Hartree-Fock-Bogoliubov Predictions for Shape Isomerism in Nonfissile Even-Even Nuclei

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Secondary minima in the potential-energy surfaces of even-even nuclei are searched for through nonaxial Hartree-Fock-Bogoliubov calculations based on a finite-range, density-dependent effective force. This study covering the mass region $64 < A < 208$ is intended to select nonfissile nuclei which would develop shape isomers. Results are presented for nuclei which seem to be the most interesting candidates for experimental investigations.

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Shape isomerism is a well-known collective phenomenon in nuclear spectroscopy. According to a geometrical description by now traditional, it can take place whenever the potential-energy surface (PES) of a nucleus displays a secondary minimum. This picture has given rise to the double-humped fission-barrier model[1] successfully adopted to describe the basic features of fission isomers. Since the early work of Polikanov *et al.*,[2] many fission isomers have been discovered in the actinide region. Among the spectroscopic properties of these excited states, the most striking one is their stability against deexcitation into the γ-ray channel.[3]

At a microscopic level, the double-humped fission barrier reflects the underlying shell structure of heavy nuclei at large deformation. Since shell structure is a feature common to all nuclei, it is of fundamental interest to investigate whether strong shell effects at large deformation would also exist for nuclei spread over the rest of the periodic table, where fission is generally inhibited. In this broad mass region, γ decay would be the most probable deexcitation mode available to shape isomers unless these states take place as first excited levels. Until now, shape isomers have generally escaped experimental identification. However, a notable exception exists, that of ^{68}Ni for which the first excited state with spin and parity $I^{\pi}=0^{+}$ has recently been identified in heavy-ion collisions as a shape isomer. This level decays to the ground state via internal conversion and e^{+}-e^{-} pair creation.[4]

It is the purpose of the present work to predict which nonfissile even-even nuclei would display shape isomers. If such nuclear excitations with $I^{\pi}=0^{+}$ do actually exist at large quadrupole deformation β (i.e., $\beta > 0.4$), they might serve as storage states for the electromagnetic energy in a γ-ray laser.[5] In a broader perspective, our study may also be viewed as supplementing the investigations on superdeformed bands recently discovered at high spin and large deformation in some nuclei.[6–8]

Early studies of shape isomerism in heavy nuclei have been performed using the Strutinsky method.[1,9] Here, the Hartree-Fock-Bogoliubov (HFB) method, which treats in a self-consistent manner both mean and pairing fields in nuclei, is used. This mean-field theory is a fundamental parameter-free approach to nuclear structure since the nucleon dynamics is only governed by the effective nucleon-nucleon interaction.[10]

Since HFB calculations are time consuming, the Strutinsky method has been used in the first stage of our study as a guide for deciding which nuclei spread over the periodic table would display shape isomers. During that systematic study,[11] over seventy nuclei with masses $64 < A < 208$ have been found as possible candidates for shape isomerism, out of which approximately twenty have been selected as the most interesting ones for experimental investigations. This selection based upon whether the difference in energy between the principal and secondary PES minima is smaller than approximately 5 MeV includes the following nuclei: ^{66,68}Ni, ^{76}Kr, ^{78,80}Sr, ^{80,82}Zr, ^{86,100}Mo, ^{88}Ru, ^{116,118}Sn, ^{142}Sm, ^{144}Gd, ^{152}Dy, ^{188}Pt, ^{190}Hg, and ^{192}Pb. Most of these guesses are proton-rich nuclei located either in the vicinity of, or not too far away from, the β stability line.[11] They are presently considered in constrained HFB calculations preserving or breaking axial symmetry to achieve a better knowledge of their static properties and determine the collective masses and moments of inertia which, together with the PES's, govern their collective dynamics. To render this study as complete as possible, our calculations have also been extended to other even-even nuclei, (i.e., ^{74}Kr, ^{98}Sr, ^{100}Zr, ^{110,112}Pd, ^{150}Gd, ^{154}Dy, and ^{192,194}Hg) which do not belong to the above selection. Some of the HFB results are presented and discussed below.

In the constrained triaxial HFB approach,[10] the total energy of a system made up of A nucleons is minimized according to the variational principle:

$$\delta[\langle\phi\,|\,\hat{H}-\lambda_Z\hat{Z}-\lambda_N\hat{N}-\mu_0\hat{Q}_{20}-\mu_2\hat{Q}_{22}\,|\,\phi\rangle]=0\,, \quad (1)$$

where $\hat{H}$ is the effective nuclear Hamiltonian, $\hat{Z}$ and $\hat{N}$ are the proton and neutron number operators, respectively, and $\hat{Q}_{20}$ and $\hat{Q}_{22}$ are the quadrupole operators simulating the action of external fields on the nucleus. In Eq.

(1), ϕ is the quasiparticle vacuum state and the λ's and μ's are Lagrange multipliers that allow the nucleon numbers and the quadrupole moments q_{20} and q_{22} to be fixed. Here, q_{20} measures the elongation of a nucleus along the Z axis, and q_{22} measures the deviation of its shape from axial symmetry. In this framework, the potential-energy surface $V(q_{20},q_{22})$ of a nucleus is defined as the HFB energy $\langle\phi|\hat{H}|\phi\rangle$ corrected for the zero-point energy (ZPE) arising from the fluctuations of the collective variables. As discussed in Ref. 12, $V(q_{20},q_{22})$ does actually represent the collective potential governing the nuclear dynamics for quadrupole motion. In the present work, the PES's are also labeled in terms of the Bohr coordinates

$$\beta=(\pi/5)^{1/2}(q_{20}^2+3q_{22}^2)^{1/2}A^{-1}\langle r^2\rangle^{-1}$$

and

$$\gamma=\arctan(\sqrt{3}q_{20}q_{22}^{-1}),$$

and are represented as $V(\beta,\gamma)$. The finite-range, density-dependent effective force $D1S$ has been used throughout this work.[13] Of course, no inert core has been assumed.

In Fig. 1 are shown the potential-energy surfaces obtained for ^{66}Ni, ^{76}Kr, ^{78}Sr, ^{82}Zr, ^{142}Sm, ^{152}Dy, ^{188}Pt, and ^{190}Hg. These surfaces display complex patterns, all showing distinct principal and secondary minima (whether or not ZPE corrections are included). The difference in energy between them is neither lower than 1.5 MeV nor higher than 5 MeV. Moreover, the PES minima are separated by barriers with heights ranging from 2 to 4 MeV. For the nuclei with $A\simeq80$, these barriers are in fact saddle points located at $\gamma\simeq30°$ and are 1 to 2 MeV lower than the axial barriers. Furthermore, a few nuclei like ^{82}Zr possess PES showing a third, shallow minimum for γ near 30°. All these features suggest that shape isomers might take place in the nuclei indicated in Fig. 1. Secondary PES minima lower than 5 MeV also occur in ^{68}Ni, ^{74}Kr, ^{80,98}Sr, ^{80,100}Zr, ^{86}Mo, ^{110}Pd, ^{116,118}Sn, ^{150}Gd, ^{154}Dy, ^{192,194}Hg, and ^{192}Pb, nuclei for which no PES's are shown here. Finally, one can observe in Fig. 1 that the secondary PES minima found for the four heavier nuclei at $\beta\simeq0.6$ are stiff in the direction of triaxiality.

For heavier nuclei, present PES predictions are compatible with the information deduced from experimental level spectra available at low energy. On the other hand, experimental information indicate that the light Kr, Sr, and Zr isotopes are deformed in their ground states. These features are in contrast with the PES shapes, all showing spherical principal minima. However, this apparent contradiction can be removed by solving the collective Hamiltonian for quadrupole motion. Preliminary calculations indicate that all these nuclei have quasirotational bands built upon their ground states. Finally, let us mention that most of our results are in qualitative

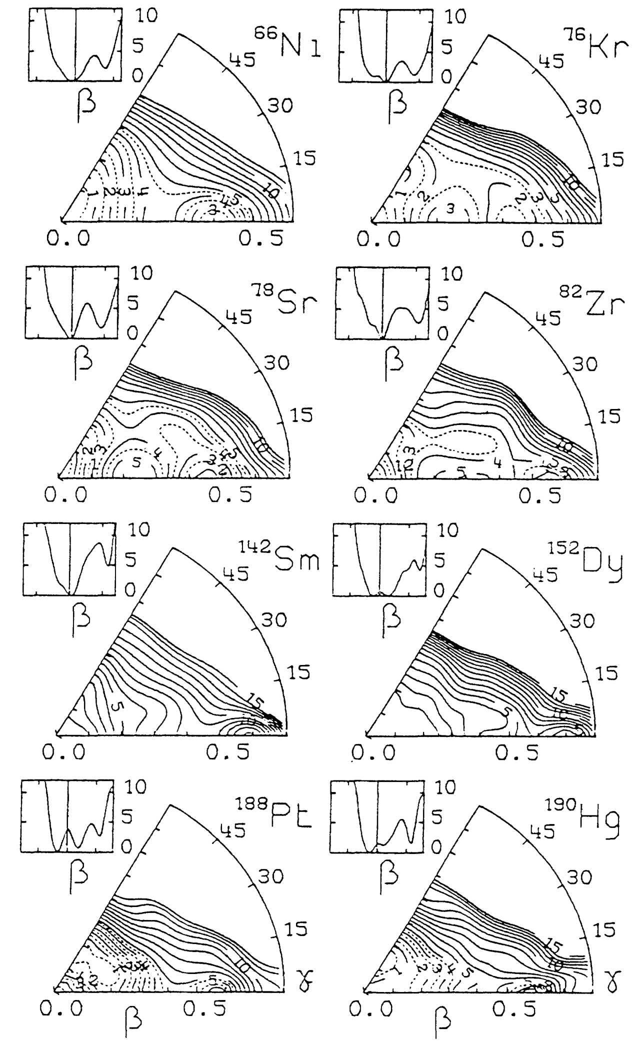

FIG. 1. Potential-energy surfaces (MeV) including zero-point-energy corrections as calculated in the (β,γ) plane for ^{66}Ni, ^{76}Kr, ^{78}Sr, ^{82}Zr, ^{142}Sm, ^{152}Dy, ^{188}Pt, and ^{190}Hg. Insets: Cuts across these surfaces along $\gamma=0°$ and $\gamma=60°$.

agreement with (i) Hartree-Fock calculations performed with the Skyrme force SIII (Ref. 14) in the $A=80$–100 mass region, and (ii) early Strutinsky calculations in the Hg region.[9]

One of our candidates to shape isomerism is ^{152}Dy, a nucleus for which superdeformed states with high spin values have recently been found.[6] These levels form a superdeformed band which occurs at a deformation corresponding to a ratio of 2:1 between the major and minor axes of an ellipsoid, that is for an axial deformation $\beta\simeq0.7$. In our study conducted for $I=0$, the PES of this nucleus shows a second minimum 2 MeV in depth. This is in qualitative agreement with the $I=0$ Strutinsky calculations of Ref. 15, but in contrast with those of Ref. 16 which only indicate a PES shoulder at null spin. The

HFB minimum is located at a charge quadrupole moment $q_{20}(\text{th}) = 18.8\ e\text{b}$, a value in good agreement with the estimate value $q_{20}(\text{expt}) = 19 \pm 3\ e\text{b}$ of the superdeformed band as deduced from measurements.[7] On the other hand, no superdeformed bands have yet been observed for ^{142}Sm, ^{144,150}Gd, and ^{154}Dy, nuclei for which we predict the formation of shape isomers. Furthermore, extending the HFB calculations beyond $\beta = 0.7$ suggests that hyperdeformed states at excitation energies higher than 8 MeV might form and coexist with shape isomers corresponding to a major-to-minor axis ratio of 2:1. If shape isomers were to take place at such hyperdeformations (i.e., $q_{20} \simeq 85$ b and $\beta \simeq 0.9$) as found for ^{188}Pt, ^{190}Hg, and ^{192}Pb (see Fig. 2), their decay would preferentially proceed via particle emission. These findings are in keeping with recent empirical predictions[17] according to which hyperdeformed states with high spin values might take place in some nuclei with semiaxes in a ratio larger than 2:1. All these examples illustrate that a close connection seems to exist between superdeformed and hyperdeformed bands seen or expected to show up in properly selected nuclei, on the one hand, and shape isomers at large or hyperlarge deformations, on the other hand.

In summary, a number of nonfissile even-even nuclei for which a secondary minimum exists in their potential-energy surfaces at large deformation have been found using constrained Hartree-Fock-Bogoliubov calculations covering the (β, γ) plane. This study (i) confirms most of the nuclei previously selected using the phenomenological Strutinsky method as possible candidates to shape isomerism, (ii) enlarges our former selection, and (iii) does suggest that a connection exists between shape isomerism at null spin and superdeformation phenomenon taking place at high spin. Furthermore, our present candidates might be classified in two families, depending upon whether their PES's are soft along γ deformation (i.e., ^{66,68}Ni, ^{74,76}Kr, ^{78,80,98}Sr, ^{80,82,100}Zr, ^{86}Mo, ^{110}Pd, and ^{116,118}Sn) or stiff against it (i.e., ^{142}Sm, ^{150}Gd, ^{152,154}Dy, ^{188}Pt, ^{190,192,194}Hg, and ^{192}Pb) whenever β gets large. The former family is that for which the barrier located in between the principal and secondary PES minima is lowest. These features together with the γ softness found for the PES's of nuclei in the $A \simeq 70$–100 region should favor triaxiality and shape isomerism at relatively low excitation energy (i.e., $E_x \lesssim 2$ MeV). It is worth pointing out that shape coexistence phenomena are taking place in a number of nuclei spread over this mass region.[18] There, even though 0^+ excited states could form at excitation energy as low as $E_x \simeq 200$ keV, none possesses the characteristic features expected for a shape isomer: To our knowledge, their half-lives never exceed a few tens of ns. Finally, the stiffness against the γ degree of freedom as found for the nuclei of the second family seems less favorable to the formation of shape isomers at relatively low excitation energy. Unless the nuclear dynamics is solved for the collective quadrupole motion, there is no way to draw more definite conclusions on this issue. This remark points to the conclusion that only an accurate description of the collective wave functions provides a reliable identification of an excited level as a possible shape isomer. If such an excitation is to exist, its wave function should have a large component near the secondary PES minimum and overlap only weakly with those of the low-lying states that form in the principal PES minimum. This is a necessary condition to prevent a shape isomer from too fast an electromagnetic decay.

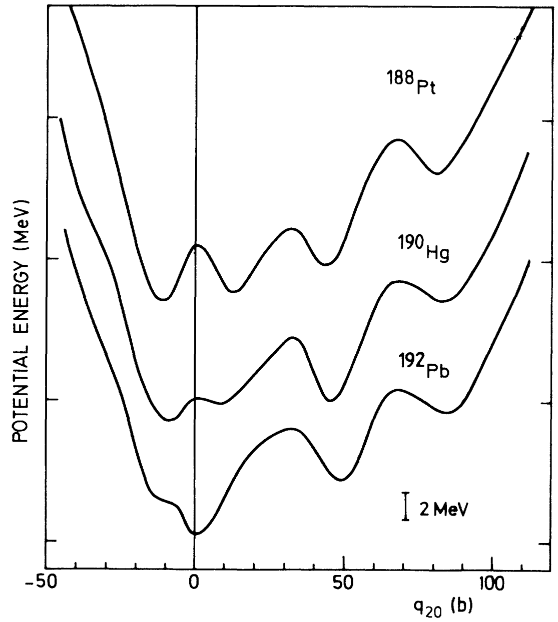

FIG. 2. Potential-energy surfaces (MeV) including zero-point-energy corrections for ^{188}Pt, ^{190}Hg, and ^{192}Pb as functions of the axial mass quadrupole moment q_{20} (b). The first secondary minima found for $q_{20} \simeq 45$ b corresponds to the respective minima shown for these nuclei at $\beta \simeq 0.6$ and $\gamma = 0$ in Fig. 1.

Beside these considerations, it must be emphasized that proper predictions for shape isomerism at large deformation might require that collective coordinates other than the quadrupole ones also be considered in the collective dynamics. For instance, a microscopic study[13] of the fission of ^{240}Pu suggests that collective octupole modes are favored for quadrupole deformations in the vicinity of and beyond the second PES minimum. Preliminary calculations seem to indicate that such modes actually are softer than those associated with triaxial oscillations in the heavier nuclei of our selection. If this feature were to be confirmed, the identification and characterization of shape isomeric states in these nuclei would require that both octupole and quadrupole degrees of freedom as well as their coupling be explicitly treated.

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