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Shape phase transition in odd-even nuclei: From spherical to deformed y-unstable shapes

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Shape phase transitions in odd-A nuclei are investigated within the framework of the interacting boson-fermion model. The case of a single j = 9/2 fermion coupled to an even-even boson core is considered. This boson core transits from spherical to γ -unstable shapes depending on the value of a control parameter in the boson Hamiltonian. The effect of the coupling of the odd particle to this core along the shape transition and, in particular, at the critical point is discussed. For that purpose, the ground-state energy surface in terms of the β and γ shape variables for the even core and odd-even energy surfaces for the different K states coming from j = 9/2 are constructed. The evolution of each individual coupled state along the transition from the spherical [U(5)] to the γ -unstable [O(6)] situation is investigated. One finds that the core-fermion coupling gives rise to a smoother transition than in the even-core case.

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I. INTRODUCTION

The study of phase transitions in finite nuclear quantal systems has been the subject of many investigations of the nuclear physics many-body problem. Recent review articles about the quantum phase transitions (QPTs) in nuclei, mostly on even-even systems, can be found in Refs. [1-5]. Phase transitions can be classified into two classes. The first of them is known as first-order phase transition and includes those for which two different phases coexist in an interval of the control parameters. The absolute minimum of the energy surface as a function of the order variables changes discontinuously for given values of the control parameters. The critical point in this case is the point in the parameter space for which the two coexisting minima (representing different phases) of the energy surface have the same energy. The second kind of phase transition is called the continuous phase transition and embraces all the cases for which the phase change occurs very softly (there is no coexistence) in a continuous way from one phase to the other as the control parameters are varied.

In the last few years, there has been a revival in the study of quantum phase shape transitions in mesoscopic systems after the introduction of the concept of the critical point symmetry (CPS). The CPS concept, first introduced by Iachello [6], applies when a quantal system undergoes transitions between traditional dynamical symmetries (definite shapes) and is designed to apply at the critical point of the shape phase transition. In the context of nuclear physics, both first-order and continuous shape phase transitions have been modeled within the geometric collective model (GCM) [7]. The CPSs proposed up to now are known as E(5) [6], X(5) [8], and Y(5) [9] and correspond to the transition from spherical to γ -unstable shapes (continuous), from spherical to axially deformed shapes (first order), and from axially deformed to triaxial shapes (continuous), respectively. Although these symmetries have been obtained within the formalism based on the Bohr Hamiltonian [7], similar ideas have also been used

in connection with the interacting boson model (IBM) [10]. Both in the GCM and in the IBM, nuclei can be classified according to their equilibrium shapes. In the GCM, collective deformations are described by introducing two collective variables, called deformation parameters or shape variables (β, γ) . The β variable measures the axial deviation from sphericity and the angle variable γ controls the departure from axial deformation. Although the IBM is formulated from the beginning in an abstract second quantized form, shape information can be introduced in the model by resorting to the intrinsic state formalism [11–13]. In this formalism, shape variables β and γ with the same interpretation as in the GCM, are introduced. Within this formalism, it has been shown that the three IBM dynamical symmetries [14] [U(5), SU(3), and O(6)] correspond to three analytical solutions for the collective Bohr Hamiltonian: the vibrational, rotational, and γ -unstable limits [7]. This correspondence has also been further explored by Rowe and collaborators in a series of papers [15–17].

Phase diagrams for both the GCM and the IBM, for the case of even-even nuclei, have been extensively studied [3-5]. However, few studies have been done on the corresponding phase transitions in Bose-Fermi systems. Recent studies of shape phase transitions in odd-even nuclei have been presented in the GCM and in the interacting boson-fermion model (IBFM) [18] in Refs. [19–23]. The CPS E(5/4) symmetry [19] has been discussed for the critical point of a single i = 3/2fermion coupled to a boson core that undergoes a transition from spherical to γ unstable. In Ref. [20], the corresponding transition has been studied in the framework of the IBFM. A more complex case of the CPS, called E(5/12) symmetry, has been described for the richer case of a fermion that can occupy single-particle states with angular momenta i = 1/2, 3/2, and 5/2 coupled to a core undergoing the transition from spherical to deformed γ unstable [21–23]. Both the E(5/4) and the E(5/12) models [19,21,22] were obtained starting from the

Bohr Hamiltonian, but comparable results are obtained within the IBFM for energy spectra and electromagnetic transitions. The role of an additional fermion at the critical point for the transition from spherical to axially deformed shapes has recently been described within the framework of the IBFM [23,24]. In Ref. [25], a supersymmetric approach was used to study phase transitions in odd-even nuclei.

In this paper, we focus on the effect of the coupling between a fermion in orbit of definite angular momentum *j* and an eveneven boson core that performs the transition from spherical to γ -unstable shapes upon variation of a control parameter. This situation is described within the framework of the intrinsic frame formalism for the IBFM [26–28]. The aim of this work is to understand how the coupling of the odd particle modifies the geometry imposed by the core, how each of the individual coupled states behaves at the transitional region, and how the critical point is affected by the inclusion of the odd particle.

The paper is structured as follows. In Sec. II, the model boson-fermion Hamiltonian is described. Section III presents the intrinsic frame formalism for odd-even systems. In Sec. IV, the results of this study are presented. Finally, in Sec. V, our main conclusions are summarized.

II. THE IBFM HAMILTONIAN

In general, the interacting boson-fermion model (IBFM) Hamiltonian is written as

$$H = H_B + H_F + V_{BF}, (2.1)$$

where H_B is the bosonic part, H_F is the fermionic part, and the V_{BF} term couples the boson and fermion degrees of freedom. We want to consider the spherical to deformed γ -unstable shape phase transition in a mixed Bose-Fermi system. For that purpose, a single fermion with j = 9/2 is coupled to an even-even boson core that undergoes the shape phase transition from spherical to deformed γ -unstable shapes. The IBFM Hamiltonian that describes the transition from U(5) to O(6) is parametrized as follows:

$$H = (1 - c)\hat{n}_d - \frac{c}{4N_B}\hat{Q}_{BF} \cdot \hat{Q}_{BF}, \qquad (2.2)$$

where N_B is the total boson number, *c* is the control parameter, and the operators in this Hamiltonian are the *d*-boson number

$$\hat{n}_d = \sum_{\mu} d^{\dagger}_{\mu} d_{\mu}, \qquad (2.3)$$

and the quadrupole operator for the odd-even system, which is the sum of the boson and fermion quadrupole operators

$$\hat{Q}_{BF} = \hat{Q}_B + \hat{q}_F. \tag{2.4}$$

With these definitions, expression (2.2) can be split into the three terms of Eq. (2.1).

For the case under study, the boson quadrupole operator reads

$$\hat{Q}_B = (s^{\dagger} \times \tilde{d} + d^{\dagger} \times \tilde{s})^{(2)}, \qquad (2.5)$$

while the fermion quadrupole operator is

$$\hat{q}_F = t_j (a_j^{\dagger} \times \tilde{a}_j)^{(2)}. \tag{2.6}$$

The coefficients t_j are the single-particle matrix elements of the *E*2 fermion operator

$$t_j = -\sqrt{\frac{1}{5}} \langle j || r^2 Y^{(2)} || j \rangle.$$
(2.7)

Since here a single-*j* shell case is considered, the only t_j will be taken as unity. It is worth noting that the boson and fermion quadrupole operators can be multiplied by boson and fermion effective charges, respectively. For the purpose of this work, they have been set to unity.

With the above-mentioned definitions, the boson Hamiltonian in Eq. (2.1) is given by

$$H_B = (1 - c)\hat{n}_d - \frac{c}{4N_B}\hat{Q}_B \cdot \hat{Q}_B.$$
 (2.8)

The IBM U(5) situation is recovered for c = 0, while c = 1 reproduces the O(6) limit. By changing *c* between these two limits, a continuous (second-order) shape phase transition is observed with the critical point at $c_c = N_B/(2N_B - 2)$. In addition to H_B , in Eq. (2.1), the fermion part H_F and the boson-fermion interaction V_{BF} are included. The pure fermion part is a constant for the single-*j* shell case, and the boson-fermion interaction obtained from Eq. (2.2) is

$$\hat{V}_{BF} = -\frac{c}{2N_B}\hat{Q}_B \cdot \hat{q}_F.$$
(2.9)

III. THE INTRINSIC FRAME FORMALISM

A useful way of looking at phase transitions is to apply the concept of the intrinsic frame which allows one to associate a potential energy surface to a Hamiltonian as (2.1) or (2.2) depending on shape variables. Within the IBM, the intrinsic state for the ground-state band for an even-even nucleus is written as

$$\Phi_{\text{g.s.}}(\beta,\gamma) = \frac{1}{\sqrt{N_B!}} [b_{\text{g.s.}}^{\dagger}(\beta,\gamma)]^{N_B} |0\rangle, \qquad (3.1)$$

where $|0\rangle$ is the boson vacuum. The ground-state boson creation operator is given by

$$b_{\text{g.s.}}^{\dagger}(\beta,\gamma) = \frac{1}{\sqrt{1+\beta^2}} \left[s^{\dagger} + \beta \cos \gamma d_0^{\dagger} + \frac{\beta}{\sqrt{2}} \sin \gamma (d_2^{\dagger} + d_{-2}^{\dagger}) \right].$$
(3.2)

The ground-state energy surface is obtained by calculating the expectation value of the boson Hamiltonian (2.8) in the intrinsic state (3.1):

$$E_{\text{g.s.}}(\beta,\gamma) = \langle \Phi_{\text{g.s.}}(\beta,\gamma) | H_B | \Phi_{\text{g.s.}}(\beta,\gamma) \rangle.$$
(3.3)

The variational parameters β and γ play a similar role to the one of the intrinsic collective shape variables in the Bohr Hamiltonian.

Intrinsic frame states for the mixed boson-fermion system can be constructed by coupling the odd single-particle states to the intrinsic states of the even core. The lowest states of the odd nucleus are expected to originate from the above-mentioned coupling to the intrinsic ground-state $\Phi_{g.s.}(\beta, \gamma)$. To obtain them, we first construct the coupled states

$$\Psi_{jK}(\beta,\gamma) = \Phi_{g.s.}(\beta,\gamma) \otimes |jK\rangle, \qquad (3.4)$$

and then diagonalize the total boson-fermion Hamiltonian in this basis, giving a set of energy eigenvalues $E_n(\beta, \gamma)$, where *n* is an index to count solutions in the odd-even system. In our case, for angular momentum j = 9/2, the possible magnetic components are $K = -9/2, \ldots, 9/2$. Therefore there are ten different states that we restrict to five because of the symmetry $K \leftrightarrow -K$.

IV. RESULTS

In this section, the effect of the coupling of an odd fermion with j = 9/2 to a boson core is investigated within the formalism presented in the preceding section.

First we discuss the coupling of the odd particle to an O(6) boson core. Consider the even-even core, if in the Hamiltonian (2.8) the control parameter c is set to unity and the expectation value of the boson Hamiltonian is computed in the intrinsic ground state, Eq. (3.3), the corresponding energy function is γ independent as shown in Fig. 1(a). In our case (with $N_B = 5$) the minimum in the β variable is around 0.78 (the value will tend to unity for N_B going to infinity). Then the odd i = 9/2 particle is coupled to the γ -unstable core using interaction (2.9). In this case, the full Hamiltonian (2.1) has to be diagonalized in the basis (3.4). For j = 9/2, a 5 × 5 matrix is obtained. The eigenvalues correspond, in cases of axial symmetry ($\gamma = 0^{\circ}, 60^{\circ}, \ldots$), to states with good projection of the angular momentum on the symmetry axis K. It should be noted that in the triaxial situation, K is not a good quantum number anymore. Calculations of the energy surfaces for the five eigenvalues of the odd-even system as a function of β and γ as those presented for the even-even nucleus in Fig. 1(a) have been performed, producing in all cases the absolute minima with axial symmetry (either prolate or oblate). This means that the addition of an odd particle to a deformed γ -unstable core does not produce triaxiality in any of the resulting intrinsic odd-even states. With this in mind, we are presenting in Fig. 1(b) and in all the remaining figures in this paper, the odd-even energy surfaces only as a function of β along $\gamma = 0^{\circ}$. To produce both prolate and oblate shapes, we will consider positive and negative values of β , maintaining $\gamma = 0^{\circ}$. We make use of the equivalence between the pair of coordinates (β , $\gamma = 60^{\circ}$) (oblate shapes) and ($-\beta$, $\gamma = 0^{\circ}$) when calculating energy surfaces (strictly speaking, within the GCM, β is positively defined and γ takes care of the prolate and oblate character of the ellipsoid and its orientation in space). In Fig. 1(b) the energy surfaces obtained when coupling a j = 9/2 particle to an O(6) core are plotted as a function of β . States are labeled by the quantum number K. The minimum of each surface is marked with a dot. From this figure it is clear that, although the core is γ unstable, the odd-even system prefers prolate shapes for K = 1/2, 3/2, 5/2, while it tends to be oblate for K = 7/2, 9/2. This fact is consistent with the simple picture of a particle orbiting around the equilibrium shape: the angular momentum has a small projection on the z axis when it lies close to the xy plane and therefore the



FIG. 1. (Color online) O(6) energy surfaces: c = 1 with $N_B = 5$. (a) Energy surface for the even-even system in the β - γ plane. (b) Five energy surfaces for the different *K* states coming from j = 9/2 in the odd-even system as a function of β . In this panel, the energy surface for the even-even case is also plotted for reference. (c) Nilsson-like scheme produced when representing the odd-even energy surfaces relative to the energy of the even-even system.

orbit, perpendicular to the angular momentum vector, lies on a plane that is close to the *z* axis, favoring a prolate shape. When, instead, it is close to the *z* axis, its projection is large (*K* is large) and the orbit lies almost parallel to the *xy* plane, favoring an oblate shape. In the same figure, the corresponding even-even energy surface is plotted, and the presence of two degenerate minima with the same deformation in absolute value, one prolate and one oblate, reflects the γ independence. All odd-even states have approximately the same β_{\min} as the core, although, as mentioned, K = 7/2, 9/2 favor oblate shapes ($\gamma = \pi$), and K = 1/2, 3/2, 5/2 favor prolate ones ($\gamma = 0$). In Fig. 1(c), the same information is plotted but computing the energy of the odd-even state relative to that of the even-even core. A Nilsson-like scheme is obtained.

Having discussed the coupling of the fermion to the O(6) limit, we move now into the transitional region by changing the control parameter c. In Fig. 2, the evolution of the energy surfaces for the core and the different K states in the odd-even system is given for a set of values of c for $\gamma = 0$. From the figure, it is clear that the state K = 9/2 is always favoring



FIG. 2. (Color online) Evolution of the energy surfaces for the even-even core and for the different *K* states in the odd-even system as a function of β deformation as the control parameter *c* is changed in the Hamiltonian, for $\gamma = 0$.

oblate deformation when the core is γ unstable. The minimum moves to smaller negative values as *c* goes through the critical point until it gets to $\beta = 0$ when the core is well inside the spherical region. The situation for K = 7/2 is similar, while K = 1/2, 3/2, and 5/2 favor prolate deformation. This situation is different from the one encountered in the case of the coupling of an odd particle to a well-deformed axial nucleus [24]. In this case, the core deformation drives all odd-even states except in a small region around the critical point in the transition from spherical to axially deformed shapes.

Now we come to the situation at the critical point. For the case under study ($N_B = 5$), the critical point for the even-even system is located at c = 0.625. In Fig. 3(a), the energy surface is plotted for the even-even core as a function of β and γ . It is seen that the even-even system is γ independent and has a spherical minimum. In Fig. 3(b), the behaviors of the odd-even energy surfaces are plotted at the critical point as functions of β . The even-even surface is very flat in β as expected for the continuous critical point situation. The dots mark the minima of the even-even and the different odd-even energy surfaces. The presence of the unpaired fermion is enough to definitely drive the system, which would otherwise be critical, into either prolate or oblate shapes. Figure 3(c) is a Nilsson-like diagram of the single-particle energies relative to the even-even core for the same case.



FIG. 3. (Color online) Critical point energy surfaces: c = 0.625 for $N_B = 5$. Same as Fig. 1, but at the critical point of the even-even core in the spherical to deformed γ -unstable shape phase transition.

The overall results are summarized in Fig. 4, where the minima in β for the different odd-even states are plotted versus the control parameter c. Positive β values correspond to prolate deformation, while negative ones mean oblate shapes. The even-even case is plotted as a reference. This splits into two lines in the deformed region, since for the even-even case two degenerate minima appear. From the figure, one can see that all over the transition the states with K = 1/2, 3/2, 5/2prefer to be prolate, while K = 7/2, 9/2 are producing oblate shapes. The upper panel is for $N_B = 5$, while the lower one is for $N_B = 15$. In both cases, it is seen that the odd surfaces tend to follow the behavior of the even-even core. However, for the smaller N_B value, the deviations from the even-even case are larger for all K. As N_B grows, the transition of the odd-even system gets closer to the one in the even-even system. We would like to mention again, that for the case in which the odd particle is coupled to a core undergoing a transition from spherical to axially deformed shapes, all the states in the odd system tend to follow the core deformation either prolate or oblate [24]. In our case, the γ instability of the core allows the odd states to drive the entire system toward either a prolate or a oblate shape depending on the value of K.



FIG. 4. (Color online) Evolution of the equilibrium deformation parameter corresponding to the different *K* states in the odd-even system as a function of the control parameter *c*. The vertical scale displays the β deformation, with positive values indicating prolate deformation and negative ones oblate deformed shapes. The values for the even-even case are plotted for reference. The upper panel is for a number of bosons $N_B = 5$, and the lower one for $N_B = 15$.

V. SUMMARY AND CONCLUSIONS

In this paper, we have studied the coupling of a single j = 9/2 particle to a boson core in the situation in which it changes its shape from spherical to deformed γ unstable. The transitional behavior is studied within the interacting boson-fermion model, with a description based on the concept of intrinsic states. At variance with the case of a core undergoing a shape transition from spherical to axial deformation [U(5) to SU(3)], where the overwhelming weight of the core tends to drive all odd states to have the same deformation (either prolate or oblate), in the case of a γ -unstable deformed core the coupling to the odd particle gives rise to a set of intrinsic

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states which are partly oblate and partly prolate, maintaining the same nature all along the transitional path. For all these states, which are coexisting in the same system, the phase transition is found to be smoothed out with respect to the behavior in the even core.

It is worth mentioning that the present study is just a schematic illustration of the actual situation in odd-even nuclei. In general, there will be several open shells for the odd particle, and a realistic boson-fermion interaction will contain not only the quadrupole-quadrupole term. We think, however, that the multi-*j* case will not change the main features obtained in the single-*j* case. The exchange interaction is known to be very important for realistic applications, since it takes into account the Pauli principle in the boson-fermion space. Anyway, the case presented here should be a good starting point for the study of odd-even nuclei in the region of the Ru, Pd, and Cd isotopes where most of the proposed E(5) nuclei are located. In that region, ¹⁰⁴Ru [29], ¹⁰²Pd [30], ¹⁰⁶Cd, and ¹⁰⁸Cd [31] have been proposed as E(5) nuclei, and the relevant single-particle orbit for odd-proton isotopes is $g_{9/2}$. Consequently, ¹⁰³Tc, ¹⁰¹Rh, and ^{105,107}Ag would be good candidates for the application of the present study after the inclusion of the corresponding exchange interaction.

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