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Preliminary selection of candidates for shape isomerism from even-even nuclei with masses $A < 208$

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This theoretical work represents the first stage in our efforts to establish an extensive list of nonfissile even-even nuclei located inside or near the valley of stability which might develop shape isomers. Our selection relies upon whether a secondary minimum takes place along an elongation axis in the potential energy surfaces of nuclei spread over the mass region $A < 208$. These surfaces are determined through a joint use of the Hartree-Fock-Bogoliubov and Strutinsky methods. More than seventy nuclei located inside the region $40 < A < 208$ are suggested as possible candidates for shape isomerism.

Most nuclear isomeric states have been observed in even-even and even-odd nuclei spread over the periodic table. They are defined as excited levels having half-lives which are long compared with the characteristic times of the fast electromagnetic transitions (i.e., the collective electric transitions $E\lambda$ with $\lambda = 1$, 2, and 3). These excitations manifest as spin or shape isomers. A spin isomer is a noncollective excited state with long half-life. The first excited state ($E_x = 75$ eV, $I^\pi = \frac{1}{2}^+$) of ^{235}U is a well-known example of spin isomer.[1] On the other hand, shape isomers are collective excitations which can develop in nuclei showing secondary minima in their potential energy surfaces (PES). These states mediate delayed fission in the actinide region where they are known as fission isomers.[2-4] The γ-decay mode is rarely available to them because tunneling through the inner PES barriers is generally weak.

The actinide nuclei undergoing delayed fission are suitable grounds for the observation of shape isomers.[5] However, there exists no reason in principle which would make unlikely the formation of these excitations in nuclei spread over the rest of the periodic table where, in general, fission is considered as an inhibited mode of de-excitation. Since experimental evidence for shape isomerism outside the actinide region so far exists only in ^{68}Ni as recently found in heavy ion collisions,[6] it is of fundamental interest to predict which nuclei among the light and medium-heavy ones might possess shape isomers. This is the purpose of the present work which is restricted to the even-even nuclei with masses $A < 208$. In this region, γ decay is expected to be the most probable de-excitation mode available to shape isomers even though β-delayed fission might also occur, as recently observed in mercury isotopes.[7]

In a broader perspective, shape isomers in nuclei stable against fission would be of interest for applied physics, in particular for the design of a γ-ray layer based on nuclear transitions induced for instance by laser-electron coupling.[8] This scenario stems from the collective nature of shape isomers which would undergo stronger transitions to proximate lasing states than spin isomeric states would. In this context, shape isomers are required to be located at relatively low excitation energy. As a consequence, our selection of candidates is also limited to nuclei showing secondary PES minima at relative energies lower than, say, 5 MeV.

Searching for shape isomers in nuclei spread over a broad mass region represents a formidable task if systematic use is to be made of the most fundamental approach to PES calculations, i.e., the constrained Hartree-Fock-Bogoliubov (HFB) method.[9] We therefore proceed to the PES calculations following the twenty-year-old Strutinsky method,[3] a corner stone of the double-humped fission barrier model.[4] In contrast with the HFB calculations, which require a substantial amount of computing time, the calculations based on the Strutinsky method can be performed at a much cheaper expense, thus offering the opportunity to run these for several hundred nuclei. Unfortunately, this phenomenological method only provides gross features for potential energy surfaces. At the present stage of our investigations, this is not viewed as a major concern since our ultimate goal is to perform constrained HFB calculations for the nuclei selected with the Strutinsky method. However, the need for rendering this selection as reliable as possible implies that the Strutinsky method be worked out with realistic inputs. Therefore, shell corrections are performed using single-particle levels deduced from constrained HFB calculations instead of those from phenomenological deformed shell models which usually are adopted for that purpose.[10,11] To our knowledge, this procedure, which combines the HFB and Strutinsky methods, has never been adopted in nuclear structure calculations. It is referred to as the SHFB method or procedure in the following discussion.

In principle, the precise localization of secondary minima requires that the potential energy surfaces be explored along the quadrupole deformations preserving or breaking the axial symmetry, that is over the entire (β, γ) plane.[12] This complete study has not been performed because only qualitative information are expected from the Strutinsky method. Therefore, our investigation is restricted to the determination of $V(\beta)$, the potential energy surface as a function of the axial deformation β. Despite this restriction, it is still possible to appreciate the γ softness of nuclei from the difference in energy between the principal

minima of $V(\beta)$ at prolate and oblate deformations, when these minima exist.

The Strutinsky method relies upon the assumption that the deformation energy $V_{Z,N}(\beta)$ of a nucleus made up with Z protons and N neutrons may be written

$$V_{Z,N}(\beta)=\bar{V}_{Z,N}(\beta)+\delta V_{Z,N}(\beta)\,,$$

where $\bar{V}$ is a smooth function of Z, N, and β, and δV, a quantal fluctuation which also depends upon these parameters. Following most standard procedures, $\bar{V}$ is taken as the deformation energy[13] of a charged liquid drop, and δV is a correction term stemming from shell and pairing effects.[3,10] In our work, pairing corrections are neglected since shell effects play a dominant role in the formation of PES minima and barriers located in between any two $V(\beta)$ minima. For the shell correction, we have adopted the single-particle levels of nuclei for which HFB calculations indicate sizable pairing correlations (i.e., pairing energies are generally larger than 10 MeV), since most nuclei have this property. The selection of these nuclei, henceforth labeled as reference nuclei, is accomplished by splitting the periodic table of nuclei[14] with $A<208$ into seven $Z\times N$ sectors, each having a reference nucleus placed at its center. The reference nuclei are: ^{46}Ti, ^{80}Sr, ^{102}Ru, ^{124}Te, ^{144}Nd, ^{170}Yb, and ^{200}Hg. Their potential energy surfaces $V(\beta)$ shown in Fig. 1 are determined from the HFB equations which are solved by expanding the many body wave functions onto oscillator eigenstates.[9] Large bases are adopted to secure the convergence of the calculations: nine major shells for ^{46}Ti, eleven for ^{80}Sr, ^{102}Ru, ^{124}Te, ^{144}Nd, and thirteen for ^{170}Yb and ^{200}Hg. These are performed using the $D1S$ effective interaction,[15] i.e., Gogny's force[16] with improved surface properties included.

The validity of the SHFB procedure may be appreciated by checking whether PES predictions based on it agree with results from reference HFB calculations. In the upper portion of Fig. 2 is shown a comparison between $V(\beta)$ values for ^{200}Hg as obtained from HFB calculations (solid curve) and from the SHFB procedure (dashed curve) which uses as inputs the single-particle levels deduced from these HFB calculations. A reasonably good agreement between the two curves is achieved except for the values of β in the vicinity of the spherical point. Another comparison is shown for ^{114}Cd in the lower part of Fig. 2 where the solid curve is from HFB calculations, and the dashed curve is a SHFB prediction for this nucleus as established from the reference nucleus ^{124}Te. A deficiency of the SHFB procedure is again observed near $\beta=0$, and also towards large deformations. This method generally produces $V(\beta)$ maps which display exaggerated

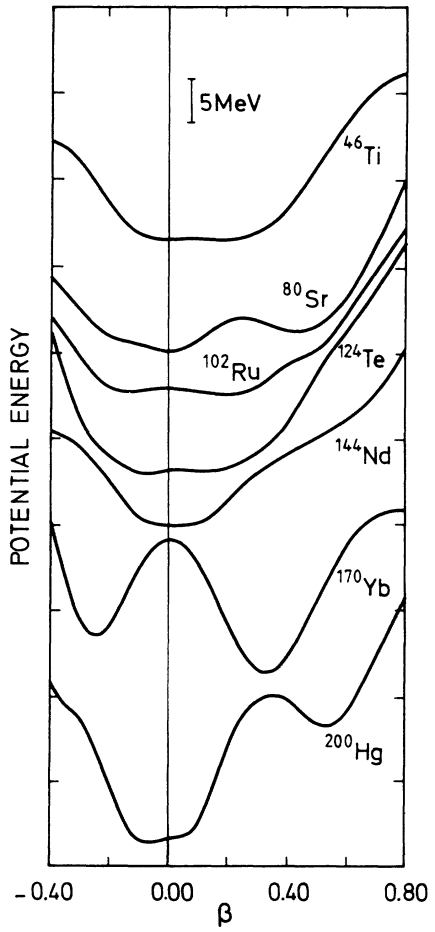

FIG. 1. Potential energy surfaces of the reference nuclei as determined from present constrained HFB calculations.

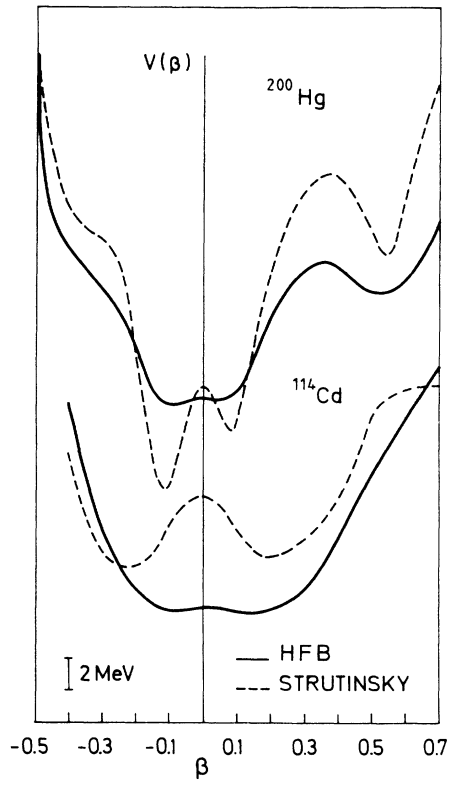

FIG. 2. Upper part: potential energy surface of ^{200}Hg. Comparison between HFB calculations (solid curve) and calculations based on the Strutinsky method (dashed curve). Lower part: potential energy surface of ^{114}Cd. For further information, see text.

structures when compared with those deduced from corresponding HFB calculations in which pairing correlations wash out sharp PES structures. In view of this, secondary minima near $\beta=0$ will be ignored. Only those appearing for deformation $\beta \geq 0.2$ will be called hereafter "secondary minimum." On the other hand, well-known shape transitions occurring for instance in the Nd-Sm region (i.e., transition from spherical to deformed shapes) and in the Os-Pt region (i.e., transition from oblate to prolate shapes) are reasonably well reproduced.[17] These illustrations as well as others not shown, indicate that the SHFB procedure is fairly reliable provided that pairing correlations are not too important. Therefore, we only expect from the SHFB procedure indications that secondary minima of $V(\beta)$ exist for some nuclei. This method is not accurate enough to provide precise estimates for the difference in energy between the principal and the secondary minima of $V(\beta)$, when this later minimum exists. Finally, our study also shows that the SHFB method is not too reliable for nuclei lighter than, say, ^{40}Ca. Meaningful searches for secondary PES minima in this region would only rely upon the HFB method, which is outside the scope of the present work.

It is impossible to show in this report the PES maps which have been systematically calculated for nearly eight-hundred nuclei.[17] As a summary, let us mention that (i) the secondary PES minima are observed for β values either near zero or within the interval $\beta=0.4-0.7$, (ii) these minima are mostly found for neutron poor nuclei in the vicinity of the stability line, and (iii) there exist some indications that shape isomers might also take place at deformations larger than $\beta=0.7$. More than seventy nuclei in the region $40<A<208$ are selected (see Fig. 3) as possible candidates to shape isomerism, among which approximately eighteen might actually be most interesting for experimental investigations. These nuclei are ^{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. Obviously, the compilation shown in Fig. 3 is not exhaustive since a number of candidates lying too far away from the valley of stability have been discarded. These candidates are not attractive unless major improvements are accomplished in the production of exotic nuclei. Figure 3 indicates that most candidates to shape isomerism are located in the vicinity of the following (Z,N) values: (40,40), (64,80), and (80,110). In addition, the shape isomers in the region defined by Z or N equal or close to 40 are expected to show up near $\beta=0$. On the other hand, those located outside this region are expected to be deformed. Finally, the shell effects giving rise to shape isomerism are strongest for Z or $N\simeq 80,82$. It is interesting to notice that the narrow mass regions where PES minima at large deformations are presently found coincide rather well with those deduced earlier from a study based on deformed shell model predictions, as shown in Fig. 6-52 of Ref. 18.

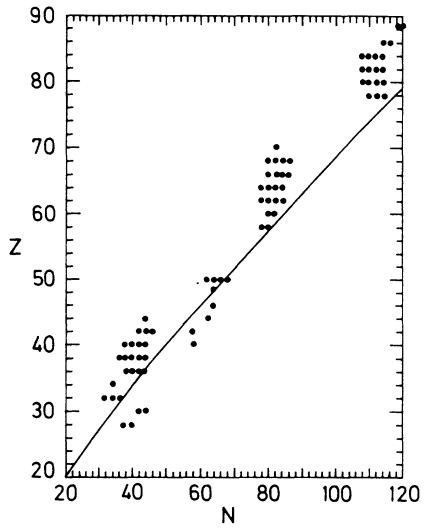

FIG. 3. List of nonfissle even-even nuclei with $A<208$ which might develop shape isomerism. The continuous curve represents the stability line.

In conclusion, the Strutinsky method implemented with results from Hartree-Fock-Bogoliubov calculations preserving axial symmetry can be considered as a useful tool for selecting nonfissile even-even nuclei which might develop shape isomers. This empirical method does not pretend to be a substitute for the fully microscopic and self-consistent HFB approach. However, our selection as it stands is valuable since it can be used as a guide for future searches based on the constrained Hartree-Fock-Bogoliubov method extended to the whole (β,γ) plane. This work is in progress.

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