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Quantization of the kinetic energy of an octupole deformed nucleus in curvilinear coordinates

M.S. Nadirbekov[1, *] and S.N. Kudiratov[1, 2, †]

[1] *Institute of Nuclear Physics, Tashkent, 100214, Uzbekistan*
[2] *Industrial, radiation and nuclear safety committee, Tashkent, 100011, Uzbekistan*

Abstract: The quantization of the kinetic energy of a deformed nucleus in curvilinear coordinates in the case of octupole vibrations of its surface has been carried out. The obtained form of the Hamiltonian differs from the previously obtained Hamiltonian for quadrupole vibrations only by factors in front of the derivatives $\partial/\partial\gamma$ and $\partial/\partial\eta$. That is because the formulas for the components of the moments of inertia of the nucleus in the cases of quadrupole and octupole vibrations have a different form. We have obtained the exact form of the complete Hamiltonian of an even-even nucleus with quadrupole and octupole deformation, which contains seven dynamical variables.

Keywords: quantization, curvilinear coordinates, quadrupole and octupole deformations, triaxiality, moment of inertia, Bohr Hamiltonian.

I. INTRODUCTION

After the discovery of the Bohr Hamiltonian [1], many solutions of the Schrödinger eigenvalue equation have been proposed, but in many cases limited to the quadrupole degree of freedom [2–4]. The total energy operator of quadrupole and octupole deformations was considered in the work [5], where the surface of the nucleus is described by seven expansion parameters corresponding to spherical harmonics of the third order. A simultaneously parametrization of octupole plus quadrupole deformation, on the intrinsic variables defined in the rest frame of the overall tensor of moment of inertia is presented in the work [6, 7].

The collective model with quadrupole and octupole deformations was applied to deformed axially symmetric nuclei in Refs. [8–13]. The importance of taking into account deformation asymmetry parameters are shown in Ref. [5, 14]. The Schrö equation with the collective Bohr Hamiltonian are analyzed in detail in Ref. [15]. In addition, it is of interest to analytical solutions of the Schrödinger equation with Bohr Hamiltonian, and to study their connection with the critical behavior of nuclei [16]. Note, that in all the above works the full form of Bohr Hamiltonian with quadrupole and octupole deformations remains undefined. But here we must take into account that it remains to quantize the classical kinetic energy associated with rotation by octupole vibrations in curvilinear coordinates. Using the Pauli procedure [17] the work [18] describes in detail the quantization of the kinetic energy of a deformed nucleus in curvilinear coordinates for quadrupole vibrations of the surface of the nucleus. Quantization of the classical kinetic energy associated with rotation by octupole vibrations of the surface of the nucleus has not been performed. The purpose of the presented work is full form of Bohr Hamiltonian with quadrupole and octupole deformations.

II. QUADRUPOLE AND OCTUPOLE VIBRATIONS OF THE NUCLEAR SURFACE

The distance from the center of the nucleus to its surface in the direction of the polar angles θ and φ measured in the laboratory coordinate system for small deviations from the sphere radius R_0, $R(\theta,\varphi)$ can be expanded into spherical functions

$$R(\theta,\varphi) = R_0\left[1+\sum_{\lambda\mu}\alpha_{\lambda\mu}Y^*_{\lambda\mu}(\theta,\varphi)\right], \tag{1}$$

* Corresponding Author: mnadirbekov@yandex.ru
† qudiratov@inp.uz

where $\alpha_{\lambda\mu}$ are dynamic variables of collective motions in the nucleus and satisfy the condition $\alpha^*_{\lambda\mu} = (-1)^\mu \alpha_{\lambda,-\mu}$, which follows from the condition that spherical functions are real

$$Y^*_{\lambda\mu}(\theta,\varphi) = (-1)^{-\mu} Y_{\lambda,-\mu}(\theta,\varphi). \tag{2}$$

In the case of quadrupole and octupole vibrations, expression (1) can be written as

$$R(\theta,\varphi) = R_0 \left[1 + \sum_{\mu=-2}^{2} \alpha_{2\mu} Y^*_{2\mu}(\theta,\varphi) + \sum_{m=-3}^{3} \alpha'_{3m} Y^*_{3m}(\theta,\varphi) \right]. \tag{3}$$

We assume that the deformation is small enough that we do not need to introduce a monopole or dipole term to keep the volume of the nucleus and the position of the center of mass constant. We use the Bohr hydrodynamic model to express the kinetic energy. Now we associate a system of orthogonal coordinate axes with the nucleus $\xi\eta\zeta$, which orientation is relative to the laboratory system is determined by three Euler angles θ_i (i=1,2 and 3),

$$R(\theta,\varphi) = R_0 \left[1 + \sum_{\nu=-2}^{2} a_\nu Y^*_{2\nu}(\theta',\varphi') + \sum_{m=-3}^{3} a'_m Y^*_{3m}(\theta',\varphi') \right], \tag{4}$$

$$a_\nu = \sum_\mu \alpha_{\lambda\mu} D^{*\lambda}_{\lambda\mu}(\theta), \qquad \alpha_{\lambda\mu} = \sum_\nu D^\lambda_{\lambda\mu}(\theta) a_\nu,$$

where $D^\lambda_{\lambda\mu}(\theta)$ is the Wigner function.

Then we choose the coordinate axes system $\xi\eta\zeta$ as follows $a_1 = a_{-1}$=0, $a_2 = a_{-2}$ and

$$a_0 = \beta_2 \cos\gamma, \qquad a_2 = a_{-2} = \frac{\beta_2 \sin\gamma}{\sqrt{2}}, \tag{5}$$

where $\beta_2 \geq 0$ is the quadrupole deformation parameter, γ ($0 \leq \gamma \leq \frac{\pi}{3}$) is the quadrupole deformation asymmetry parameter [1, 3].

We choise the body-fixed coordinate axes, and also assume that the shape of the nucleus becomes symmetrical at large octupole deformation, then the asymmetry parameters tend to zero, i.e.: [19] $a'_{3,\pm1}$=$a'_{3,\pm3}$=0, $a'_{3,2}$=$a'_{3,-2}$ and

$$a'_{30} = \beta_3 \cos\eta, \qquad a'_{32} = a'_{3,-2} = \frac{\beta_3 \sin\eta}{\sqrt{2}}, \tag{6}$$

where β_3 is the octupole deformation parameter, η ($0 \leq \eta \leq \frac{\pi}{2}$) is the octupole deformation asymmetry parameter [20].

Then the total energy of quadrupole and octupole vibrations has the form [3]

$$E = \frac{B_2}{2}(\dot\beta_2^2 + \beta_2^2 \dot\gamma^2) + \frac{B_3}{2}(\dot\beta_3^2 + \beta_3^2 \dot\eta^2) +$$

$$+ V(\beta_2,\beta_3,\gamma,\eta) + \sum_{\kappa=1}^{3} \frac{\omega_\kappa^2 J_\kappa}{2}, \tag{7}$$

where first and second terms are operators kinetic energy of quadrupole and octupole vibrations, respectively, quantities B_2 and B_3 are the quadrupole and octupole mass parameters, respectively, $V(\beta_2,\beta_3,\gamma,\eta)$ are potential energy of β_2-, β_3-, γ- and η- vibrations, the last term in (7) is the rotational energy. ω_κ (κ=1,2,3) components of angular velocities of the nucleus with quadrupole and octupole deformations in the body-fixed system, that can be expressed through time derivatives of three Euler angles [18], J_κ are components of the total moment of inertia and has the following form:

$$J_1 = B_2(3a_{20}^2 + 2\sqrt{6}a_{20}a_{22} + 2a_{22}^2) + 4B_3(3a_{30}^2 + 4a_{32}^2 + \sqrt{30}a_{30}a_{32}), \tag{8}$$

$$J_2 = B_2(33a_{20}^2 - 2\sqrt{6}a_{20}a_{22} + 2a_{22}^2) + 4B_3(3a_{30}^2 + 4a_{32}^2 - \sqrt{30}a_{30}a_{32}), \tag{9}$$

$$J_3 = 8B_2a_{22}^2 + 8B_3a_{32}^2. \tag{10}$$

To quantize the total energy (7), the following conditions must be met. Kinetic energy is expressed explicitly in terms of the time derivatives of collective variables. And potential energy must be written in the form of scalar variables. The total moment of inertia associated with the collective rotations was diagonal. Because we consider quadrupole and octupole are separately.

III. QUANTIZATION OF THE KINETIC ENERGY OF AN OCTUPOLE DEFORMED NUCLEUS IN CURVILINEAR COORDINATES

To quantize the classical kinetic energy associated with rotation and quadrupole and octupole vibrations of the surface of the nucleus, it is necessary to select the Euler angles θ_1, θ_2, θ_3 and internal variables a_{20}, a_{22}, a_{30} and a_{33}. Here curvilinear coordinates are defined as coordinates that cannot be written as linear combinations of Cartesian coordinates with fixed coefficients [21]. It should be noted that the quantization of the kinetic energy of a deformed nucleus in curvilinear coordinates for the internal variables a_{20} and a_{22} was performed in detail by Ref. [18].

Now we perform the same procedure for the variables a_{30} and a_{32}. In this paper, we consider the simultaneous occurrence of quadrupole and octupole deformationof the shape even-even nucleus. But we do not take into account their interaction, by the reason the problem becomes mathematically very complicate and we start for the beginning from the same approximation, when we can neglect by their interaction. Therefore we can write the energy of octupole vibrations by analogy with quadrupole vibrations as in [1, 3]:

$$E_{\beta_3} = \frac{B_3}{2}(\dot{\beta}_3^2 + \beta_3^2\dot{\eta}^2) + V(\beta_3,\eta) + \sum_{\kappa=1}^{3}\frac{\omega'^2_\kappa J_\kappa^{(3)}}{2}. \tag{11}$$

here $V(\beta_3,\eta)$–potential energy of β_3-and η- vibrations, the last term is the rotational energy operator in the case of octupole vibrations, ω'_κ components of angular velocities of the nucleus with octupole deformation in the body-fixed system. And components of the total moment of inertia for octupole vibrations equal to:

$$J_1^{(3)} = 4B_3\left(3a_{30}^2 + 4a_{32}^2 + \sqrt{30}a_{30}a_{32}\right), \tag{12}$$

$$J_2^{(3)} = 4B_3\left(3a_{30}^2 + 4a_{32}^2 - \sqrt{30}a_{30}a_{32}\right), \tag{13}$$

$$J_3^{(3)} = 8B_3a_{32}^2. \tag{14}$$

Write the kinetic energy operator [18]

$$\hat{T} = -\frac{1}{2}\hbar^2\sum_\mu \frac{1}{m_\mu}\frac{\partial^2}{\partial x_\mu^2}. \tag{15}$$

Now the kinetic energy operator corresponding to the classical expression (11) can be written as [18]

$$\hat{T} = -\frac{\hbar^2}{2}\frac{1}{\sqrt{G}}\sum_{ij}\frac{\partial}{\partial q_i}\left(\sqrt{G}g^{ij}\frac{\partial}{\partial q_j}\right), \tag{16}$$

where G is the determinant of the metric tensor $g_{\mu\nu}$, which is determined by following expression:

$$g_{\mu\nu} = \sum_k J_k V_{k,\mu}(\theta_i)V_{k,\nu}(\theta_i), \qquad \mu,\nu \geq 3. \tag{17}$$

where $V_{k,\nu}(\theta_i)$ as in [18]

$$V_{k,l}(\theta_1,\theta_2,\theta_3) = \begin{pmatrix} -\sin\theta_2\cos\theta_3 & \sin\theta_3 & 0 \\ \sin\theta_2\sin\theta_3 & \cos\theta_3 & 0 \\ \cos\theta_2 & 0 & 1. \end{pmatrix} \tag{18}$$

Now we get an explicit expression for the matrix (17):

$g_{\mu\nu} =$

$$= \begin{pmatrix} B_3 & 0 & 0 & 0 & 0 \\ 0 & 2B_3 & 0 & 0 & 0 \\ 0 & 0 & (J_1\cos^2\theta_3 + J_2\sin^2\theta_3)\sin^2\theta_2 + \\ & & +J_3\cos^2\theta_2 & (J_2 - J_1)\sin\theta_2\cos\theta_3\sin\theta_3 & J_3\cos\theta_2 \\ 0 & 0 & (J_2 - J_1)\sin\theta_2\cos\theta_3\sin\theta_3 & J_1\sin^2\theta_3 + J_2\cos^2\theta_3 & 0 \\ 0 & 0 & J_3\cos\theta_2 & 0 & J_3. \end{pmatrix}$$

Find the determinant of this matrix

$$G = det(g_{\mu\nu}) = 2B_3^2 \sin^2\theta_2 J_1 J_2 J_3 =$$

$$= 32B_3^5 \sin^2\theta_2 a_{32}^2 \left[\left(3a_{30}^2 + 4a_{32}^2\right)^2 - 30a_{30}^2 a_{32}^2\right]. \tag{19}$$

The matrix $g^{\mu\nu}$, the inverse of the matrix $g_{\mu\nu}$ (17), has been found from the relation

$$g^{\mu\nu} = g_{\mu\nu}^{-1} = \frac{G_{\mu\nu}}{G}, \tag{20}$$

where $G_{\mu\nu}$ is the algebraic complement of the element $g_{\mu\nu}$ in the determinant of G. Now we find non-zero matrix elements of $g_{\mu\nu}^{-1}$:

$$g_{11}^{-1} = \frac{1}{B_3}, \quad g_{22}^{-1} = \frac{1}{2B_3}, \tag{21}$$

$$g_{33}^{-1} = \frac{2B_3^2 J_3}{G}(J_1 \sin^2\theta_3 + J_2 \cos^2\theta_3), \tag{22}$$

$$g_{34}^{-1} = g_{43}^{-1} = \frac{-2B_3^2 J_3}{G} \sin\theta_2 \sin\theta_3 \cos\theta_3 (J_1 - J_2), \tag{23}$$

$$g_{35}^{-1} = g_{53}^{-1} = \frac{-2B_3^2 J_3}{G} \cos\theta_2 (J_1 \sin^2\theta_3 + J_2 \cos^2\theta_3), \tag{24}$$

$$g_{44}^{-1} = \frac{2B_3^2 J_3}{G} \sin^2\theta_2 (J_1 \cos^2\theta_3 + J_2 \sin^2\theta_3), \tag{25}$$

$$g_{45}^{-1} = g_{54}^{-1} == \frac{2B_3^2 J_3}{G} \cos\theta_2 \times$$

$$\times(-J_1 \sin\theta_2 \cos\theta_3 \sin\theta_3 + J_2 \sin\theta_2 \sin\theta_3 \cos\theta_3), \tag{26}$$

$$g_{55}^{-1} = \frac{2B_3}{G} \sin^2\theta_2 \times$$

$$\times \left[J_1 J_2 \cos^4\theta_3 + J_2 \cos^2\theta_3 (J_3 \cot\theta_2 + 2J_1 \sin^2\theta_3) +\right.$$

$$\left. + J_1 \sin^2\theta_3 (J_3 \cot^2\theta_2 + J_2 \sin^2\theta_3)\right]. \tag{27}$$

Note that the expression for g_{55}^{-1} (27) differs from that in work [18].

Further find volume element in the form

$$d\tau = |G| dq_1 ..... dq_N. \tag{28}$$

here q_i are generalized coordinates.

Using formula

$$\omega_k' = \frac{d\beta_k}{dt} = \sum_i V_{ki} \frac{\partial\theta_i}{dt}, \tag{29}$$

we rewrite the formula (11) in the form

$$E_{\beta_3} = \frac{1}{2}\sum_k J_k(a_{30}, a_{32}) \left(\sum_i V_{kl}(\theta_1, \theta_2, \theta_3) \frac{d\theta_i}{dt} \right)^2 + \frac{1}{2} B_3(\dot{a}_{30}^2 + \dot{a}_{33}^2). \tag{30}$$

We choose generalized coordinates q_i

$$q_1 = a_{30}, \quad q_2 = a_{32}, \quad q_3 = \theta_1, \quad q_4 = \theta_2 \quad q_5 = \theta_3. \tag{31}$$

We determine some matrix elements $g_{\mu\nu}$ of the matrix (19)

$$g_{11} = B_3, \quad g_{22} = 2B_3,$$

$$g_{1k} = g_{k1}, \quad \texttt{for} \quad k \neq 1,$$

$$g_{2k} = g_{k2},, \quad \texttt{for} \quad k \neq 2.$$

Now we rewrite the determinant G (19) as:

$$G^{1/2} = 16 B_3^{5/2} \sin\theta_2 \left[9a_{30}^4 a_{32}^2 - 6a_{30}^2 a_{32}^4 + 16 a_{32}^6 \right]^{1/2}.$$

We will calculate the kinetic energy operator for g_{11}^{-1} and

$$-\frac{\hbar^2}{2}\frac{1}{G^{1/2}}\frac{\partial}{\partial q_1} G^{1/2} g_{11}^{-1} \frac{\partial}{\partial q_1} = -\frac{\hbar^2}{2B_3}\left[\frac{6a_{30}\left(3a_{30}^2 - a_{32}^2\right)}{9a_{30}^4 - 6a_{30}^2 a_{32}^2 + 16 a_{32}^4} \frac{\partial}{\partial a_{30}} + \frac{\partial^2}{\partial a_{30}^2} \right].$$

Now we will calculate the kinetic energy operator for g_{22}^{-1} and

$$-\frac{\hbar^2}{2}\frac{1}{G^{1/2}}\frac{\partial}{\partial q_2} G^{1/2} g_{22}^{-1} \frac{\partial}{\partial q_2} = \left[\frac{3(3a_{30}^4 - 4a_{30}^2 a_{32}^2 + 16 a_{32}^4)}{2a_{32}(9a_{30}^4 - 6a_{30}^2 a_{32}^2 + 16 a_{32}^4)} \frac{\partial}{\partial a_{32}} + \frac{\partial^2}{2\partial a_{32}^2} \right].$$

We obtain the expression for the kinetic energy operator

$$\hat{T}_{a_{30}, a_{32}} = -\frac{\hbar^2}{2B_3}\left[\frac{6a_{30}\left(3a_{30}^2 - a_{32}^2\right)}{9a_{30}^4 - 6a_{30}^2 a_{32}^2 + 16 a_{32}^4} \frac{\partial}{\partial a_{30}} + \right.$$

$$\left. + \frac{\partial^2}{\partial a_{30}^2} + \frac{3(3a_{30}^4 - 4a_{30}^2 a_{32}^2 + 16 a_{32}^4)}{2a_{32}(9a_{30}^4 - 6a_{30}^2 a_{32}^2 + 16 a_{32}^4)} \frac{\partial}{\partial a_{32}} + \frac{\partial^2}{2\partial a_{32}^2} \right].$$

Move on from a_{30} and a_{32} to variables β_3 and η and also considering:

$$\beta_3 = \sqrt{a_{30}^2 + 2a_{32}^2}, \qquad \eta = \arctan\sqrt{2}\frac{a_{32}}{a_{30}}.$$

We obtain the final form of the expression for classical kinetic energy (11) of octupole β_3 and η vibrations of the surface of the nucleus in curvilinear coordinates. The operator of kinetic energies of β_3-vibration:

$$\hat{T}_{\beta_3} = -\frac{\hbar^2}{2B_3}\frac{1}{\beta_3^4}\frac{\partial}{\partial\beta_3}\left(\beta_3^4 \frac{\partial}{\partial\beta_3}\right) \tag{32}$$

The operator of kinetic energies of η-vibration:

$$\hat{T}_{\eta} = -\frac{\hbar^2}{2B_3\beta_3^2}\left[\frac{\partial^2}{\partial\eta^2} + \frac{24\cos^2 2\eta - 6\cos 2\eta}{5 + 5\cos 2\eta + 8\cos^2 2\eta} \frac{\cos\eta}{\sin\eta}\frac{\partial}{\partial\eta} \right]. \tag{33}$$

The resulting expressions (32) and (33) is compared with a similar expression for quadrupole β_2 and γ vibrations of the surface of the nucleus [1, 3]. The operator of kinetic energies of β_2-vibration:

$$\hat{T}_{\beta_2} = -\frac{\hbar^2}{2B_2}\frac{1}{\beta_2^4}\frac{\partial}{\partial\beta_2}\left(\beta_2^4 \frac{\partial}{\partial\beta_2}\right) \tag{34}$$

The operator of kinetic energies of γ-vibration:

$$\hat{T}_{\gamma} = -\frac{\hbar^2}{2B_2}\frac{1}{\sin 3\gamma}\frac{\partial}{\partial\gamma}\left(\sin 3\gamma \frac{\partial}{\partial\gamma}\right) \tag{35}$$

It can be seen that the last factors in the formulas (32) and (34) do not coincide. Although the dynamic variables a_{20}, a_{22} and a_{30}, a_{32} have 4similar expressions by (5) and (6), but the type of expression for the components of their moments of inertia is different, i.e. the first and second terms in formulas (8) and (9).

IV. BOHR HAMILTONIAN OF THE EVEN-EVEN NUCLEI WITH QUADRUPOLE AND OCTUPOLE DEFORMATIONS

The total energy of surface quadrupole and octupole vibrations of an even-even nuclei expressed by formula (7). Then the Bohr Hamiltonian of an even-even nucleus with quadrupole and octupole deformations in the curvilinear coordinates has the following form:

$$\hat{H} = \hat{T}_{\beta_2} + \hat{T}_{\beta_3} + \hat{T}_{\gamma} + \hat{T}_{\eta} + \hat{T}_{rot} + V(\beta_2, \beta_3, \gamma, \eta). \tag{36}$$

The general solution of the Schrödinger equation with the operator (36) depends on the chosen potential energy $V(\beta_2, \beta_3, \gamma, \eta)$. Usually this problem can be solved by choosing the phenomenological form of this potential energy. Often the general form of potential energy is expressed in following [22]:

$$V(\beta_2, \beta_3, \gamma, \eta) = V(\beta_2) + V(\beta_3) + \frac{V(\gamma)}{\beta_2^2} + \frac{V(\eta)}{\beta_3^2}, \tag{37}$$

where V(β_2), V(β_3), V(γ) and V(η) – potential energies of β_2-, β_3-, γ- and η-vibrations, separately.

A general solution to the Schrödinger equation with the operator (36) has not yet been found. Therefore, the study of collective excitations of the deformed even-even nuclei is carried out by introducing simplifying assumptions.

V. CONCLUSION

The general theory of quadrupole and octupole excitation of an even-even nuclei is described by the Hamilton operator. It is convenient to represent this operator in curvilinear coordinates. Previously, the Hamiltonian operator in curvilinear coordinates for quadrupole deformations was obtained. In this work firstly the quantization of the kinetic energy of a deformed nucleus in curvilinear coordinates in the case of octupole vibrations of its surface has been carried out. Thus, we have obtained the exact form of the complete Hamiltonian of an even-even nucleus with quadrupole and octupole deformation, which contains seven dynamical variables β_2, γ, β_3, η, θ_1, θ_2, θ_3.

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