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$K = 1, 2, 3$ OCTUPOLE VIBRATIONS

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Abstract: Applying the Bohr-Mottelson hydrodynamic model, we develop and solve a coupled Schrödinger equation yielding the $K = 1, 2, 3$ octupole vibrations in deformed even nuclei (the $K = 0$ state is obtained trivially). For higher states, K does not appear to be a good quantum number. We assume the simple rotation-vibration picture in the adiabatic approximation and neglect quadrupole-octupole coupling. The model does not fix the energies; it permits any order among the $K = 1, 2, 3$ states.

1. Introduction

For deformed even nuclei the Bohr-Mottelson collective model gives a qualitative prediction of octupole vibrations [1]) with $K = 0$ ($J^P = 1^-, 3^-, 5^-, \ldots$), $K = 1$ ($J^P = 1^-, 2^-, 3^-, \ldots$), $K = 2$ ($J^P = 2^-, 3^-, 4^-, \ldots$) and $K = 3$ ($J^P = 3^-, 4^-, 5^-, \ldots$). They correspond roughly to the surface shapes Y_{3K}. However, generally there is coupling between the multipole shapes Y_{lm}, and the goodness of the K quantum number is not evident except for the manifestly axial-symmetric case $K = 0$. Below we demonstrate that a coupled problem does yield the $K = 1, 2, 3$ vibrations.

In sect. 2 we outline the general rotation-vibration problem, state the approximations and derive a Schrödinger equation for octupole vibrations. Then, in sect. 3, we develop the solution for K, and in sect. 4 for the energy. Sect. 5 gives the discussion.

2. The rotation-vibration problem

In the laboratory coordinate system the nuclear surface is [2])

$$R(\Omega) = R_0[1 + \sum_{lm} \alpha_{lm} Y^*_{lm}(\Omega)] \tag{1}$$

with $\alpha_{l-m} = (-)^m \alpha^*_{lm}$. The corresponding coefficients a_{lm} in the body-fixed coordinate system are

$$a_{lm} = \sum_{m'} D^{(l)}_{m'm} \alpha_{lm'} . \tag{2}$$

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The classical kinetic energy for small oscillations † becomes with eq. (2)

$$T = \tfrac{1}{2}\sum_{lm} B_l|\dot{\alpha}_{lm}|^2$$

$$= \tfrac{1}{2}\sum_{k=1}^{3} \mathscr{I}_k \omega_k^2 + \tfrac{1}{2}\sum_{lm} B_l|\dot{a}_{lm}|^2 + H'. \tag{3}$$

Here the first term, where $\mathscr{I}_k \equiv \mathscr{I}_{kk}$ given by eq. (5) below, is the diagonal part of the rotational energy, the second term is the vibrational energy, and H' is the rest. Specifically, H' contains the off-diagonal rotational energy and the Coriolis-type rotation-vibration coupling :

$$H' = \tfrac{1}{2}\sum_{k\neq k'} \mathscr{I}_{kk'}\omega_k\omega_{k'} - \mathrm{Im}\sum_k \sum_{lmm'} B_l(-)^{m+m'} \dot{a}^*_{lm} a_{lm'} \langle lm|L_k|lm'\rangle \omega_k, \tag{4}$$

where

$$\mathscr{I}_{kk'} = \sum_{lmm'} B_l(-)^{m+m'} a^*_{lm} a_{lm'} \langle lm|L_k L_{k'}|lm'\rangle \tag{5}$$

(note that in the body system $[L_1, L_2] = -iL_3$ etc.).

In the quadrupole problem ($l = 2$) the shape (1) is ellipsoidal and the body axes can be taken as principal axes [3]). Then we have $a_{2\pm1} = 0$, $a_{22} = a_{2-2} = a^*_{22}$ (a_{20} is necessarily real). It follows that H' vanishes for the pure $l = 2$ problem. However, once the body axes have been so fixed, all the coefficients a_{lm} for a given $l \geqq 3$ are present and they are complex (except a_{l0}).

In earlier octupole work [4-7]), the coefficients a_{3m} have been taken as real and/or some of them have been assumed absent, in order to make the Coriolis term †† or all of H' vanish. Without such arbitrary restrictions on the degrees of freedom, H' will not vanish. Nevertheless, what little experimental information there is [8]), it supports the simple rotation-vibration picture as a reasonable first approximation for the octupole case, and we drop H' in what follows.

We make the adiabatic approximation of small vibrations about a large axial quadrupole deformation:

$$\mathscr{I}_1 = \mathscr{I}_2 = \mathscr{I}_0, \qquad \mathscr{I}_3 = 8B_2|a_{22}|^2 + 2B_3(|a_{31}|^2 + 4|a_{32}|^2 + 9|a_{33}|^2). \tag{6}$$

Upon quantization, the coupling between the a_{lm} will appear in the form $1/\mathscr{I}_3$ (see below). We note the absence of a_{l0}, which means that each axially symmetric mode ($K = 0$) is decoupled from the rest. This leads immediately to the β-vibrations and the $K = 0$ octupole vibrations (b-vibrations) [4,9]).

As we are specifically concerned with the octupole states, we neglect for simplicity the quadrupole-octupole coupling by dropping the a_{22} term from eq. (6); this coupling is considered in ref. [9]). (Accordingly γ-vibrations will not appear in the present problem.)

† We assume mass parameters B_l rather than B_{lm}, even though deformed nuclei are considered [1]).

†† Davidson's argument [6]) for the vanishing of the Coriolis term fails upon quantizing the vibrations because the matrix of $\dot{a}$ is pure imaginary.

We now take x, y, z, defined by

$$x^2 = 2|a_{31}|^2, \qquad y^2 = 2|a_{32}|^2, \qquad z^2 = 2|a_{33}|^2, \tag{7}$$

for the coordinate variables of our vibrational problem and perform canonical quantization as in refs. [3,9]), finding

$$T_{\text{vib}} = -\frac{\hbar^2}{2B_3}\left[\nabla^2 + \frac{1}{x^2+4y^2+9z^2}\left(x\frac{\partial}{\partial x} + 4y\frac{\partial}{\partial y} + 9z\frac{\partial}{\partial z}\right)\right]. \tag{8}$$

In the approximation $H' = 0$ the body axes are principal axes, and we have with eq. (6)

$$\begin{aligned} T_{\text{rot}} &= \frac{\hbar^2}{2}\sum_k \frac{J_k^2}{\mathscr{I}_k} \\ &= \frac{\hbar^2}{2\mathscr{I}_0}[J(J+1) - K^2] + \frac{\hbar^2}{2B_3}\frac{K^2}{x^2+4y^2+9z^2}. \end{aligned} \tag{9}$$

For the potential we write

$$V = \tfrac{1}{2}C_x x^2 + \tfrac{1}{2}C_y y^2 + \tfrac{1}{2}C_z z^2. \tag{10}$$

Defining

$$T'_{\text{vib}} = T_{\text{vib}} + \frac{\hbar^2}{2B_3}\frac{K^2}{x^2+4y^2+9z^2}, \tag{11}$$

we have the vibrational Schrödinger equation

$$(T'_{\text{vib}} + V)\psi = E\psi. \tag{12}$$

3. The eigenvalue problem for K

We write the potential (10) in the form

$$\begin{aligned} V &= \tfrac{1}{2}C_3 r^2 + \tfrac{1}{2}c_x x^2 + \tfrac{1}{2}c_y y^2 + \tfrac{1}{2}c_z z^2 \\ &\equiv \tfrac{1}{2}C_3 r^2 + V' \end{aligned} \tag{13}$$

and treat V' as a perturbation. With the substitution

$$\psi = (x^2+4y^2+9z^2)^{-\frac{1}{4}} v \tag{14}$$

the unperturbed problem becomes

$$\left\{-\frac{\hbar^2}{2B_3}\left[\nabla^2 - \frac{f_K(\theta,\phi)}{r^2}\right] + \tfrac{1}{2}C_3 r^2\right\} v = Ev, \tag{15}$$

where

$$\frac{f_K(\theta,\phi)}{r^2} = \frac{25x^2+64y^2+9z^2}{4(x^2+4y^2+9z^2)^2} + \frac{K^2}{x^2+4y^2+9z^2}. \tag{16}$$

Writing

$$v = R(r)\mathscr{Y}(\theta, \phi)$$

we obtain the separation

$$\left\{-\frac{\hbar^2}{2B_3}\left[\nabla_r^2 - \frac{\lambda(\lambda+1)}{r^2}\right] + \tfrac{1}{2}C_3 r^2\right\} R = ER, \tag{17}$$

$$[\boldsymbol{L}^2 - \lambda(\lambda+1) + f_K(\theta, \phi)]\mathscr{Y} = 0, \tag{18}$$

where λ is a so far undetermined separation constant.

The requirement that ψ be analytic at the origin [10]) determines the eigenvalues of λ. As $r \to 0$, the asymptotic solution of eq. (17) is r^λ. According to eq. (14), ψ then has the asymptotic radial behaviour $r^{\lambda-\frac{1}{2}}$, which allows $\lambda = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$. However, the angular function $\mathscr{Y}$ imposes a further restriction. We shall find $\mathscr{Y}$ as a series in the spherical harmonics Y_{lm}. Analyticity requires that an even (odd) radial exponent $\lambda - \frac{1}{2}$ be taken together with even (odd) values of l. Thus for $\lambda = \frac{1}{2}$ we have $l = 0, 2, 4, \ldots$ and for $\lambda = \frac{3}{2}$ the values † $l = 1, 3, 5, \ldots$.

We seek solutions to eq. (18) in the form

$$\mathscr{Y} = \sum_{lm\sigma} c_{lm}^{\sigma} Y_{lm}^{\sigma}, \tag{19}$$

$$Y_{lm}^{\sigma} \equiv \frac{Y_{lm} + \sigma(-)^m Y_{l-m}}{\sqrt{2i^{1-\sigma}(1+\delta_{m0})}},$$

$$\sigma = \pm(1), \qquad m \geqq 0. \tag{20}$$

We note that the functions Y_{lm}^{σ} are orthonormal and real, and

$$Y_{l0}^{+} = Y_{l0}, \qquad Y_{l0}^{-} = 0.$$

These functions prove convenient because $f_K(\theta, \phi)$ contains only Y_{LM}^{+} with $L, M = 0, 2, 4$.

We clear the denominator of eq. (18), substitute in eq. (19) and form the secular equation, which will give the eigenvalues of K for a given λ. The matrix is reduced to eight unconnected submatrices by the selection rules $\Delta\sigma = 0$, $\Delta l =$ even, $\Delta m =$ even, which follow from the form of $f_K(\theta, \phi)$. Thus each submatrix, labelled I to VIII, is characterized by a certain set of l, m, σ values, as shown in table 1. We note that $\lambda = \frac{1}{2}, \frac{5}{2}, \frac{9}{2}, \ldots$ can be used in submatrices I, V, VI, VII and $\lambda = \frac{3}{2}, \frac{7}{2}, \frac{11}{2}, \ldots$ in II, III, IV, VIII.

In practice the matrices must be truncated after some l-value. Only the first approximation, involving a single matrix element, can be calculated conveniently by hand. In that approximation I, II, III and IV *with the lowest values of* λ give real values of K: 1.57, 3.34, 2.19 and 2.43, respectively. (Submatrices V–VIII give $K^2 < 0$.) Machine calculations of higher approximations showed that these K-values

† In familiar point-particle quantum mechanics the proper matching of radial and angular functions near the origin ($r^l Y_{lm}$) is automatic.

converge to 0, 3, 1 and 2. Below (sect. 4) the corresponding states are identified as the ground state and the sought one-quantum octupole states.

The machine calculations were done on an Elliott 503 at the State Computing Centre, Helsinki. Since the secular matrix is not symmetric, the diagonalization was done by Eberlein's method [11]). All submatrices were taken as large as 28×28. Convergence was rapid for II and IV, slow for I and intermediate for III.

TABLE 1

The l, m, σ values of the eight submatrices

I	II	III	IV	V	VI	VII	VIII
0 0+	1 0+	1 1+	1 1−	2 1+	2 1−	2 2−	3 2−
2 0+	3 0+	3 1+	3 1−	4 1+	4 1−	4 2−	5 2−
2 2+	3 2+	3 3+	3 3−	4 3+	4 3−	4 4−	5 4−
4 0+	5 0+	5 1+	5 1−	6 1+	6 1−	6 2−	7 2−
4 2+	5 2+	5 3+	5 3−	6 3+	6 3−	6 3−	7 4−
4 4+	5 4+	5 5+	5 5−	6 5+	6 5−	6 6−	7 6−
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

An easy approximation to eq. (18) is obtained by replacing $f_K(\theta, \phi)$ by its average value

$$\frac{1}{4\pi}\int d\Omega f_K(\theta, \phi) = 0.864 + 0.279K^2, \tag{21}$$

whence

$$K^2 \approx 3.6[\lambda(\lambda+1) - l(l+1)] - 3.1. \tag{22}$$

With lowest possible λ and l, this gives $K^2 = -0.4$ for I, $K = 1.8$ for II, III and IV, $K^2 = -22$ for V, VI and VII, and $K^2 = -33$ for VIII. This approximation is poor but provides some guidance at a glance.

For *higher values of* λ, eq. (22) gives further real K-values: e.g. $K = 5.3$ for $\lambda = \frac{5}{2}$, $l = 0$; these λ- and l-values can occur only in submatrix I. Numerically (28×28 matrix) we find $K = 6.5519$ as the largest K for I with $\lambda = \frac{5}{2}$. This is obtained already with the 10×10 matrix, so it is clear that this K does not converge to an integer. The same seems to hold for all K-values obtained with higher values of λ. The couplings contained in our T'_{vib} evidently mix K-values for the higher states, and the calculations give rms expectation values.

4. The energy problem

The radial equation (17) is that for a three-dimensional harmonic oscillator (except that λ is half-integral). Hence we have immediately

$$E_n^{(0)} = \hbar\omega(2k + \lambda + \tfrac{3}{2}) = \hbar\omega(n + \tfrac{3}{2}), \tag{23}$$

where

$$\omega = \sqrt{\frac{C_3}{B_3}}, \qquad k = 0, 1, 2, \ldots, \qquad n = \tfrac{1}{2}, \tfrac{3}{2}, \tfrac{5}{2}, \ldots;$$

we have added the superscript 0 to indicate that this is the *unperturbed* energy. We see that the state $\lambda = \frac{1}{2}$, $K = 0$ is the ground state for these vibrations, and the three states $\lambda = \frac{3}{2}$, $K = 1, 2, 3$ are degenerate at the energy $\hbar\omega$.

The degeneracy is removed by the perturbation V', defined in eq. (13), in first order. For the unperturbed angular functions $\mathscr{Y}(K)$ (eq. (19)) we take simply

$$\mathscr{Y}(1) = Y_{11}^{+}, \qquad \mathscr{Y}(2) = Y_{11}^{-}, \qquad \mathscr{Y}(3) = Y_{10}. \tag{24}$$

This is a good approximation since the next-largest amplitudes c_{lm}^{σ} are only of the order 0.1; this was established by computing the c_{lm}^{σ} from the 28×28 matrices. As the result of the perturbation calculation we find the ratios of the energy shifts $\Delta E(K)$:

$$\Delta E(1) : \Delta E(2) : \Delta E(3) = (3c_x + c_y + c_z) : (c_x + 3c_y + c_z) : (c_x + c_y + 3c_z). \tag{25}$$

This allows any order for the three levels.

We finally note that the wave functions $\psi(\lambda, K)$ have the rough asymptotic behaviour ($r \to 0$)

$$\begin{aligned} &\psi(\tfrac{1}{2}, 0) \sim \text{const.}, \\ &\psi(\tfrac{3}{2}, 1) \sim rY_{11}^{+} \propto x, \\ &\psi(\tfrac{3}{2}, 2) \sim rY_{11}^{-} \propto y, \\ &\psi(\tfrac{3}{2}, 3) \sim rY_{10} \propto z. \end{aligned} \tag{26}$$

In view of the definitions (7), we have here the pure multipole vibrations [1]). However, eqs. (26) are obtained only by neglecting the angular dependence of the factor $(x^2 + 4y^2 + 9z^2)^{-\frac{1}{4}}$ in eq. (14) and by making the approximation (24).

5. Discussion

We have demonstrated above that the macroscopic collective model predicts the one-quantum octupole states with good K in deformed nuclei. The singular $1/\mathscr{I}_3$ coupling between the octupole coordinates was taken as the only coupling.

The states $K^P = 2^+$ (γ-vibration), 1^- and 3^- are obtained from a mathematically identical problem. This problem was posed in ref. [9]), which contains the solution of the similar $K^P = 2^+, 2^-$ problem. The general quadrupole-octupole problem of this type would contain $K^P = 2^+, 1^-, 2^-, 3^-$. Such a four-dimensional problem could be solved by generalizing the techniques of the present study. Also, in that context it would be appropriate to trace the evolution of the solutions as couplings are introduced. To complete the problem, one should finally include the term H' defined by eqs. (3) to (5).

Experimental evidence on $K = 1, 2, 3$ octupole vibrations is scant [8]). The isotopes ^{182}W, ^{228,230}Th and ^{246}Cm have well-established $K^P = 1^-, 2^-$ bands. However, some of them are based on two-quasiparticle states rather than on octupole vibrations [12,13]). Of course, in final analysis all collective states too must be derivable from particle excitations.

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