Phase transitions versus shape coexistence

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In the present paper, we discuss the differences that underlie a topic of current intensive research and debate, e.g., the appearance of phase transitions and shape coexistence in atomic nuclei. Besides a formulation of the basic differences, we discuss on one hand some typical examples of shape coexistence (near the Sn and Pb closed shell regions) and, on the other hand, of phase transitions. The present discussion should allow a more transparent way to analyze nuclear structure changes in particular mass regions.

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I. INTRODUCTION

The concept of deformed shapes and the appearance of different shapes in a given nucleus was introduced in nuclear physics as early as 1937 by the work of Bohr and Kalckar [1]. In those early days, little did one expect how fruitful these ideas would turn out to be. The discovery of the first excited state with spin 0^+ in the doubly magic nucleus ^{16}O and its subsequent interpretation, starting from rearranging four particles from occupied into empty orbitals above the Fermi level, resulted in a cooperative strong binding energy effect. A subsequent highly deformed shape, coexisting with the spherical ground state [2], opened up a new field in nuclear physics research, devoted to the investigation and understanding of shape coexistence. Soon after, it was realized that the atomic nucleus, on its way to fission, had to undergo a number of shape changes in which a specific shape could be trapped as an isomeric state in a secondary potential minimum, called fission isomers [3]. Shape coexistence, invoking multiple shapes, was predicted and also observed in many spherical nuclei near magic shells and these particular phases could be linked to the occupation of very specific up- and/or downsloping orbitals, coined "intruder orbitals," which allowed for a simple understanding of the phenomenon of shape coexistence [4,5]. The method put forward in those papers could be used to predict shape coexistence, e.g., in the Sn nuclei, around mass number $A=116$ and in the Pb nuclei from mass number $A=196$ and below. Once fast rotation was employed as a new tool to study nuclear shapes spinning up nuclei very fast, like in the case of ^{152}Dy, a "superdeformed" shape was discovered with axis ratios for the prolate deformed ellipsoid of 2:1, coexisting with single-particle excitations corresponding to oblate shapes [6]. This research field has exploded in recent years due to the highly increased technical capabilities in detecting gamma radiation emitted during the slowing down of the rapid rotation (Gammasphere, Euroball, …).

Shape changes also occur in another way in atomic nuclei when one considers only the ground state and low-lying excitations. There exists extensive experimental and theoretical information about nuclei that seem to form a transition in between a spherical phase (exhibiting anharmonic quadrupole vibrational energy spectra) and a more deformed collective phase that is often associated with energy spectra exhibiting rotational properties. Some of these clear-cut examples are situated at the neutron number $N=90$ for the rare-earth nuclei Nd, Sm, Gd [7–12], and also in the region of Ru, Pd even-even nuclei [13,14] in which a transition is observed between anharmonic vibrations and γ-soft vibrational motion when progressing from lighter to neutron-rich nuclei.

These transitional regions have been quite well studied in terms of algebraic models (notably within the framework of the interacting boson model) [15–24], but also within the collective model [25] leading to the idea of critical point symmetries [26–28].

The variety of shapes occurring in atomic nuclei continues to be a topic of active and rapidly evolving research as exemplified in the recent papers by Andreyev *et al.* [29] and Warner [30]. It is the purpose of this paper to clearly outline the differences between shape coexistence and phase transitions.

II. PHASE TRANSITIONS VERSUS SHAPE COEXISTENCE

The flexibility of the interacting boson model (IBM) allows an easy parametrization for the study of phase transitions on the extended Casten triangle [31,32]. The Hamiltonian that incorporates the two opposite forces, one driving to spherical shapes and one driving to deformation, can be constructed in the *s,d* IBM as follows:

$$\hat{H} = a\left[\eta\hat{n}_d - \frac{(1-\eta)}{N}\hat{Q}_\chi\hat{Q}_\chi\right], \tag{1}$$

where the quadrupole operator is given by

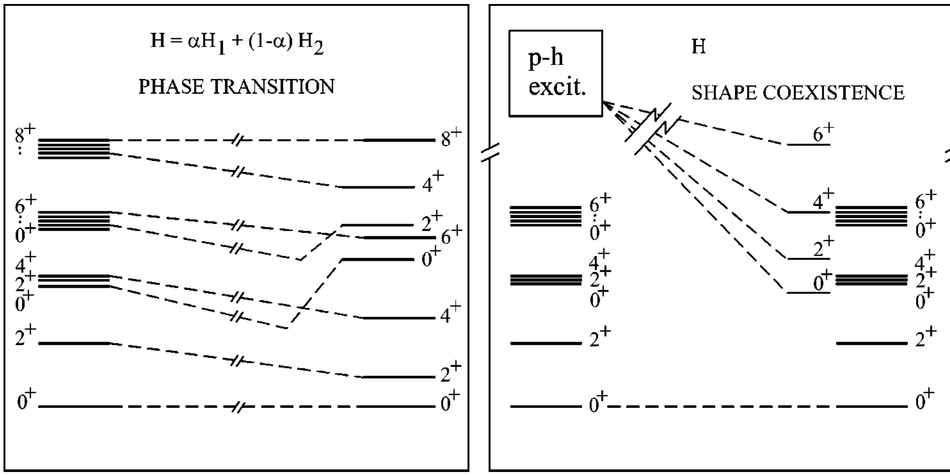

FIG. 1. Schematic illustration for a possible shape transition (left-hand side) and for the situation where next to a family of regular states, another class of states can result as an example of shape coexistence (right-hand side).

$$\hat{Q} = (s^\dagger\tilde{d} + d^\dagger s)^{(2)} + \chi(d^\dagger\tilde{d})^{(2)}. \qquad (2)$$

The parameter a is a general energy scaling factor, N the number of s and d bosons, and η and χ are two structural parameters, describing the spherical-deformed transition and the prolate-oblate transition, respectively. In order to visualize this simple parametrization, the Casten triangle is used in which one axis is formed by η and the other one by χ. As a concrete example by varying η from one to zero a spherical-deformed phase transition is crossed.

The Hamiltonian (1) is of the type that in a general way, can be parametrized by means of a Hamiltonian

$$H = \alpha H_1 + (1-\alpha)H_2, \qquad (3)$$

in which the separate Hamiltonians H_1 and H_2 describe two different types of motion that are basically incompatible with one another (e.g., the example of vibrational excitations on one side and the states of an axially symmetric rotor on the other side). This means that the Hamiltonians do not commute. Otherwise the states of both Hamiltonians would not interact with each other, e.g., H_1 made out of s,d boson operators and H_2 out of f,p boson operators. Explicitly one needs nevertheless that both Hamiltonians work in the same Hilbert space $\mathcal{H}$. This means they are acting on states which can be expanded in the same set of basis states. Generally speaking one could state that we deal with a system with $\mathcal{H}=\mathcal{H}_1=\mathcal{H}_2$. The parameter α then allows for a smooth transition between the two limiting cases in order to describe the transition. Studying the ground-state properties along the transition (binding energy and other observables) one can even get interesting information on the order of the transition between the two phases. Much attention has been given to this issue recently, in particular using the IBM and its underlying symmetries ([15–24]).

The point we like to stress here is that in such a study, the number of basis states is preserved through the transition and progressing from one limiting case into the other (see Fig. 1, left-hand part). One notices that the eigenstates of one limit will be spread out and finally end up as the eigenstates of the other limit. The way in which this happens depends on the structure of the Hamiltonians and can be measured using the concept of Shannon information or wave function entropy (see, e.g., Ref. [33]).

On the other hand, phase coexistence can appear when a number of basis states, appearing at very high excitation energy (outside of the model space that is regularly considered as the space of low-lying configurations) under normal circumstances (such as particle-hole excitations across closed shells), can profit from residual proton-neutron interactions. This can be the case in nuclei with $a(n)$ (almost) closed shell of protons (or neutrons), on one hand, and a large number of valence neutrons (or protons), on the other hand. In such a situation, the proton-neutron correlation energy in the p-h excited high-lying configurations can become competitive with the energy needed to create this family of extra states and so see the energy drops towards the low-energy regime [4,5]. Such classes of states are also quite often called "intruder" excitations (see Fig. 1, right-hand part). In this situation, one essentially makes use of a single Hamiltonian H but extends the model space by including (various) a different phase and its associated basis states. Therefore one has a coupling of two different Hilbert spaces and $\mathcal{H}=\mathcal{H}_1\otimes\mathcal{H}_2$. Mostly, this concerns, in practical applications, an N s,d boson space coupled to an $N+2$ s,d boson space. They are used to describe shape coexistence between normal (valence) excitations and intruder excitations that include $2p$-$2h$ excitations. It should be mentioned that both sets of states can interact and mix with each other via a mixing Hamiltonian that does not conserve the boson number.

To distinguish between phase transition and phase coexistence, the essential feature is that in the case of phase transitions the two different types of motion can only develop subsets of states resembling the motion generated by H_1 and H_2. On the other hand of phase coexistence, *complete* structures can be generated in each space (compare, e.g., the phase transition in the even-even Sm nuclei in which all the states in the vibrational region smoothly go over into states in the deformed region, contrasting with the situation like in the even-even Cd nuclei near mass number $A\approx 112$ and in the neutron-deficient Pb nuclei, in which different classes of states do appear in each given nucleus). Therefore, the use of spectroscopic methods providing a complete data set is of the utmost importance. Here, light-ion induced reactions and thermal neutron capture provide essential tools [34].

Finally, it should be mentioned that a complete different approach can be used. This approach concerns the use of crancking in the IBM [20,35] and is a semiclassical approach. Here, phase transitions are obtained as a function of angular frequency ω, and the changes which occur when the *mp-mh* states become yrast states, like in the Cd and Pd isotopes [36], can be described as a phase transition [37] between a spherical (vibrational, mainly) and a deformed phase.

III. EXAMPLES OF PHASE TRANSITIONS AND SHAPE COEXISTENCE

Excellent examples of complete structures representing shape coexistence have been observed in the last decade in the Cd isotopes. These isotopes form an excellent test of shape coexistence as here the intruder states have their lowest excitation energy (at midshell) exactly at the line of stability. This allows the unique possibility to study the six stable even-even Cd isotopes in an as complete way as possible. Studies like those of the structure of ^{112}Cd [38–40] revealed that these isotopes have complete three-phonon spherical structures together with complete more deformed O(6)-like intruder excitations, leading to very specific interactions between both [41].

As these collective, intruder configurations most probably involve proton $2p$-$4h$ excitations across the $Z=50$ shell closure, it might be speculated that their behavior would be very similar to the properties of the ground-state bands in the adjacent Ru and Ba nuclei, with the constraint of considering the same number of neutrons. Such *mp-nh* excitations can now be handled within the algebraic framework of the IBM [15,42]. In this approach, explored in detail in a series of papers [43–46], both particle and hole shell-model configurations are approximately handled as interacting particle and holelike *s* and *d* bosons. A particular symmetry that allows the transformation of particle into hole bosons (or the other way around), and is formally like the isospin transformation that allows protons to be transformed into neutrons (or the other way around), here called *I*-spin or intruder spin, was suggested [47]. Its presence results in *I*-spin multiplets (formally analogous to isospin multiplets in light nuclei) and some interesting realizations of this symmetry were discussed in, e.g., the Sn region [40,48]. This symmetry then implies strong similarities for both excitation energies (see Fig. 2) as well as for $B(E2)$ transition probabilities to hold between the $2p$-$4h$ intruder bands in the Cd nuclei and the $6h$ and $6p$ ground-state bands in the Ru and Ba nuclei, respectively. This would hold for an unbroken I-spin multiplet structure. A very recent analysis [49] in the Ru, Ba, and Cd nuclei has given extra information to strengthen this idea through $B(E2)$ values (see Table I). Experiments are planned to study the very neutron-rich ^{124,126,128}Cd isotopes in order to explore the behavior of the family of intruder states [50].

Another more dramatic but less detailed (in terms of spectroscopic information on energy spectra, transition probabilities, …) example of shape coexistence shows up in the data for the Pb region when removing neutrons from the closed shell at $N=126$. These data point towards the appearance of specific particle-hole $(p$-$h)$ excitations across the closed shell at $Z=82$. It is precisely the energy gap at the $Z=82$, $N=126$ closed shell of only approximately 3.5 MeV, combined with a very large open neutron shell (filling the 82–126 orbitals) that enables the proton-neutron quadrupole-quadrupole force to lower the excitation energy of $2p$-$2h$, $4p$-$4h$, … configurations as much as to approach the ground state (for the Pb and Hg nuclei) and even cross it (for the Pt and possibly the Po nuclei, too) [4,5]. Because of the increased quadrupole collectivity associated with these *p-h* excitations, collective bands are observed on top of the low-lying 0^+ intruder excitations and so indicates the presence of shape coexistence (see Fig. 3 for the most recent systematics). A discussion, using *I*-spin symmetry arguments, has been used also [45,46,51], and a very detailed study, using configuration mixing within the interacting boson model, has been carried out by Fossion *et al.* [52].

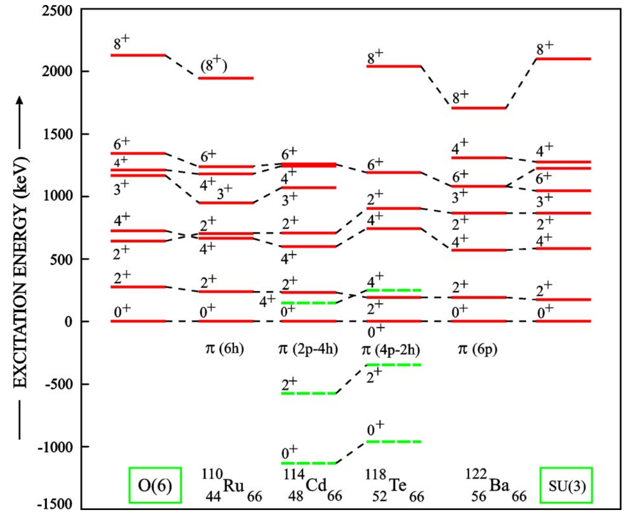

FIG. 2. (Color online) Systematics of the lowest family of intruder states in ^{114}Cd and in ^{118}Te compared with the regular configurations in ^{110}Ru and in ^{122}Ba. The energies of the *I*-spin 3/2 multiplet are normalized in energy. A smooth transition from and O(6) into a SU(3) structure is indicated with these two limits drawn at the extreme left and right of the figure.

Calculations, making use of a deformed mean-field approach that study the possible equilibrium states [53–56] have indicated the possibilities of producing rather close-

TABLE I. Comparison of the $B(E2;2_1^+\to 0_1^+)$ values in the even-even Ru and Ba nuclei with the corresponding $B(E2;2_3^+\to 0_I^+)$ intruder $E2$ transition in the Cd nuclei with the same neutron number [49].

Neutron number	Cd intruder $B(E2;2_3^+\to 0_A^+)$	Ru $B(E2;2_1^+\to 0_1^+)$	Ba $B(E2;2_1^+\to 0_1^+)$
62	23^{+27}_{-18}		
64	56 ± 17	58 ± 5	
66	61 ± 8	70 ± 5	154 ± 14
68	86^{+24}_{-30}	74 ± 7	116 ± 6
70			98 ± 16

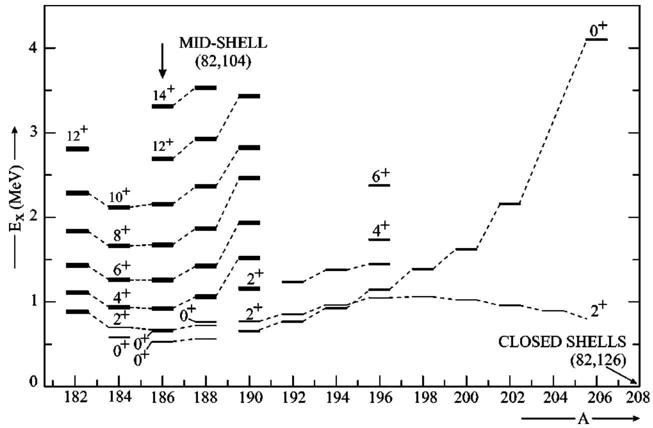

FIG. 3. Systematics of the lowest 0^+ states in the even-even Pb nuclei. The first excited 2^+ state is also given for reference. The band members of the yrast structure are given in the mass region $182 \leqslant A \leqslant 190$. The references are denoted in the introductory part of the present article.

lying oblate and prolate minima in the total energy surface for the Pb nuclei while approaching the neutron midshell region at $N=104$, next to the spherical ground-state configuration. In the Hg nuclei with a ground state corresponding to a slightly deformed oblate configuration, a second prolate configuration is predicted, mimimizing its energy near midshell ($N=104$), whereas for the Pt nuclei, a crossing of both minima is implied and the prolate deformed minimum becomes the lowest configuration at midshell. For the Po nuclei, the situation looks somewhat more complicated [51] with an oblate minimum, approaching the spherical ground-state configuration near $N=110$, and a prolate minimum, becoming dominant in the ground state for even lower neutron numbers. Very recently, detailed studies using configuration mixing starting from Hartree-Fock-Bogoliubov (HFB) [57] and HF+BCS [58–60] calculations have come to the same conclusion for the presence of shape coexistence in the very neutron-deficient Pb nuclei, albeit starting from a microscopic mean-field approach.

The characterization of phase transitions in transitional regions has been amply discussed using algebraic methods (more in particular using the IBM) [15–24]. In those studies, arguments for possible phase transitions have been presented. Illustrations are ample and concentrate on the Sm, Gd region when passing the $N=90$ neutron number [7–12] and the Hf-Hg region with possible prolate-oblate phase transitions [21]. Irrespective of the precise type of transition occurring, the Hamiltionian as depicted in Eq. (1) allows a good overall description of those transitions. One should, however, be careful in making a conclusion as to what precisely is happening: even though the $N=90$ region seems very indicative of a phase transition, recent experiments in ^{154}Gd have shown evidence for a low-energy coexisting band [61]. Interesting other regions to study are the Sr,Zr nuclei in passing the $N=56$ subshell closure. There are strong indications that here, too, a spherical to deformed phase transition is happening, much like in the $N=90$ rare-earth mass region. More detailed calculations of this mass region will be carried out.

Using algebraic methods, very interesting calculations have been carried out studying different types of phase transitions [62,63]. Here, the transition between a superconducting phase, described by the Hamiltonian

$$H_2 = -GS_+S_-, \tag{4}$$

with

$$S_+ = \sum_{j,m>0} (-1)^{j+m} a^\dagger_{j,m} a^\dagger_{j,-m}, \tag{5}$$

$$S_- = \sum_{j,m>0} (-1)^{j+m} a_{j,-m} a_{j,m}, \tag{6}$$

and a rotational phase described by the Hamiltonian

$$H_1 = -\chi Q \cdot Q, \tag{7}$$

with Q the SU(3) quadrupole tensor operator has been explored. In this particular case, analytical solutions exist in the two limits but no simple analytical solution exists in the intermediate situation. In this situation, eigenstates from one limit are spread out thinly over the eigenstates of the other limit and a sharp phase transition in many-fermion systems results and no clear case of phase coexistence shows up.

IV. CONCLUSION

In the study of extended regions in the nuclear mass for a given isotope (or isotone), ample evidence has resulted for either smooth transitions from one phase into another one (with the number of levels being the same on both sides of the transition) like, e.g., in the Sm, Gd nuclei *or* for situations in which a particular class of excitations are dropping quickly in energy thereby bringing a new phase of nuclear structure and resulting in shape coexistence with the regular low-lying states (see, e.g., the region near closed shells at $Z=50$ and $Z=82$ while approaching the midshell neutron regions at $N=66$ and $N=104$, respectively).

In the present paper we have discussed the salient features that allow to discriminate between a region in which phase transitions appear and a region that exhibits shape coexisting phenomena. In Sec. II, we have discussed a simple Hamiltonian that allows us to describe phase transitions within the IBM irrespective of the mass region one is concentrating on [see the Hamiltonian of Eq. (1)] and in which the two different limiting cases on separate sides of the transition form incomplete sets of states. On the other hand, when shape coexistence appears, complete sets of states can be generated. In the latter case, the nuclear structure is determined by the direct product of the Hilbert spaces describing the various phases like $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3 \ldots$. In Sec. III we have described some very recent and at the same time typical examples of both shape coexistence and phase transitions in order to elucidate differences between the two forms of shape changes that might occur when changing through a series of isotopes or isotones compared to having different shapes in a given nucleus.

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