GCM study of hexadecapole correlations in superdeformed $^{194}$Hg.

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Abstract

The role of hexadecapole correlations in the lowest superdeformed band of $^{194}$Hg is studied by self consistent mean field methods. The generator coordinate method with particle number projection has been applied using Hartree-Fock wave functions defined along three different hexadecapole paths. In all cases, the ground state is not significantly affected by hexadecapole correlations and the energies of the corresponding first excited hexadecapole vibrational states lie high in energy. The effect of rotation is investigated with the Skyrme-Hartree-Fock-Bogolyubov method and a zero range density-dependent pairing interaction.

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I. INTRODUCTION

Recent experimental data on the spectra of superdeformed (SD) bands in $^{149}$Gd [1], $^{153}$Dy [2], $^{194}$Hg [3], and $^{131,132}$Ce [4] have put into evidence a $\Delta I = 4$ staggering of the dynamical moment of inertia of these bands. It manifests itself in systematic shifts of the energy levels which are alternately pushed down and up with respect to a purely rotational sequence. The amplitude of this staggering is of the order of 50 eV. Since these oscillations distinguish states differing by four units of angular momentum, it seems natural to explain their origin by a coupling between the rotational motion and hexadecapole vibrations [1,5]. This scenario requires the presence in the mean field of the nucleus of a small component with a four-fold rotational symmetry, i.e., a symmetry associated with a $\frac{\pi}{2}$ rotation around one of the principal axes of the quadrupole tensor. The strongly prolate-deformed intrinsic Hamiltonian is then slightly perturbed by a term with the $C_4$ symmetry.

The effect of such terms has been investigated in phenomenological models with the $C_4$ symmetry axis coinciding either with the symmetry axis ($z$-axis) of the quadrupole tensor [6–8] or with the $C_4$ perturbation quantized along the rotation axis ($x$-axis) [1,9]. Hamamoto and Mottelson [8] have studied the properties of a quartic rotational Hamiltonian. Staggering appears then as a result of tunneling between the four equivalent minima of the total energy surface of the Hamiltonian due to the $K$-mixing. Burzyński et al. [10] have obtained the exact solutions for a system of $N$ identical particles in a single $j$-shell interacting through a multipole-multipole Hamiltonian with quadrupole and hexadecapole terms. They have shown that the staggering in $J^{(2)}$ may occur in certain cases.

All these studies have assumed the presence of a hexadecapole term in the Hamiltonian of the SD nucleus. It still remains to explain the origin of such a term. Ragnarsson [11] has considered triaxial hexadecapole deformations in a study at high spins of SD bands in the $A=150$ mass region using the shell correction approach with a Nilsson potential. The effect of $\epsilon_{44}$ deformation has been found extremely small. Frauendorf et al. [12] have applied the tilted axis cranking formalism also to a Nilsson Hamiltonian with a hexadecapole field, $Y_{44} + Y_{4,4}$, and have concluded that it is impossible to generate a staggering of the observed order of magnitude even assuming $\epsilon_{44}$ values as large as 0.1.

In the present work, based on self-consistent methods with Skyrme interactions, the importance of hexadecapole correlations in the lowest SD band of $^{194}$Hg is investigated. Firstly, we analyze dynamical hexadecapole correlations without rotation by means of the generator coordinate method (GCM) with particle number projection [13]. Secondly, cranking calculations have been performed within the Hartree-Fock-Bogoliubov + Lipkin Nogami (HFBLN) method [14,15] with a zero-range density dependent interaction [16] in the pairing channel.

II. THE METHODS

A. The Generator Coordinate method

The GCM formalism used in this study has been presented in detail in Ref. [13]. It permits one to study the dynamics of the nucleus as a function of one or several collective coordinates using generating functions with good particle number. The intrinsic wave functions, $|\Phi\rangle$, are obtained by constrained HF+BCS calculations with the Routhian
\[ E' = \langle \Phi | \hat{H} | \Phi \rangle - \lambda \langle \Phi | \hat{N} | \Phi \rangle - \lambda_2 \langle \Delta \hat{N}^2 \rangle - q_{i44}^i (\langle \Phi | \hat{Q}_{i44}^i | \Phi \rangle - Q_{i44}^i)^2. \]  

In Eq. (1) \( \hat{N} \) is the particle number operator and \( Q_{i44}^i \) denotes the hexadecapole moment quantized along the \( i \) axis, i.e.,

\[ Q_{i44}^i = \frac{1}{2} \int r^4 (Y_{i44}^x + Y_{i44}^z) \rho(r) d^3 r, \]

where \( i = x, z \) and \( \rho \) denotes the selfconsistent HFBCS density distribution. The functions \( Y_{i44}^x \) and \( Y_{i44}^z \) are the spherical harmonics along the \( x \) and \( z \) axis respectively. Thus \( Q_{i44}^i \) has a fourfold \((C_4)\) symmetry along the \( i \)th axis. The energy dependence on hexadecapole distortions around the SD minimum of \(^{194}\text{Hg}\) is determined using constraints on either \( Q_{i44}^z \) or \( Q_{i44}^x \). We have chosen \( z \) as the symmetry axis of the quadrupole tensor, whereas \( x \) denotes the perpendicular axis.

In the particle-hole channel, we employ the Skyrme interaction \( \text{SkM}^*[17] \). In the particle-particle (pairing) channel, the state-independent seniority interaction is used. An approximate variation after projection on particle number is performed by means of the Lipkin-Nogami method \[18\].

In this study it is assumed that the density distribution has three symmetry planes. The HF equations have then been solved on a rectangular mesh \( 12 \times 12 \times 16 \text{fm}^3 \), corresponding to the octant with positive values of the three cartesian coordinates. Single-particle wave functions are discretized with a mesh size of 1 fm. We have checked that the results are not qualitatively modified when increasing the size of the box or changing the mesh size.

From the HFBCS wave functions, states \( |NZ\rangle \) with the correct number of particles are obtained by projection:

\[ |NZ\rangle = \hat{P}_{NZ}|\Phi\rangle, \]

where

\[ \hat{P}_{NZ} = \frac{1}{\pi} \int_0^\pi \exp \left\{ i \phi_N (\hat{N} - N) \right\} d\phi_N \frac{1}{\pi} \int_0^\pi \exp \left\{ i \phi_Z (\hat{Z} - Z) \right\} d\phi_Z \]

is the projection operator on neutron and proton numbers. The integrations over the gauge angles are approximated by \( n \)-point trapeze formulae. The choice \( n = 7 \) ensures that the particle number dispersion never exceeds 0.001.

The GCM wave function is a superposition of projected wave functions corresponding to different hexadecapole deformations:

\[ |\Phi\rangle_{\text{GCM}} = \int f(Q_{i44}^i) |NZ; Q_{i44}^i\rangle dQ_{i44}^i \]

The weight function \( f \) is obtained from the Hill-Wheeler equation:

\[ \int \left[ \langle NZ; Q_{i44}^i | \hat{H} | NZ; Q_{i44}^i \rangle - E_{NZ; Q_{i44}^i} |NZ; Q_{i44}^i\rangle \right] f(Q_{i44}^i) dQ_{i44}^i = 0 \]

where \( \hat{H} \) is the many-body Skyrme+pairing Hamiltonian. Finally, the collective wave functions, \( g \), can be obtained by an integral transformation of \( f(Q_{i44}^i) \):

\[ g(Q_{i44}^i) = \int \langle NZ; Q_{i44}^i |NZ; Q_{i44}^i \rangle^{1/2} f(Q_{i44}^i) dQ_{i44}^i. \]
B. The cranked HFBLN method

The HFBLN method for rotating nuclei has been presented in Refs. \[14,15\]. As in the GCM calculations without rotation, the SkM* parametrization of the Skyrme force has been used in the particle-hole channel. In the pairing channel, the density-dependent pairing interaction,

$$V_P = \frac{V_0}{2} (1 - P_\sigma) \delta(\vec{r}_1 - \vec{r}_2) \left[ 1 - \alpha \rho \left( \frac{\vec{r}_1 + \vec{r}_2}{2} \right) \right]$$

(8)

has been employed. The strength $V_0$ has been chosen equal to 880 MeV and the reference density, $\rho_c = \alpha^{-1}$, to 0.16 fm$^{-3}$. It has been shown recently \[16\] that the introduction of a zero-range density dependent pairing interaction improves considerably the agreement between the HFBLN calculation and the experimental data for SD bands in the $A=190$ mass region. In particular, the experimental transition energies in the SD band of $^{194}$Hg are reproduced with a systematic error lower than 10 keV over 12 transitions.

Hexadecapole constraints have been introduced in the cranked HFBLN equations in the same way as in the nonrotating case.

III. RESULTS

The GCM collective path is determined by a full minimization of the energy with constraints on the hexadecapole moment alone, as defined by Eq. (1). This does not guarantee that other collective variables do not change along the path, i.e., that the hexadecapole mode is decoupled from all the other modes. In the case of such a coupling, one should in principle enlarge the collective subspace and include other variables as generator coordinates.

In our GCM calculations with the $Q_{44}$ constraint, the quadrupole-hexadecapole coupling is very weak. Namely, the mass quadrupole moment, $Q_{20} = Q_{20}^z = r^2 Y_{20}^z$, does not vary by more than 1$b$ in the whole considered range of $Q_{44}^z$ values. This is not true for the $Q_{44}^x$ trajectory. Indeed, the $Q_{44}^x$ moment can be expressed in terms of hexadecapole moments $Q_{4\mu}^z$ quantized along the z-axis:

$$Q_{44}^x = \frac{1}{8} Q_{44}^z + \frac{\sqrt{7}}{4} Q_{42}^z + \frac{\sqrt{70}}{16} Q_{40}^z.$$  

(9)

Consequently, $Q_{44}^x$ has $\mu=0$ and 2 components along the z axis which are strongly coupled to the quadrupole moments $Q_{20}^z$ and $Q_{22}^z$. To avoid many-dimensional GCM calculations in the $Q_{44}^x$ direction, we have defined two different trajectories. In the first version, the quadrupole moment varies self-consistently as a function of $Q_{44}^z$. In the second version, the quadrupole moment is constrained to its value at the SD minimum.

The potential energy curves corresponding to projected wave functions (3) are plotted in Fig. 1 as functions of $Q_{44}^z$ (top) and $Q_{44}^x$ (bottom). The evolution of the quadrupole moment $Q_{20}^z$ as a function of $Q_{44}^z$ is plotted on Fig. 2. In the same figures are shown the results of the HFBLN calculation performed at $I=42$.

According to the calculations, the collective motions along the $Q_{44}^z$ and $Q_{44}^x$ paths are decoupled. Namely, in the $Q_{44}^z$ version of the calculations, the value of $Q_{44}^x$ does not vary.
by more than 1000 fm$^4$ along the collective path. Also in the $Q_{44}$ version the value of $Q_{44}$ remains always compatible with zero.

The potential energy curves shown in Fig. 1 exhibit similar dependences as functions of the hexadecapole constraints. This means that, qualitatively, the response of the nucleus to the hexadecapole perturbation of the average field is the same in both cases. As expected, relaxing the constraint on the quadrupole moment (solid line in Fig. 1) leads to a slight decrease of the energy. In spite of the fact that the quadrupole moment shows large variation along the unconstrained path (see Fig. 2), the corresponding gain in energy never exceeds a few hundred keV.

The effect of rotation on total potential energies seems to be fairly weak, although the conditions of the calculations with or without rotation are not exactly the same. The curves are surprisingly close in the $Q_{44}$ variant. In the calculations with a constraint along the rotation axis, there is a slight shift of the minimum toward smaller hexadecapole moments at $I=42$ but the hexadecapole stiffness is very similar. The small shift in the equilibrium value of $Q_{44}$ with angular momentum can be attributed to the rotation-induced shape change in the SD yrast band of $^{194}$Hg. As discussed in Ref. [19], a systematic decrease in both a $Q_{50}$ and $Q_{40}$ with rotational frequency is expected for SD yrast band in $^{194}$Hg. According to the self-consistent calculations, the expectation value of $Q_{42}$ is almost zero (i.e., at least two orders of magnitude smaller than $Q_{40}$). Consequently, according to Eq (9), the equilibrium value of $Q_{44}$ should follow closely the value of $Q_{40}$. Indeed, the shift in $Q_{40}$ from approximately 38000 ($I=0$) to 35300 ($I=42$) fm$^4$ is consistent with the results displayed in Fig. 1.

It is worth noting that the quadrupole moments minimizing the energy for small values of $Q_{44}$ are rather different for $I=0$ and $I=42$ (see Fig. 2). This is probably more related to the different pairing interactions employed and to particle number projection than to rotation. Indeed, the quadrupole moments of the unprojected HFBCS states $|\Phi\rangle$ with and without rotation vary in a similar manner as functions of $Q_{44}$. On the other hand, the neutron pairing energy which is of the order of 4.0 MeV for both pairing interactions around the SD minimum, increases up to 6.5 MeV for a seniority interaction at small $Q_{44}$ values. This leads to large differences between the projected and unprojected wave functions.

A static calculation does not give access to a scale parameter which would permit one to compare directly the evolution of the energy as a function of $Q_{44}$ and $Q_{44}$. As discussed above, the large values of $Q_{44}$ are related to the large hexadecapole moment of the nucleus along the $z$ axis, while the mean value of $Q_{44}$ at the SD minimum is compatible with 0. A first crude measure of the variation of the collective wave functions along the collective path is given by the variation of the overlap between the wave functions corresponding to different values of $Q_{44}$. According to calculations, the overlaps between the wave functions corresponding to the SD minimum and the extreme hexadecapole deformations considered ($E^*\sim 4$ MeV) vary between 0.1 and 0.3. These rather large values imply the rigidity of SD states with respect to the hexadecapole fields with $\mu=4$.

A better way of comparing the collectivity along the collective paths considered is to perform the full GCM calculation. This calculation gives at the same time the distribution of the lowest wave function as a function of hexadecapole deformations and the excitation energies of the associated modes. We have performed GCM calculations along the three collective paths defined above. The $Q_{44}$ path with a constrained quadrupole deformation has been used to test the discretization of the hexadecapole moments, with up to 17 wave
functions corresponding to hexadecapole moments ranging from 4000 to 36000 fm$^4$. These tests have shown that eight to ten discretization points lead to an accuracy of the order of 100 keV, which is sufficient for our purpose.

The results for the three collective trajectories are summarized in Table I. The HFBCS SD state is predicted at an energy of 1519.41 MeV and its hexadecapole moments $Q_{44}^z$ and $Q_{44}^x$ are 0 and 20000 fm$^4$, respectively. These values are not strongly modified by the collective correlations. The predicted gain in energy due to dynamical correlations for the collective lowest state is in all cases lower than 1.0 MeV, which is much smaller than the typical energy gains associated with the quadrupole and octupole degrees of freedom (see for instance Ref. [20]). Also the quadrupole and hexadecapole moments of the first excited collective states are not significantly different from the values obtained for the static minimum. The energies of the first excited state are large, $E^* > 3$ MeV. The slightly lower value obtained in the unconstrained $Q_{44}^x$ path is probably more due to the variation of the quadrupole moment along the path than to a genuine hexadecapole effect.

In Fig. 3 are shown the squared moduli of the collective wave functions $g$, Eq. (7), corresponding to the lowest GCM state along the $Q_{44}^z$ (top) and $Q_{44}^x$ (bottom) trajectories discussed above. It is seen that the collective ground states do not show any significant distortion with respect to $Q_{44}$. The distributions are centered around the static minimum. The collective wave function obtained in the unconstrained $Q_{44}^x$ calculations is slightly asymmetric, i.e., components with lower hexadecapole moments have a slightly larger weight, but this effect is not large enough to modify the total hexadecapole moment.

The GCM results that we have discussed show that hexadecapole correlations are rather weak. In particular, no hexadecapole excitations at low energies have been found. However, the wave functions considered do not belong to a $C_4v$ irreducible representation. To construct such wave functions, one should consider the mixing of the four wave functions obtained by rotations of $\frac{\pi}{2}$ around the quantization axis of the hexadecapole tensor. For instance, for the $C_4$ symmetry associated with the $z$ axis, the four corresponding transformations of the HFBCS wave function $|\Phi\rangle$ can be expressed as permutations of coordinates:

$$
(x, y, z) \Rightarrow (y, -x, z) \Rightarrow (-x, -y, z) \Rightarrow (-y, x, z).
$$

(10)

Let us recall that if one imposes the condition that the nuclear density is symmetric with respect to the three planes $x = 0$, $y = 0$, $z = 0$, one can decompose the single particle wave function $\Phi_k$ into four components with definite parities with respect to these planes [21]. Namely, the wave function $\Phi_k$ can be written as:

$$
\Phi_k = \begin{pmatrix}
\Phi_{k,1} \\
\Phi_{k,2} \\
\Phi_{k,3} \\
\Phi_{k,4}
\end{pmatrix} = \begin{pmatrix}
Re\Phi_k(\vec{r}, +) \\
Im\Phi_k(\vec{r}, +) \\
Re\Phi_k(\vec{r}, -) \\
Im\Phi_k(\vec{r}, -)
\end{pmatrix}.
$$

(11)

This choice ensures that the parities of the components $\Phi_{k,\alpha}$ with respect to plane symmetries about $x$, $y$ and $z$ planes depend only on the label $\alpha$ and the parity $p_k$ as indicated in Table II. Up to an irrelevant phase factor, the permutation of $x$ and $y$ in wave function (11) gives rise to (for positive signature):

\...
where $\vec{r}'$ is obtained from $\vec{r}$ by the permutation of $x$ and $y$. Using relation (12) and Table II, one immediately sees that the second and fourth symmetry operations in Eq. (10) lead to wave functions with spin-down component orthogonal to the spin-down component of $\Phi_k$, provided that the $\Phi_{k,\alpha}$ have axial symmetry with respect to the $z$-axis. The overlap between the original HFBCS state and the total wave function obtained by the third transformation of Eq. (10) is equal to the third component of the vector density which is exactly zero for time reversal invariant wave functions.

The above symmetry properties lead to extremely small overlaps between the four wave functions generated by the $C_{4v}$ symmetry operations: they are lower than $10^{-5}$ for all the wave functions that we have used in our GCM calculation with a collective path defined along the $z$-axis. Our calculation has been performed without rotation. Two factors may increase these overlaps when the nucleus rotates. The first factor is the change in the spin content of the wave functions due to the Coriolis coupling. The second factor is the slight breaking of axial symmetry due to rotation. The importance of these effects remains to be studied quantitatively.

\section*{IV. CONCLUSIONS}

In this work we have analyzed the presence of hexadecapole correlations in the mean fields created by Skyrme like effective interactions. Hexadecapole deformations have been introduced by the addition of hexadecapole constraints aligned either along the symmetry axis or the axis of rotation.

The static effects of these correlations turn out to be very weak in SD $^{194}$Hg and do not seem to be enhanced by rotation. We have also tried to put into evidence dynamical effects thanks the generator coordinate method. The GCM ground states obtained along the three collectives paths introduced do not show any fingerprint of polarisation due to the hexadecapole modes. The first GCM excited modes appear also rather high in energy, at 3-4 MeV. The lowest energy has been obtained in a GCM calculation along an $x$-path with relaxed quadrupole moment. We have interpreted this result as being due mainly to quadrupole correlations. However, it remains to be verified in a more complete study whether hexadecapole correlations are enhanced by a direct coupling between quadrupole and hexadecapole modes.

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FIGURES

FIG. 1. Potential energy curve as a function of the $Q_{44}^{z}$ moment (top) and the $Q_{44}^{x}$ moment (bottom). The solid line represents the result obtained from particle-number-projected wave functions without rotation and the dashed line represents the HFBLN results at $I=42$. The dash-dotted line (bottom) represents the $I=0$ results with a fixed quadrupole moment.

FIG. 2. Mass quadrupole moment, $\langle r^2 Y_{20}^z \rangle$, versus $Q_{44}^{x}$ in the nonrotating case (solid line) and at $I=42$ (dashed line).

FIG. 3. Squared moduli of the collective GCM wave functions plotted versus the $Q_{44}^{z}$ moment (top) and the $Q_{44}^{x}$ moment (bottom). Solid and dashed lines represent the results obtained with unconstrained and constrained quadrupole moments, respectively.
TABLE I. The GCM results for the three collective paths specified by $Q_{44}^z$, $Q_{44}^x$ and $Q_{44}^{xz}$, where superscript $c$ denotes the collective path with constrained quadrupole moment. Excitation energies are denoted by $e^*$. Energies are given in MeV units and hexadecapole moments in fm$^4$ for the $Q_{44}^z$ path and in 1000 fm$^4$ in the two other cases.

| $n$ | $Q_{44}^z$ | Energy | $e^*$ | $Q_{44}^x$ | Energy | $e^*$ | $Q_{44}^{xz}$ | Energy | $e^*$ |
|-----|-----------|--------|------|-----------|--------|------|-------------|--------|------|
| 1   | 3.5       | -1520.12 | 0.00 | 21.2      | -1520.15 | 0.00 | 20.4        | -1520.36 | 0.00 |
| 2   | -27.0     | -1516.10 | 4.02 | 20.1      | -1516.95 | 3.21 | 23.6        | -1516.17 | 4.19 |
| 3   | 31.9      | -1514.47 | 5.65 | 15.5      | -1515.19 | 4.97 | 24.1        | -1515.14 | 5.22 |

TABLE II. Parities of the components $\Phi_{k,\alpha}$ of a function $\Phi_k$ of parity $p_k$, with respect to the $x = 0$, $y = 0$ and $z = 0$ planes.