Octupole excitations in light xenon and barium nuclei

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The properties of light even and odd Xe and Ba nuclei (N and Z close to 56) with respect to octupole deformation have been studied by the Hartree-Fock+BCS and the generator coordinate methods. None of the considered nuclei possess a stable static octupole deformation. However, we find that octupole collectivity is enhanced by dynamical correlations. Cranked shell model calculations indicate that octupole effects should persist at least up to spins around $10\hbar$.

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I. INTRODUCTION

The existence of octupole deformations in ground states of atomic nuclei is believed to occur predominantly when the numbers of neutrons and of protons are close to 56, 88, 136 [1,2]. These three numbers correspond to situations where the Fermi level lies between the intruder subshell $(N+1, l, j)$ and the normal parity subshell $(N, l-3, j-3)$. Manifestations of octupole deformation or strong octupole correlations have been observed in the regions of the light Ra and Th ($Z \approx 88, N \approx 136$), and of the heavy Xe and Ba nuclei ($Z \approx 56, N \approx 88$). The very light Xe and Ba isotopes with $Z \approx N \approx 56$ have also been suggested as candidates for enhanced octupole collectivity on the basis of Strutinsky-type calculations [3]. With the coming availability of highly granulated multidetector systems and of radioactive nuclear beams, it should now be possible to reach experimentally this mass region close to the proton drip line.

In the present work, we investigate whether the prediction of octupole deformation or softness near ^{112}Ba [3] is confirmed by a more microscopic approach. We also wish to provide a more quantitative analysis of the characteristics of octupole collectivity than that provided by the Strutinsky-type approach. In particular, we study the properties which may be of relevance for an experimental determination of the presence of octupole correlation effects: (i) the magnitude of the $E3$ and octupole-induced dipole transitions, (ii) octupole correlations in odd sytems, and (iii) influence of rotation on octupole correlations. In the present work, we have considered several approaches: first, the constrained Hartree-Fock + BCS method (HFBCS), which provides static deformation energy surfaces directly comparable with those found by the Strutinsky method, second, the generator coordinate method (GCM) at spin zero in order to study the magnitude of dynamical correlations, and third a cranking calculation using a Woods-Saxon potential to study the rotation effects.

The question of dipole transitions is an important one since they might be the most prominent experimental feature pointing to the existence of octupole correlations. Because it is likely that $E1$ transition rates in light Xe and Ba isotopes are hindered, their theoretical determination is rather a subtle matter. Two factors play a crucial role: octupole-induced dipole moments are expected to be much reduced for $N \approx Z$, but in addition, octupole softness is predicted to disappear when N or Z differ from 56 by more than a few units [3]. Therefore it would be very fortunate if strong enough $E1$ transitions could exist in a $N > 56$ system, still showing octupole softness.

The approach that we use to determine these $E1$ transition rates relies on GCM calculations based on a collective space determined by means of the HFBCS approximation using the same Hamiltonian. We believe that it is the most coherent scheme presently available to investigate the presence of octupole-induced $E1$ collectivity.

II. CALCULATIONS

First, we consider the deformation energy surfaces for axial quadrupole and octupole deformations. Then, octupole excitations are analyzed within the HF-BCS+GCM method, as described in Ref. [4], and applied for the first time to the case of octupole vibrations in Refs. [5,6]. These dynamical calculations are limited to octupole deformation, neglecting possible couplings to the quadrupole modes.

The first step consists in the determination of a set of HFBCS states with specified expectation values of the octupole moment $q_3 = \langle r^3 Y_{30} \rangle$. When the calculation does not include a constraint on the quadrupole moment $q_2 = \langle 2z^2 - x^2 - y^2 \rangle$, the variational nature of the HFBCS equations ensures that the function $q_2(q_3)$ corresponds to the lowest energy associated with a given octupole moment q_3. We use the Skyrme force SIII for the mean field. In the pairing channel, the interaction is of a seniority type with strengths $G_n = \frac{16.5}{(11+N)}$, $G_p = \frac{16.5}{(11+Z)}$. The

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high energy single particle space used to solve the BCS equations is truncated as described in Ref. [7]. In odd-neutron nuclei, the blocking is effected approximately by assuming 1/2 occupancy for both of the degenerate levels belonging to the selected orbital. This amounts to neglecting the small terms of the Skyrme functional associated with time reversal breaking. Moreover, in the treatment of pairing correlations, we use the blocking approximation by excluding the contribution of this orbital to the sums in the BCS equations.

In a second part, the set of HFBCS states with octupole moments q_3 ranging from -1600 fm^3 to $+1600$ fm^3 by steps of 200 fm^3 is used as a nonorthogonal basis for the diagonalization of the same Skyrme SIII + seniority force Hamiltonian. We interpret the lowest energy eigenstate as the intrinsic ground state (with K half integer for an odd-neutron system). The first excited state of negative parity is then considered as describing the lowest intrinsic octupole vibrational state on which a negative parity rotational band can be built. Since the GCM provides collective wave functions, we can evaluate the matrix elements of the proton octupole and dipole moments from which the $B(E3)$ and $B(E1)$ reduced transition probabilities are obtained.

In a previous study of even-even $N \approx Z \approx 56$ nuclei using the Strutinsky method [3], static octupole deformations were found for a rather limited number of isotopes. The energy gain due to octupole deformation exceeded 100 keV only in $^{108-112}$Xe and ^{112,114}Ba. In addition, ^{108}Xe and ^{112}Ba were predicted to be proton emitters in Ref. [1]. For these reasons this study has been restricted to the sequences $^{110-114}$Xe and $^{113-115}$Ba, which are anyhow the most likely isotopes to be investigated experimentally. Some experimental results concerning ^{114}Xe have been published recently [8].

III. RESULTS

A. HFBCS deformation energy surfaces

The HFBCS energy of ^{112}Xe is shown as a function of the quadrupole and octupole moments, (q_2, q_3), in Fig. 1. In order to relate the microscopically calculated values of the moments q_2 and q_3 with the conventional deformation parameters β_2, β_3, the following approximate relations have been used:

$$\beta_2 \approx 1.387\left\{\left(1+\frac{40}{21}\frac{q_2}{r_0^2 A^{5/3}}\right)^{1/2}-1\right\},$$

$$\beta_3 \approx \frac{2.424 q_3}{A^2(1+0.84\beta_2)}.$$

The relation between β_2 and q_2 does not take into account a hexadecapole deformation β_4, which in the Strutinsky calculations comes out between 0.06 and 0.08 near the ^{112}Xe minimum. Compared to the $\beta_4 = 0$ case, introducing the effect of β_4 would reduce slightly our values of β_2. To give an order of magnitude of the correspondence between the (q_2, q_3) and the (β_2, β_4) scales, in

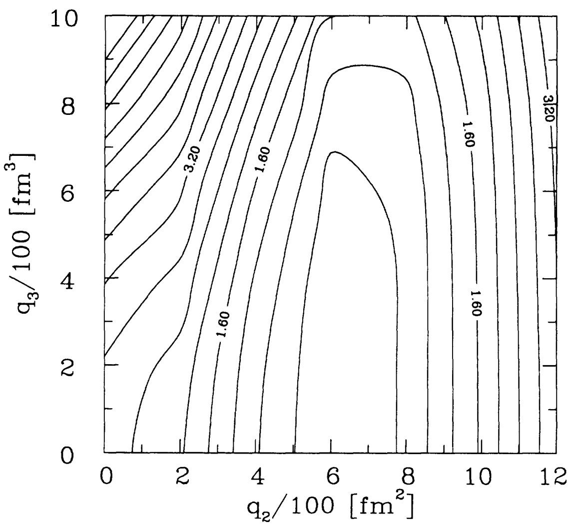

FIG. 1. Contour map in the (q_2, q_3) plane of the HFBCS energy calculated for the ^{112}Xe nucleus with the SIII force. The contour line spacing is 400 keV.

^{112}Xe, $q_2 = 600$ fm^2 corresponds to $\beta_2 \approx 0.2$ while $q_3 = 1000$ fm^3 corresponds to $\beta_3 \approx 0.19$ (at $\beta_2 = 0$).

The shallow minimum predicted in Ref. [3] is not present in the surface given by the HFBCS calculation. However, the octupole softness remains pronounced. For instance, at $q_2 = 600$ fm^2 the energy rises only by 240 keV when q_3 increases from 0 to 600 fm^3. Up to now, our calculations for other nuclei have shown that HFBCS produces at most very shallow octupole minima. Nonetheless, differences between the present method and that of Ref. [3] as regards octupole softness are limited and the overall agreement remains satisfactory.

In Fig. 2, neutron levels in ^{112}Xe are displayed as a function of quadrupole moment (at q_3=0). Levels responsible for the octupole deformation properties of the light

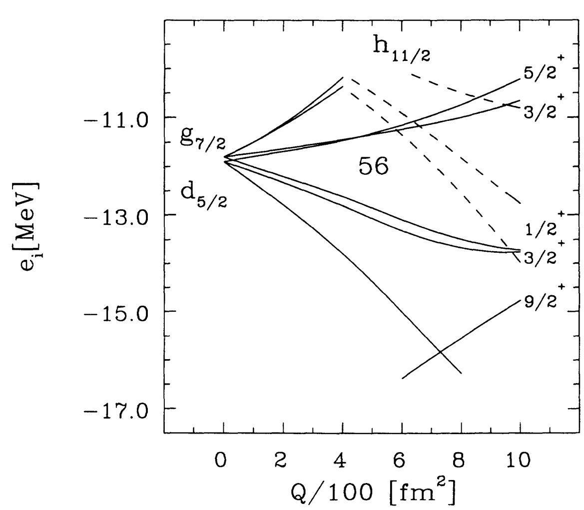

FIG. 2. Single particle neutron levels in ^{112}Xe vs quadrupole moment q_2 in the vicinity of the deformed $N = 56$ gap; continuous (dashed) lines denote positive (negative) parity levels. Spins and parities of positive parity levels are indicated.

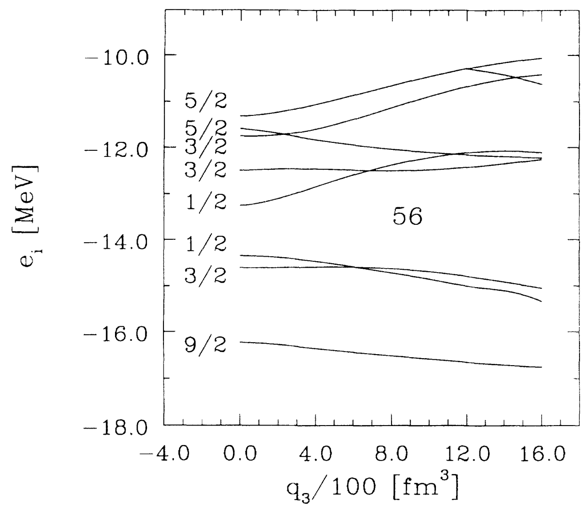

FIG. 3. Single particle neutron levels in ^{113}Ba vs octupole moment q_3; the quadrupole moment resulting from the HF-BCS calculation increases with q_3 from 800 to 950 fm^2.

Xe and Ba nuclei are the four $d_{5/2}, g_{7/2}$ orbitals together with the negative parity, low Ω $h_{11/2}$ orbitals. The gap at $N = 56$ stabilizes a moderate quadrupole deformation $q_2 \approx 600-700$ fm^2. The effect of octupole deformation on the ^{113}Ba s.p. levels is shown in Fig. 3. This spectrum correponds to a calculation in which the first $\Omega = 3/2$ level above the $N = 56$ gap is blocked. The value of the quadrupole moment which minimizes the energy for each octupole deformation increases from 800 fm^2 at $q_3 = 0$ to 950 fm^2 at $q_3 = 1600$ fm^3. Due to the interaction of the opposite parity $\Omega = 1/2$ and 3/2 orbitals the $N = 56$ gap becomes wider as the octupole moment increases creating either octupole softness or a shallow minimum. In the odd-neutron systems, the octupole $N = 56$ gap is large enough to destroy BCS pairing correlations for q_3 larger than 800 fm^3.

B. GCM dynamics

The GCM results are presented in Table I. As explained in Sec. II, the GCM basis is generated by HFBCS calculations with constraint on q_3 only, the value of the quadrupole moment corresponding to the minimum of the energy for each q_3 value. Thanks to our blocking approximation, the GCM matrix elements can be calculated for odd nuclei using the formalism presented in Ref. [4].

In all odd-neutron isotopes we have studied the $\Omega = 3/2$ band head by blocking the first level above the $N = 56$ gap (see Fig. 3). In ^{113}Ba, we have also calculated the octupole excitation properties of the $\Omega = 1/2$ state by using a HFBCS basis obtained by blocking the first $\Omega = 1/2$ orbital above the $N = 56$ gap. Since the energy of this orbital rises with q_3 (see Fig. 3), we find as expected that the corresponding GCM energy is larger than for the blocked $\Omega = 3/2$ state. The enhancement of octupole correlations caused by the particle number 56 is apparent in the set of excitation energies of the negative parity states in Table I.

TABLE I. For each nucleus indicated in the first column are given the GCM excitation energy of the negative parity intrinsic state, the transition dipole moment, and the $B(E3; K = 0, I = 0 \rightarrow K = 0, I = 3)$ value (in single particle units).

Nucleus	E (MeV)	D (e fm)	$B(E3)$ (s.p.u.)
^{110}Xe	1.59	0.01	17.3
^{111}Xe ($K = 3/2$)	1.47	−0.06	17.3
^{112}Xe	2.00	−0.04	16.8
^{113}Xe ($K = 3/2$)	1.85	−0.10	18.9
^{114}Xe	2.07	−0.17	18.0
^{113}Ba ($K = 3/2$)	0.97	0.06	22.0
^{113}Ba ($K = 1/2$)	1.46	0.06	18.8
^{114}Ba	1.21	0.03	21.9
^{115}Ba ($K = 3/2$)	1.24	−0.05	24.0

In the odd-neutron systems, energies of octupole phonons built on the $K = 3/2$ configuration are reduced with respect to their even neighbors. This is probably due to the quenching of neutron pair correlations caused by the blocking of a single particle. Indeed, the energy of the lowest two-quasiparticle (2qp) excitation is decreased in the odd system compared to its even neighbors, and one can expect in a dynamical calculation that this 2qp energy is an upper bound of the energy of the octupole phonon. In the HFBCS calculations, odd systems show also enhanced octupole softness, developing sometimes shallow octupole minima. This is visible in Fig. 4, where the HFBCS energy and the energies of the parity-projected states corresponding to fixed values of q_3 are shown for ^{113,114}Ba. Note also that the energy gain due to parity projection in the positive parity ground state is larger in the even systems than in the odd ones. The same is true for all the Xe and Ba isotopes that we have

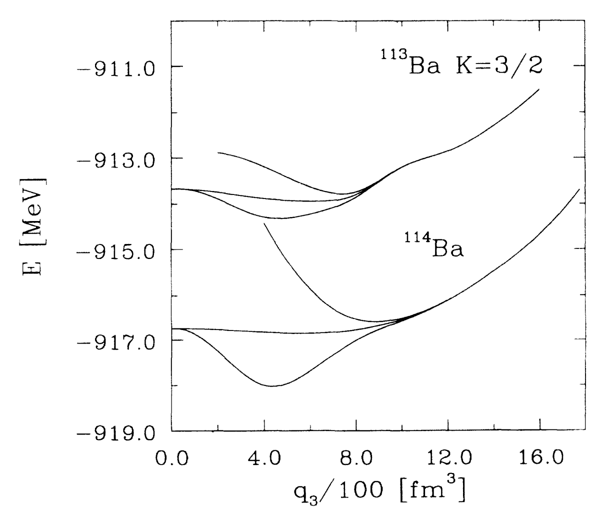

FIG. 4. HFBCS energy and energies of the parity-projected states ($\pi-$, the upper one; $\pi+$, the lower one) of ^{114}Ba and of the $K = 3/2$ configuration in ^{113}Ba (shifted down by 10 MeV) as a function of the octupole moment q_3.

considered, although the Ba case shown in Fig. 4 is the most pronounced one. It is probably due to the narrowing of the width of the GCM overlap kernel caused by the decrease of pairing correlations in odd isotopes.

We find very similar GCM $B(E3)$ values for all the isotopes. Transition dipole moments, on the other hand, do vary, especially in Xe isotopes where they show increase in magnitude with $N - 56$ with some even-odd staggering. They even change sign, as a function of the neutron number, and become negative in ^{111}Xe and ^{115}Ba. As expected, HFBCS intrinsic dipole moments increase in magnitude with q_3. In ^{110}Xe, intrinsic dipole moments are positive and smaller than 0.01 e fm for q_3 smaller than 1000 fm^3. They are also positive in ^{113,114}Ba. In all cases, the GCM transition dipole moments are very close to the HFBCS intrinsic dipole moments at $q_3 = 600$ fm^3, which is roughly the arithmetic mean of the q_3 equilibrium values of positive and negative parity energy curves (see Fig. 4).

We have also calculated the intrinsic dipole moments for the same nuclei within the shell correction method of Ref. [9] (with the macroscopic contribution discussed in Ref. [10] and the parameters of Ref. [11]). We have obtained results very similar to that of HFBCS, in particular, the negative signs of intrinsic dipole moments for the heaviest isotopes studied here. It follows from these calculations that the macroscopic contribution to the dipole moment comes out positive but in heavier isotopes it is dominated by the negative fluctuating part.

C. Effect of rotation

In order to appreciate the stability of octupole deformation or softness with respect to rotation we have performed some cranked Strutinsky calculations. Our model is based on the deformed Woods-Saxon potential [12] and the method of calculation is analogous to that of Ref. [13]. We have performed a detailed investigation of ^{112}Xe. The Routhians E^ω have been calculated as the sum of the energy at spin zero and of the relative Routhian, $\langle H^\omega\rangle - \langle H^{\omega=0}\rangle$. They have been minimized on a grid in the $(\beta_2, \beta_3, \beta_4)$ space with a value of β_5 fixed to $0.5\beta_3$. The values of β_2, β_3, and β_4 have been allowed to vary respectively from 0.10 to 0.26, 0 to 0.12, and 0.04 to 0.08. The pairing has been treated within the BCS approximation for $I = 0$ and the following parametrization of the pairing gap Δ has been used for $\omega > 0$:

$$\Delta(\omega) = \begin{cases} \Delta(0)[1 - \frac{1}{2}(\frac{\omega}{\omega_c})^2], & \omega < \omega_c, \\ \frac{1}{2}\Delta(0)(\frac{\omega_c}{\omega})^2, & \omega > \omega_c. \end{cases}$$

The parameter $\hbar\omega_c$ was fixed at 0.6 MeV for neutrons and 0.7 MeV for protons. Pairing strengths from Ref. [14] have been used. Since the mesh covers only the vicinity of the spin-zero equilibrium deformation [3], any minima which may exist outside this mesh (secondary at $I = 0$) are not considered in this study. We have checked that equilibrium values (β_2, β_3) minimizing the total Routhian are always in the interior of the grid.

With increasing ω, the reflection asymmetric minimum which at $I = 0$ corresponds to ($\beta_2 \approx 0.18$, $\beta_3 \approx 0.08$, $\beta_4 \approx 0.06$) shifts slightly towards larger β_2 and β_4 and smaller β_3. At $\hbar\omega = 0.3$ MeV ($I \approx 6 - 8\hbar$) it still corresponds to $\beta_3 \approx 0.06$ and is about 200 keV lower than the reflection symmetric one. For $\hbar\omega = 0.35$ MeV, after the $h_{11/2}$ neutron pair alignment, the Routhian minimum on the mesh shifts to $\beta_3 = 0.04$; however, the reflection symmetric point $\beta_3 = 0$ has nearly the same energy. This situation persists after the proton pair alignment.

A similar calculation for ^{114}Xe within a smaller mesh shows that the octupole deformed shape is energetically favored up to the first neutron pair alignment ($I \approx 10$), then the reflection symmetric shape becomes a minimum. One has to emphasize that the triaxial quadrupole effects, known to be important after the alignment of the first neutron pair in some other nuclei, have not been taken into account in the present calculation. Still, one can expect that octupole softness persists up to the first band crossing.

IV. CONCLUSIONS

We have studied the octupole deformation properties of light isotopes of Xe and Ba with $N \approx Z \approx 56$. Using the HFBCS+GCM method, we have calculated the energies, transition dipole moments and $B(E3)$ transition probabilities for the octupole phonon states. The prediction of octupole softness of these nuclei made in Ref. [3] is supported by this study and has been extended to odd-neutron isotopes. The predicted $B(E3)$ values are close to 20 W.u. for all isotopes whereas the transition dipole moments show large variations with the neutron number. Odd nuclei are in general more favorable to detect $E1$ transitions than their even neighbors. Except in ^{113,114}Xe, the magnitude of these $E1$ transitions is rather small. However, it should still be investigated whether the explicit introduction of the dipole degree of freedom in the GCM dynamics would not lead to a change of the predicted $E1$ transition rates. Using the Woods-Saxon Strutinsky cranking method, we have also found that octupole softness should persist at least up to spins $I \leq 10$.

The breaking of reflection symmetry in ^{114}Xe has been recently suggested by experimental data [8]. The excitation energy found for the 3^- state (1.62 MeV) is slightly lower than our GCM energy of the negative parity intrinsic state. The $B(E1)$ values have been estimated from the $B(E1)/B(E2)$ ratios and the Grodzins systematics. The magnitude of the $5^- \to 6^+ B(E1)$ is compatible with the value given in Table I. However, the $B(E1)$ value extracted from the $5^- \to 4^+$ transition is two orders of magnitude smaller [8], which contradicts a simple interpretation based on fixed intrinsic octupole deformation.

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