right) X, \]
\[ b_{33} = -\left( \sqrt{2} \cos \gamma + \sqrt{3/2} \sin \gamma \right) Y, \]
\[ a_{32} = \sin \gamma \cdot Z, \]
\[ b_{32} = 0, \]
\[ a_{31} = \frac{\sqrt{5}}{2} \sin \gamma \cdot X, \]
\[ b_{31} = -\frac{\sqrt{5}}{2} \sin \gamma \cdot Y, \]
\[ a_{30} = \sqrt{5} \cos \gamma \cdot Z. \]

Putting Eqs. (33) into Eqs. (29, 30), for a pure octupole deformed system, we 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:

\[ J_{12} = 2 \sqrt{15} a_{30} b_{32} - 6 a_{31} b_{31} + \sqrt{15} a_{31} b_{33} - \sqrt{15} a_{33} b_{31} \]
\[ = -6 \left( \sqrt{\frac{5}{2}} \sin \gamma \cdot X \right) \left( -\sqrt{\frac{5}{2}} \sin \gamma \cdot Y \right) \]
\[ + \sqrt{15} \left( \sqrt{\frac{5}{2}} \sin \gamma \cdot X \right) \left( -\sqrt{2} \cos \gamma - \sqrt{\frac{3}{2}} \sin \gamma \right) Y \]
\[ - \sqrt{15} \left( \sqrt{2} \cos \gamma - \sqrt{\frac{3}{2}} \sin \gamma \right) X \left( -\sqrt{\frac{5}{2}} \sin \gamma \cdot Y \right) \]
\[ = 0. \]

Similarly, we can also reproduce the inertia tensor in Refs. [29, 34, 35] by a correct replacement of deformation parameters in the present formalism.

From these discussions, we have known that there are simple relations between the parameters in Refs. [29, 31–33] and \( (a_{lm}, b_{lm}) \) in the present formalism. Hence, the results in these literatures [29, 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. [29, 31–33] but also those with other deformations, which is useful to investigate the atomic nuclei with some special deformations.

In real nuclei, octupole deformations always coexist with quadrupole deformations. Many researches [13, 29]
have been performed for the system with the coexistence of quadrupole and octupole deformations. The present formalism is convenient to describe 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. [13, 27, 30, 33, 38] can be obtained using the present formalism.

Similarly, hexadecapole deformations always coexist with quadrupole deformations in real nuclei. Many researches 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 realistic mean-field method [65, 67], and verified in recent experiment [67], the present formalism is convenient to take the quadrupole and hexadecapole degrees of freedom simultaneously into account. When $a_{lm}$ and $b_{lm}$ are re-parameterized 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 parametrization of pure hexadecapole deformations is 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

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

Here, the definitions of $Y_{4\mu}^{(+)}(\theta, \phi)$ and $Y_{4\mu}^{(-)}(\theta, \phi)$ are the same as those in Eqs. (33). It shows that the parameters $(a_{40}, a_{4\mu}, b_{4\mu}, \mu = 1, 2, 3, 4)$ are just some special sampling of $(a_{lm} \text{ and } b_{lm})$. To make the system obey relatively simple transformation rules under the $O_h$ group, this set of parameters $(a_{40}, a_{4\mu}, b_{4\mu})$ have been reparameterized with a set of biharmonic coordinates. As 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, 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, we derive out 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, we need to remove off three superfluous variables among $a_{lm}$ and $b_{lm}$ in order to quantify the collective Hamiltonian. For a quadrupole deformed system, we can regard $a_{21}$, $b_{21}$, and $b_{22}$ as superfluous variables. When $a_{21}$, $b_{21}$, and $b_{22}$ are removed off, $T_{\text{co}}$ 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 in order to remove off $T_{\text{co}}$. Even a octupole deformed system, a set of internal parameters that make $T_{\text{co}}$ disappear, is not still found up to now. Here, we adopt an approximate method to eliminate $T_{\text{co}}$ by freezing a part of deformation parameters. From Eqs. (22, 24), we can see, to make $T_{\text{co}}$ 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 $a_{10}, a_{12}, a_{14}, \ldots, a_{4l}$ or $l = 1$ are reserved and the rest are removed off. Then, the kinetic energy becomes

$$T = \frac{1}{2} B_2 (\dot{a}_{20}^2 + \dot{a}_{22}^2) + \frac{1}{2} B_3 (\dot{a}_{30}^2 + \dot{a}_{32}^2)$$

$$+ \frac{1}{2} B_4 (\dot{a}_{40}^2 + \dot{a}_{42}^2 + \dot{a}_{44}^2) + \cdots$$

$$+ \frac{1}{2} \left( J_1 \dot{\omega}_1^2 + J_2 \dot{\omega}_2^2 + J_3 \dot{\omega}_3^2 \right), \tag{36}$$

with the moments of inertia

$$J_1 = \frac{1}{4} \sum_{l} B_l \left\{ 2(l+1)a_{10}^2 + \sqrt{2 l(l^2 - 1)(l + 2)} a_{10}a_{12} \right.$$

$$+ \sum_{m=2}^{l-1} (a_{m}^l a_{lm+1} - a_{m}^{l-1} a_{lm-1} + a_{m}^{l'} a_{lm+1} - a_{m}^{l'} a_{lm-1})$$

$$+ \sum_{m=2}^{l-1} [l(l + 1) - m^2] a_{lm}^2 \right\}, \tag{37}$$

$$J_2 = \frac{1}{4} \sum_{l} B_l \left\{ 2(l+1)a_{10}^2 - \sqrt{2 l(l^2 - 1)(l + 2)} a_{10}a_{12}$$

$$+ \sum_{m=2}^{l-1} (a_{m}^l a_{lm+1} + a_{m}^{l-1} a_{lm-1} + a_{m}^{l'} a_{lm+1} + a_{m}^{l'} a_{lm-1})$$

$$+ \sum_{m=2}^{l-1} [l(l + 1) - m^2] a_{lm}^2 \right\}, \tag{38}$$

and

$$J_3 = \sum_{l} B_l \sum_{m=2}^{l-1} m^2 a_{lm}^2. \tag{39}$$

To obtain a quantized Hamiltonian, we write the kinetic energy as

$$T = \frac{1}{2} g_{ij} \dot{q}_i \dot{q}_j, \tag{40}$$
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.,

\[
G = \begin{bmatrix} B_2 & B_2 & B_3 & B_3 & \cdots & \mathcal{J}_1 & \mathcal{J}_2 & \mathcal{J}_3 \end{bmatrix},
\]

its determinant

\[
g = \det G = B_2^2 B_3^2 \cdots \mathcal{J}_1 \mathcal{J}_2 \mathcal{J}_3.
\]

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

\[
T = -\frac{\hbar^2}{2} \sum_{i=1}^{3} \frac{1}{\sqrt{B_i}} \frac{\partial}{\partial q_i} G^{-1}_{ij} \frac{\partial}{\partial q_j}
\]

\[
= -\frac{\hbar^2}{2 B_i} \frac{1}{\sqrt{B_1 \mathcal{J}_2 \mathcal{J}_3}} \frac{\partial}{\partial q_i} \mathcal{J}_2 \mathcal{J}_3 \frac{\partial}{\partial q_i}
\]

\[
+ \sum_{i=1}^{3} \frac{R_i^2}{2 \mathcal{J}_i}.
\]

where \( q_i = a_{20}, a_{22}, a_{30}, a_{32}, a_{40}, a_{42}, a_{44}, \ldots \), and \( R_i = -i \hbar \frac{\partial}{\partial q_i} \), \( i = 1, 2, 3 \) 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

\[
a_{20} = \beta_2 \cos \gamma_2, \\
a_{22} = \beta_2 \sin \gamma_2, \\
a_{30} = \beta_3 \cos \gamma_3, \\
a_{32} = \beta_3 \sin \gamma_3, \\
a_{40} = \beta_4 \cos \gamma_4, \\
a_{42} = \beta_4 \cos \delta_4 \sin \gamma_4, \\
a_{44} = \beta_4 \sin \delta_4 \sin \gamma_4,
\]

the quantized kinetic operator in the curve coordinates is obtained.

For a pure quadrupole deformed system, we obtain immediately

\[
T_2 = -\frac{\hbar^2}{2 B_2} \left( \frac{1}{\beta_2^2} \frac{\partial}{\beta_2} \beta_2^2 \frac{\partial}{\beta_2} \frac{1}{\beta_2^2 \sin 3 \gamma_2} \frac{\partial}{\beta_2} \sin 3 \gamma_2 \frac{\partial}{\beta_2} \right)
\]

\[
+ \sum_{i=1}^{3} \frac{R_i^2}{2 \mathcal{J}_i},
\]

with

\[
\mathcal{J}_i = 4 B_2 \beta_2^2 \sin^2 \left( \gamma_2 - \frac{2 \pi}{3} \right), \quad (i = 1, 2, 3).
\]

\( T_2 \) is the kinetic energy operator in Bohr Hamiltonian.

For a pure octupole deformed system, we obtain

\[
T_3 = -\frac{\hbar^2}{2 B_3} \left( \frac{1}{\beta_3^2} \frac{\partial}{\beta_3} \beta_3^2 \frac{\partial}{\beta_3} \frac{1}{\beta_3^2 w(\gamma_3)} \frac{\partial}{\beta_3} w(\gamma_3) \frac{\partial}{\beta_3} \right)
\]

\[
+ \sum_{i=1}^{3} \frac{R_i^2}{2 \mathcal{J}_i},
\]

with

\[
w(\gamma_3) = \sin \gamma_3 \sqrt{9 - 21 \sin^2 \gamma_3 + 16 \sin^4 \gamma_3},
\]

and the moments of inertia

\[
\mathcal{J}_1 = B_3 \beta_2^2 \left[ 1 + 8 \sin^2 (\gamma_3 + \gamma_0) \right], \\
\mathcal{J}_2 = B_3 \beta_2^2 \left[ 1 + 8 \sin^2 (\gamma_3 - \gamma_0) \right], \\
\mathcal{J}_3 = 4 B_3 \beta_2^2 \sin^2 \gamma_3,
\]

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

For a pure hexadecapole deformed system, we obtain

\[
T_4 = -\frac{\hbar^2}{2 B_4} \left[ \frac{1}{\beta_4^2} \frac{\partial}{\beta_4} \beta_4^2 \frac{\partial}{\beta_4} \frac{1}{\beta_4^2 \sin 4 \gamma_4} \frac{\partial}{\beta_4} \sin 4 \gamma_4 \frac{\partial}{\beta_4} \right]
\]

\[
+ \sum_{i=1}^{3} \frac{R_i^2}{2 \mathcal{J}_i},
\]

with

\[
w(\gamma_4, \delta_4) = \sqrt{\mathcal{J}_1' \mathcal{J}_2' \mathcal{J}_3'},
\]

and the moments of inertia

\[
\mathcal{J}_i = B_4 \beta_4^2 \mathcal{J}_i', \quad (i = 1, 2, 3).
\]

Here

\[
\mathcal{J}_1' = 10 + 3 \sqrt{5} \cos \delta_4 \sin 2 \gamma_4 + \left( 3 \cos \delta_4 + \sqrt{7} \sin \delta_4 - 5 \right) \sin^2 \gamma_4,
\]

\[
\mathcal{J}_2' = 10 - 3 \sqrt{5} \cos \delta_4 \sin 2 \gamma_4 + \left( 3 \cos \delta_4 + \sqrt{7} \sin \delta_4 - 5 \right) \sin^2 \gamma_4,
\]

\[
\mathcal{J}_3' = \left( \cos^2 \delta_4 + 4 \sin^2 \delta_4 \right) \sin^2 \gamma_4.
\]

From Eq. (44), we notice that the 4th power of \( \beta_2 \) appears in the first term of the kinetic energy. The same case also appears in Eq. (47) for \( \beta_3 \). Different from Eqs. (45) and (47), the 5th power of \( \beta_4 \) appears in the first term of the kinetic energy. It 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 \( (a_{20}, a_{22}, a_{42}) \) are taken into account.

**IV. THE ROTATIONAL SPECTRA FOR SOME SPECIAL DEFORMED SYSTEMS**

In the preceding section, we 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 we do not discuss in details solution of the general Hamiltonian. Follow Davydov’s assumption, we regard the deformation variables as parameters, and investigate the rotation of multipolar deformed systems, which is very interesting to study the rotational spectra in atomic nuclei.

In order to obtain the rotational spectra for some special deformed systems, we introduce the axially symmetrical spheroidal wave functions

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

(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, we 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), we obtain the following equations:

$$R_{1}^{2}|IK\pm\rangle = \frac{1}{2} \left[ I(I+1) - K^2 \right] |IK\pm\rangle + \frac{1}{4} o'_{K}o'_{K+1} |I, K + 2\pm\rangle + \frac{1}{4} o'_{K-1}o'_{K-2} |I, K - 2\pm\rangle,$$

(55)

$$R_{2}^{2}|IK\pm\rangle = \frac{1}{2} \left[ I(I+1) - K^2 \right] |IK\pm\rangle - \frac{1}{4} o'_{K}o'_{K+1} |I, K + 2\pm\rangle - \frac{1}{4} o'_{K-1}o'_{K-2} |I, K - 2\pm\rangle,$$

(56)

$$R_{3}^{2}|IK\pm\rangle = K^2 |IK\pm\rangle,$$

(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 $o'_{K}$ is the same as $o'_{m}$ in Eq. (51). With the relations, the matrix elements of the rotational operator are obtained as

$$\langle IK'| \sum_{i=1}^{3} \frac{R_{i}^{2}}{2 J_{i}} |IK\rangle$$

$$= \frac{1}{4} \left( \frac{1}{J_{1}} + \frac{1}{J_{2}} \right) I(I+1) \delta_{K'K} + \frac{1}{2} \left( \frac{1}{J_{3}} \frac{1}{2 J_{1}} - \frac{1}{2 J_{2}} \right) K^2 \delta_{K'K} + \frac{1}{8} \left( \frac{1}{J_{1}} - \frac{1}{J_{2}} \right) \sqrt{1 + \delta_{K0}o'_{K}o'_{K+1}\delta_{K'K+2}} + \frac{1}{8} \left( \frac{1}{J_{1}} - \frac{1}{J_{2}} \right) \sqrt{1 + \delta_{K0}o'_{K-1}o'_{K-2}\delta_{K'K-2}}.$$

(58)

By using Eq. (58), we can study the collective rotation for the system with the deformations $a_{0}, a_{2}, a_{4}, \ldots, a_{I} \approx 0$. Here, we do not focus on the full spectrum of a deformed nucleus with dominant quadrupole deformation. We are 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, our studies can provide some information on rotational spectra for octupole and hexadecapole deformed systems, which are helpful to know the properties of atomic nuclei with octupole or hexadecapole deformations coexisting with quadrupole deformations.

Considering that the most interesting rotational spectra are those with the lowest $K$, we have calculated the rotational spectra with the lowest $K$ for the octupole and hexadecapole deformed systems. In Fig. 1, we have shown the variation of rotational spectra with $\gamma_{3}$ for an octupole deformed system. For simplicity, we take $2^{+}$ state as an example to analyze the relationship between the level energy and $\gamma_{3}$ deformation. For $2^{+}$ 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 $\gamma_{3}$, the first $2^{+}$ level varies slowly. In the vicinity of $\gamma_{3} = 0^\circ$, the first $2^{+}$ level appears a little decreasing with the increasing $\gamma_{3}$, while that appears a little increasing with the increasing $\gamma_{3}$ close to $\gamma_{3} = 90^\circ$. In the range of $\gamma_{3} = 20^\circ$ and $70^\circ$, 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 $\gamma_{3}$. Different from these lowest levels, the second and third levels in every angular momentum and parity go to infinity with $\gamma_{3}$ going to zero. With the increasing of $\gamma_{3}$, the second and third levels appear valleys, i.e., metastable states, which may be the isomers of $\gamma_{3}$ deformation. When $\gamma_{3} = \gamma_{0}$, the second and/or third levels appear peaks, i.e., $\gamma_{3}$ unstable states. When $\gamma_{3} = 90^\circ$, $a_{30}$ disappears, only $a_{32}$ deformation exists in the nuclei, the shape of this system possesses $T_{d}$ symmetry, 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 octupole term will be added to the dominant quadrupole contribution, thus it will most probably result to some small deviations from quadrupole spectrum. But, the character of octupole spectrum can reflect the information on the properties of real nuclei with octupole deformations coexisting with the quadrupole deformations.

Besides of the octupole deformed system, we have also calculated the rotational spectra for a hexadecapole deformed system. In Fig. 2, we demonstrate the evolution of rotational spectra to $\gamma_{4}$ with $\delta_{4}$ fixed to 0, i.e., only
a_{40} and a_{42} deformations under consideration. Over the range of \( \gamma_4 \), the lowest levels of even angular momentum states are almost independent of \( \gamma_4 \). Only in the vicinity of \( \gamma_4 = 0^\circ \) and \( \gamma_4 = 90^\circ \), these levels appear a little decreasing or increasing with \( \gamma_4 \). However for these levels corresponding to the odd and higher even angular momentum states, their energies are sensitive to \( \gamma_4 \). Similar to that of octupole deformation, these levels go to infinity when \( \gamma_4 \) goes to \( 0^\circ \). With the increasing of \( \gamma_4 \), these levels drop quickly, but not monotonously, appear valley: metastable state, which may be the isomer of \( \gamma_4 \) deformation, and peak: unstable state. When \( \gamma_4 \) is added to \( 90^\circ \), \( a_{40} \) disappears, all the rotational levels become relatively low, which implies that it is relatively easy to appear \( a_{42} \) deformation in real nuclei.

When \( \delta_4 \) is fixed to \( 45^\circ \), the rotational spectra varying with \( \gamma_4 \) is displayed in Fig. 3. Except for the lowest levels of \( 2^+ \) and \( 4^+ \) states, the other levels depend remarkably on \( \gamma_4 \). Only in the vicinity of \( \gamma_4 = 0^\circ \), 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 \( \gamma_4 \), these levels corresponding to the odd and higher even angular momentum states change dramatically. In the region around \( \gamma_4 = 30^\circ \) 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 that it is difficult to appear these levels in real nuclei. Furthermore, a sharp peak appears in these levels, which corresponds to \( \gamma_4 \) unstable state. As the peak is too high, it is impossible to appear the \( \gamma_4 \) unstable state in real nuclei, which is different from that in Fig. 2.

In Fig. 4, we show the variation of rotational spectra with \( \gamma_4 \) for \( \delta_4 = 90^\circ \). In the case, only \( a_{40} \) and \( a_{44} \) deformations are concerned, the shape of system possesses \( D_{4h} \) symmetry and the corresponding moments of inertia \( J_1 = J_2 \). From Fig. 4, we can see that there exists a critical point of \( \gamma_4 \) deformation \( (\gamma_4^c \approx 40.2^\circ) \). In the point, \( J_1 = J_2 = J_3 \), the rotational Hamiltonian is reduced to a spherical top, the rotational levels with the same angular momentum are 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 $\gamma_4$. However for the odd angular momentum states, their energies go to infinity when $\gamma_4$ 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 appear 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 $\gamma_4$, which shows that it is more unstable for the nuclei with a larger $\gamma_4$ deformation.

Over Figs. 2-4, we 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. But, 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 Bohr model, we 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, we have derived the quantized Hamiltonian operator. Based on the operator, we 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 $\gamma_3$, and all the lowest levels form a regular rotational spectrum. Different from the lowest levels, the higher levels depend remarkably on $\gamma_3$. In the vicinity of $\gamma_3 = 0^\circ$, these higher levels go to infinity. With the increasing of $\gamma_3$, these levels drop quickly, but not monotonously. There appear peak (unstable state) and valley (metastable state) in these levels over the range of $\gamma_3$. These metastable states may form the isomers of $\gamma_3$ deformation. The 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 $\gamma_4$ and form a regular rotational band. For the odd and higher even angular momentum states, the corresponding levels are sensitive to $\gamma_4$. They go to infinity closing to $\gamma_4 = 0^\circ$, and decline fast with the increasing $\gamma_4$. Similarly, there appear $\gamma_4$ unstable and metastable states in the range of $\gamma_4$. For the hexadecapole deformations with $\delta_4$ 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 $\gamma_4$, 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 to understand the properties of real nuclei with octupole and/or hexadecapole coexisting with the quadrupole deformations.

VI. ACKNOWLEDGMENTS

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[1] A. Bohr, Mat. Fys. Medd. K. Dan. Vidensk. Selsk. 26, 14 (1952).
[2] A. Bohr and B. Mottelson, Mat. Fys. Medd. K. Dan. Vidensk. Selsk. 27, 16 (1952).
