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Test of two-level crossing at the $N=90$ spherical-deformed critical point

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It is shown that the empirical transition region near neutron number $N=90$ can be described in terms of the crossing of configurations in a two-level system, as expected for a first order phase transition.

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Nuclear collectivity is often described in the context of harmonic vibrator, deformed symmetric rotor, and γ-unstable models which constitute a set of basic structures with analytical solutions. These three models have been described in the framework of the interacting boson approximation (IBA) model [1] as the U(5), SU(3), and O(6) dynamical symmetries of IBA, respectively. There are only a few nuclei that are very close to the dynamical symmetry limits. The vast majority of nuclei are transitional and must therefore be described by numerical diagonalizations of the Hamiltonian.

It has been known for a long time [2–4], based on the intrinsic state formalism, that the spherical-deformed transition regions in the IBA from U(5) to SU(3) and from U(5) to O(6) behave, in the large boson number limit, as first and second order phase transitions, respectively. The equilibrium configurations were also classified by means of the separatrix of the catastrophe formalism [5]. Of course, phase transitional behavior in finite nuclei will be smoothed out compared to infinite (macroscopic) systems, but finite nuclei have also been recently shown by experiments and analysis to exhibit characteristics of a phase/shape transition [6], including a critical point. Nuclei at a critical point have recently been described by a new class of symmetry [7,8] and empirical examples of the two symmetries in this class, denoted E(5) and X(5), have been identified [9,10]. These critical points can be characterized [11] as that stage in the transitional region where changes in the structure, as manifested in simple observables, Q invariants, and the wave function entropy, occur more rapidly (e.g., with neutron number or model parameters) than at any other stage. That is, these are the singular points where the derivatives of these quantities have an extremum and the second derivatives change sign.

The critical point for a vibrator to axial rotor transition, which is described by the symmetry X(5), is the focus of this Rapid Communication. It is manifested in the spherical-deformed $N=90$ region [10]. While many observables change rapidly with neutron number in the $N=90$ region, this is, however, not a direct proof that a phase transitional description is appropriate, as opposed, for example, to simply a rapid structural change. However, one particular unique characteristic of a first order phase transition [the case described by X(5)] does provide such a test. A first order phase transition entails a crossing of the energies of the two coexisting phases [12]. (Phase transitions and the symmetry breaking they entail have been discussed, for example, in Refs. [13].) In such a case of coexisting phases, the nuclear wave functions at and near the critical point can be described in terms of a mixing and (virtual) crossing of two specific configurations. The idea is illustrated in Fig. 1.

The purpose of this Rapid Communication is to show that this is indeed the case in the $N=90$ vibrator-to-axial-rotor transition region in which the near-critical-point nuclei ^{152}Sm and ^{150}Nd have been excellently described by the X(5) description. We shall do this by modeling the transition region with the IBA model and then by quantitatively analyzing the resulting IBA wave functions before and after the critical point.

In order to study the phase/shape transition from U(5) to SU(3), we use the extended consistent Q formalism (ECQF) [14] of the IBA in which the Hamiltonian takes the form

$$H=\epsilon_d\hat{n}_d-\kappa\hat{Q}^{\chi}\cdot\hat{Q}^{\chi}, \tag{1}$$

where $\hat{n}_d=d^{\dagger}\cdot\tilde{d}$ and $\hat{Q}^{\chi}=(s^{\dagger}\tilde{d}+d^{\dagger}s)+\chi(d^{\dagger}\tilde{d})^{(2)}$.

In order to exhibit the phase transitional behavior, it is convenient to rewrite this Hamiltonian in terms of a new parameter, $\zeta=4N_B/(\epsilon_d/\kappa+4N_B)$ [11], with N_B the number of bosons, as

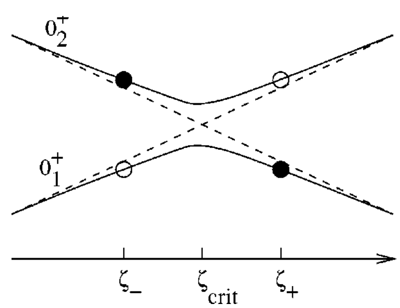

FIG. 1. Illustration of the idea of mixing and (virtual) crossing of two configurations as a function of a control parameter (called ζ, see below) near the critical point of a first order phase transition. The points ζ_{crit} and $\zeta_{\pm}$ are discussed in the text. The interchange of characters at the crossing is schematically illustrated by using similar symbols (open or closed dots) to indicate similarity of structure.

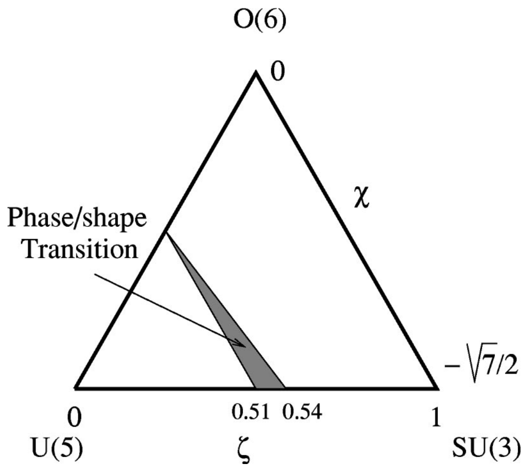

FIG. 2. The schematic representation of the IBA parameter space. The range of ζ values for the phase/shape transition is given for $N_B=10$. Adopted from Ref. [15].

$$H(\zeta)=c\left[(1-\zeta)\hat{n}_d-\frac{\zeta}{4N_B}\hat{Q}^{\chi}\cdot\hat{Q}^{\chi}\right], \tag{2}$$

where c is a scaling factor. This Hamiltonian describes the entire U(5)-SU(3) transition by varying only the parameter ζ between 0 [in the U(5) limit] and 1 [in the SU(3)] with a critical phase transition at $\zeta_{crit}=16N_B/(32N_B-25)\rightarrow 0.5$ for $N_B\rightarrow\infty$ [11]. Figure 2 shows schematically the IBA parameter space with the U(5) ($\zeta=0$) to SU(3) ($\zeta=1$) transition as the bottom leg of the triangle. The figure also shows (as a shaded area) the region in which a spherical 0^+ state coexists with a deformed 0^+ state [15]. This phase/shape coexistence region starts where the deformed minimum develops in addition to the spherical one and ends where the spherical minimum disappears and only the deformed minimum remains. For $N_B=10$ (appropriate for ^{152}Sm) and $\chi=-\sqrt{7}/2$ the coexistence region corresponds to $\zeta=0.51$–0.54, and the critical point is $\zeta_{crit}=0.54$.

We performed IBA calculations for the Nd, Sm, Gd, and Dy isotopes with $N>82$, centered on the critical point at $N=90$, using an extremely simple parametrization of the Hamiltonian, namely, $\zeta=0.23+0.085N_\nu$, where N_ν is the number of neutron bosons. This N_ν dependence is similar to that of Scholten *et al.* [16] for the Sm isotopes. The parameter κ was set equal to 0.0195 MeV and $\chi=-\sqrt{7}/2$.

Despite the simplicity of this parametrization, the calculations reproduce the transitional region quite well. As two examples, we show in Fig. 3 the data and calculations for $R_{4/2}\equiv E(4_1^+)/E(2_1^+)$ and for $E(0_2^+)$, in order to illustrate the typical finite-body phase transitionlike trajectory of an observable through the transition region. The excitation energy minimum for the 0_2^+ state near the critical point reflects the crossing of spherical and deformed configurations (see below).

In order to study whether the behavior of the system is indeed that of a first order phase transition, we investigate whether the wave functions can be expressed in terms of two-level mixing and whether the spherical and deformed

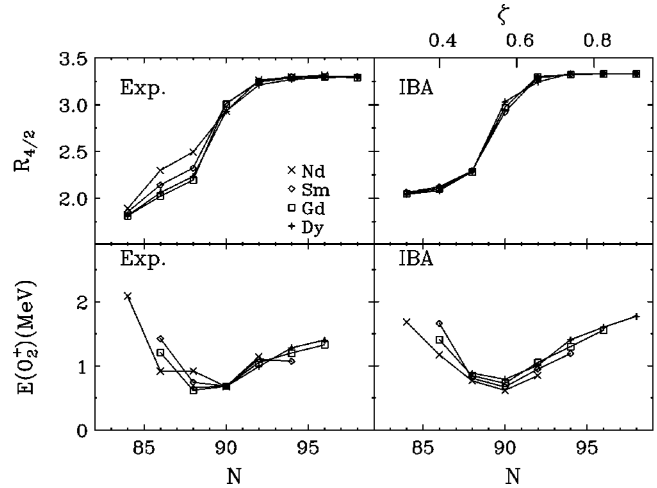

FIG. 3. The evolution of empirical $R_{4/2}\equiv E(4_1^+)/E(2_1^+)$ and $E(0_2^+)$ in the Nd-Dy isotopic chains with $N>82$ compared with the IBA results (see text).

configurations interchange as one traverses the critical point, as illustrated schematically in Fig. 1. To do so, we focus on the 0_1^+ and 0_2^+ states. (Similar results should apply for other spins.) The $N=90$ transition region is rapid, but, as seen in Fig. 3, the results have only a small dependence on the boson number N_B for a given ζ. This allows us to simplify the analysis by studying the wave functions for a constant N_B. We choose $N_B=10$, appropriate to ^{152}Sm.

The system is a two level system in the vicinity of the critical point ζ_{crit} if the first two 0^+ eigenstates of the Hamiltonian $H(\zeta)$ span a "universal" two-dimensional vector space. One can write the wave vectors of the first two $0_{1,2}^+(\zeta)$ states of the Hamiltonian $H(\zeta)$ as an expansion in any complete orthonormal set of wave functions. We choose the set corresponding to the critical point ζ_{crit}. That is, we write

$$0_i^+(\zeta)=\sum_n a_{n,i}|0_n^+(\zeta_{crit})\rangle, \tag{3}$$

where $\Sigma_n(a_{n,i})^2=1$. To focus on the two-level aspect, we write this as

$$0_i^+(\zeta)=a_{1,i}|0_1^+(\zeta_{crit})\rangle+a_{2,i}|0_2^+(\zeta_{crit})\rangle+a_{R,i}|R(\zeta_{crit})\rangle \tag{4}$$

for $i=1,2$, where R stands for the "rest" of the wave function, that is, for all the components $|0_n^+(\zeta_{crit})\rangle$ with $n>2$, where $a_{R,i}=\pm\sqrt{\Sigma_{j>2}a_{j,i}^2}$, and $(a_{1,i})^2+(a_{2,i})^2+(a_{R\cdot i})^2=1$.

We now ask whether the physical 0_1^+ and 0_2^+ states in effect span only a two level basis in the vicinity of ζ_{crit}. Of course, far from ζ_{crit}, both 0_1^+ and 0_2^+ would be described by many terms in an expansion in the ζ_{crit} basis. Indeed, well beyond the region of phase coexistence there is only one well-developed minimum. For example, near U(5)[SU(3)], there is no deformed [spherical] configuration, and the 0_1^+ state in either limit would have significant components of many ζ_{crit} wave functions. It is therefore appro-

TABLE I. Wave functions of the 0_1^+ and 0_2^+ states near the critical point in terms of the basis $0_m^+(\zeta_{crit})$. The values for the "rest" vector R are given as $\sqrt{a_{R,i}^2}$, see Eq. (4). The values are given for $\zeta_-=\zeta_{crit}-0.1$ and $\zeta_+=\zeta_{crit}+0.1$ where $\zeta_{crit}=0.54$ for $N_B=10$.

Physical state	Basis		
	$0_1^+(\zeta_{crit})$	$0_2^+(\zeta_{crit})$	R
$0_1^+(\zeta_-)$	-0.864	$+0.495$	0.092
$0_2^+(\zeta_-)$	$+0.488$	$+0.782$	0.388
$0_1^+(\zeta_+)$	-0.861	-0.477	0.176
$0_2^+(\zeta_+)$	-0.498	$+0.713$	0.494

priate to choose a range of ζ values large enough that the structural changes are significant but small enough that a two-level description might apply. Specifically, we look at the wave functions of the $0_{1,2}^+$ states at $\zeta_\pm=\zeta_{crit}\pm\Delta_\zeta$ and we have taken $\zeta_{crit}=0.54$ and $\Delta_\zeta=0.1$. From the IBA wave functions we obtain the results in Table I.

The two-level character of the system in the vicinity of the critical point is demonstrated by the small component of the "rest" vectors R and by the fact that the wave functions of the 0_1^+ and 0_2^+ states, for both ζ_+ and ζ_-, are close to the form for two-state mixing, namely,

$$|0_1^+(\zeta)\rangle=+a_1|0_1^+(\zeta_{crit})\rangle+a_2|0_2^+(\zeta_{crit})\rangle, \tag{5}$$

$$|0_2^+(\zeta)\rangle=+a_2|0_1^+(\zeta_{crit})\rangle-a_1|0_2^+(\zeta_{crit})\rangle, \tag{6}$$

that is $a_{1,1}=-a_{2,2}\equiv a_1$ and $a_{1,2}=a_{2,1}\equiv a_2$.

We note that the amplitude of the "rest" vector $|R\rangle$ is larger for the 0_2^+ state, which is not surprising since this state is much closer in energy to the other $0_i^+, i>2$ states and will mix to some degree with them. Nevertheless, the predominantly two-state mixing character of the solutions near ζ_{crit} is clear from the table.

It may at first appear from the overlaps in Table I that the structures of the 0_1^+ states before and after the critical point are similar, and the same for the 0_2^+ states. However, this is not true as can be seen from Table I itself, where the relative signs of the main components of the $0_1^+(\zeta_-)$ and $0_1^+(\zeta_+)$ states are not the same. In fact, the interchange of character at a virtual crossing that we wanted to test (see earlier discussion of Fig. 1) is clear if the overlap of the 0_1^+ state at ζ_- is taken with the 0_1^+ and 0_2^+ states at ζ_+. These overlaps are $\langle 0_1^+(\zeta_-)|0_1^+(\zeta_+)\rangle=0.51$ and $\langle 0_1^+(\zeta_-)|0_2^+(\zeta_+)\rangle=0.78$. These numbers show that the $0_1^+(\zeta_-)$ state more closely resembles the $0_2^+(\zeta_+)$ state rather than the $0_1^+(\zeta_+)$ ground state. The idea is illustrated in Fig. 1, where similarity in the dots (solid or open) indicates similarity in structure.

The evolution of structure with ζ and the interchange of character around the critical point may also be seen from the calculated values of characteristic observables and from the overlaps of the wave functions near ζ_{crit} with spherical and deformed wave functions. The calculated values for $R_{4/2}$ and $E(2_1^+)$, for $N_B=10$ and $\kappa=0.0195$ MeV, for $\zeta=\zeta_-$, are

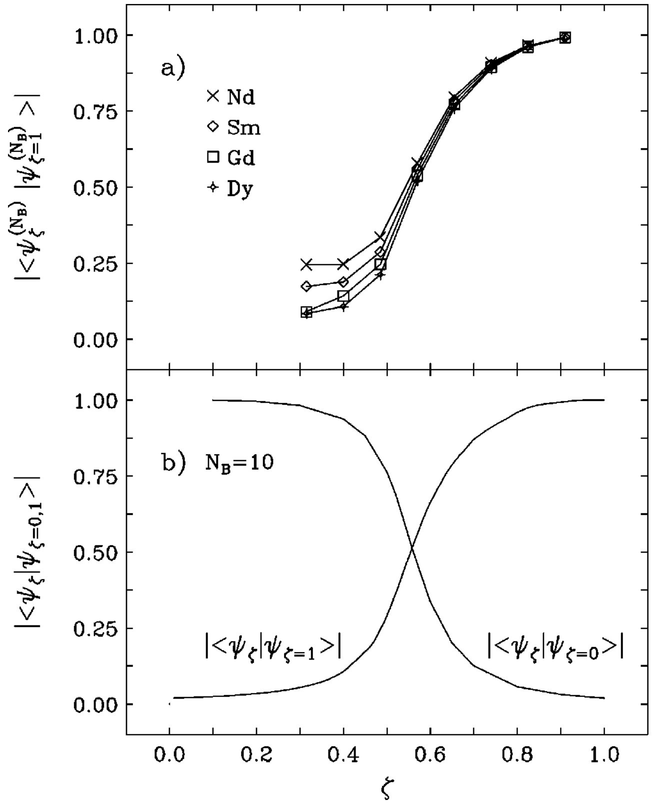

FIG. 4. (a) Overlaps of the ground state wave functions $\psi_\zeta^{(N_B)}$ obtained from the fit of the Nd-Dy nuclei (the same calculations as in Fig. 3) with the SU(3) ground state wave function for the same N_B. (b) Overlaps of the ground state wave function $\psi_\zeta(0_1^+)$ as a function of ζ with the SU(3) ($\zeta=1$) ground state wave function and the U(5) ($\zeta=0$) ground state wave function for $N_B=10$. Note the change of character from predominantly vibrator to predominantly rotor as ζ passes $\zeta_{crit}=0.54$.

2.14 and 0.562 MeV, respectively. In contrast, for $\zeta>\zeta_{crit}$ we have, at $\zeta=\zeta_+$: $R_{4/2}=3.24$ and $E(2_1^+)=0.089$ MeV.

Concerning the wave functions themselves, Fig. 4(a) shows the overlaps of the actual ground state wave functions from the fits with the SU(3) ground state (each overlap is extracted for the appropriate boson number N_B). This figure shows both the evolution towards a deformed SU(3) ground state and the remarkable similarity in the behavior of adjacent elements near $N=90$.

The trend in Fig. 4(a) is isolated more cleanly if calculations as a function of ζ are carried out for a constant boson number so that different overlaps are taken with the same set of limiting basis states. To this end, we show, in Fig. 4(b), the overlaps of the ground state wave functions with both the U(5) ($\zeta=0$) and SU(3) ($\zeta=1$) wave functions for $N_B=10$. Again, there is clearly a crossing near ζ_{crit} where the 0_1^+ state changes from predominantly of U(5), or vibrator character, to SU(3), or rotor character.

In conclusion, from a simple analysis of the wave functions of IBA calculations that reproduce quite well the extensive data in the Nd-Dy isotopes in the spherical-deformed transition region near $N=90$, we have shown that, near the critical point, the wave functions comprise a two-level system that mixes and that the structural change at the critical point corresponds to a (virtual) crossing of the spherical and deformed configurations. These are, in fact, characteristic signatures of a first order phase transition.

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