Singular Character of Critical Points in Nuclei

V. Werner\textsuperscript{1)}, P. von Brentano\textsuperscript{1)}, R.F. Casten\textsuperscript{2)}, and J. Jolie\textsuperscript{1)}

\textsuperscript{1)} Institut für Kernphysik, Universität zu Köln, Germany
\textsuperscript{2)} WNSL, Yale University, New Haven, CT 06520-8124, USA

Abstract

The concept of critical points in nuclear phase transitional regions is discussed from the standpoints of Q-invariants, simple observables and wave function entropy. It is shown that these critical points very closely coincide with the turning points of the discussed quantities, establishing the singular character of these points in nuclear phase transition regions between vibrational and rotational nuclei, with a finite number of particles.

Key words: Critical Point Symmetry, phase transition, shape transition, quadrupole shape invariants, wave function entropy, IBA
PACS number(s): 21.60.-n, 21.60.Ev, 21.60.Fw

Nuclear structural evolution in transitional regions is often thought of as a continuous variation of properties, as a function of nucleon number, from one idealized limit (e.g., vibrator, rotor) to another. The rapidity of structural change may vary across a transitional sequence of nuclei, and different mass regions exhibit different rates of change but, until recently, no individual point along these evolutionary trajectories could be singled out with special observational properties.

In the last years, however, the concept of critical points in shape/phase transition regions has been much discussed [1–5]. While the concept itself is well known in nuclei (in the context of the coherent state formalism [6,7] of the IBA model [8]), it is only very recently that analytic descriptions of critical point nuclei have been given [9,10]. This is a significant point since, historically, such nuclei have been the most difficult to treat: they exhibit competing degrees of freedom, and one has had to resort to numerical calculations.

Two critical point symmetries, called E(5) and X(5), have been proposed [9,10], giving analytic expressions for observables which are exactly at the
critical points of a vibrator to axially asymmetric ($\gamma$-soft) rotor transition region, and of a vibrator to symmetric rotor transition region, respectively, for an infinite number of nucleons. An important aspect of this is that, for the first time, one is able to associate special observational characteristics to a specific point along a trajectory from one structural limit to another. Recently [11], using the methods presented here, the well-known O(6) limit of the IBA has also been identified as another, heretofore unrecognized, critical point symmetry, for the transition between prolate and oblate nuclei. This is an important result since the O(6) symmetry can be calculated in the IBA for finite nucleon numbers, in contrast to the non-IBA symmetries E(5) and X(5). So far only two examples for nuclei [12,13] which lie close to the X(5) and E(5) symmetries are known while, interestingly, there are many examples for O(6) like nuclei. In the present work we will restrict our discussion to prolate nuclei.

To understand the evolution of structure in real nuclei, with a finite number of nucleons, it is important to gather information about systematic changes of observables at or near such critical points. This aim can be achieved by the use of a model that is able to describe limiting cases of nuclear structure - vibrators, rotors and $\gamma$-soft nuclei - and a large variety of nuclei between these limits. Such a model is given by the IBA, which - in the expansion of the coherent state formalism - exhibits critical points as has been discussed in refs. [6,7,14,15]. We stress that the critical point descriptions X(5) and E(5) are defined in terms of a geometrical approach, not the IBA. Nevertheless the IBA provides a convenient tool to span a range of structure, including phase transitions, and also to assess effects of finite particle numbers.

It is the purpose of this Letter to show, from several complementary theoretical approaches, that there is independent evidence for the singular character of these critical points, and independent ways of identifying them in observables calculated in collective models. To do so we bring together three major themes: the already mentioned study of phase transitional regions and critical point nuclei, the behavior of quadrupole shape ($Q$)-invariants, and the study of chaos and entropy in nuclear systems. We show that the critical points occur very near to the turning points (points of steepest descent or ascent) of these $Q$-invariants – that is, at the extrema of their first derivatives. The same behavior will also be shown to hold for some more easily accessible observables.

To span the transition regions, it is convenient to use the IBA Hamiltonian in the following form

$$H = a[(1 - \zeta)n_d - \frac{\zeta}{4N}Q \cdot Q] \quad (1)$$

where $Q = s^\dagger \tilde{d} + d^\dagger s + \chi[d^\dagger \tilde{d}]^{(2)}$ and we consider the well known parameter space of the extended consistent Q formalism (ECQF) varying $\zeta$ between 0
and 1, and \( \chi \) from 0 to \(-\sqrt{7}/2 = -1.32\), while \( a \) is a scaling factor. This parametrization is equivalent to the more commonly encountered (equivalent) ECQF [16,17] form of \( H \), which includes the parameters \( \epsilon \) and \( \kappa \).

Figure 1 illustrates the three dynamical symmetries of the IBA in terms of a triangle. With the Hamiltonian of Eq. (1) it is easy to calculate the structure for any point in the triangle. For \( \zeta = 0 \) one obtains a U(5) structure (for any \( \chi \)), and \( \zeta = 1, \chi = -\sqrt{7}/2 \) gives SU(3). Thus, a U(5)\( \leftrightarrow \)SU(3) transition region is defined by \( \chi = -\sqrt{7}/2 \) and \( \zeta \) varying from 0 to 1, while a U(5)\( \leftrightarrow \)O(6) region has \( \chi = 0 \) and \( \zeta \) varying from 0 to 1.

One can use the coherent state formalism [6,7] of the IBA model to identify the critical points in the ECQF space. In this approach, the energy functional for the ECQF Hamiltonian is given by

\[
E(\zeta, \chi, \beta, \gamma) = \frac{N\beta^2(1 - \frac{\zeta(\chi^2 - 3)}{4N - 4N\zeta + \zeta})}{1 + \beta^2} - \frac{N(N-1)\zeta}{4N - 4N\zeta + \zeta} \left( 4\beta^2 - 4\sqrt{7}\chi^3 \cos 3\gamma + 2\chi^2\beta^4 \right) \div \left(1 + \beta^2\right)^2
\]  

(2)

The variation of \( \zeta \) changes the structure between the vibrator limit and rotational nuclei – both axially symmetric and axially asymmetric – which are the transitions we will focus on. Critical points in \( \zeta \) are found where \( E \) becomes flat at \( \beta = 0 \). These points, which we refer to as \( \zeta_c \), can be derived by evaluating the condition

\[
\left| \frac{\partial^2 E(\zeta_c)}{\partial \beta^2} \right|_{\beta=0} = 0 .
\]  

(3)

On the transition path from U(5) to O(6) (for \( \chi = 0 \)) exactly one critical point is found, namely where a second, deformed, minimum in \( \beta \) of the energy functional emerges.

The situation becomes more complicated for transitions with \( \chi \neq 0 \). In these cases, the spherical minimum is joined by a deformed minimum and both minima coexist in a very close parameter range in \( \zeta \), converging to one point when approaching \( \chi = 0 \). Thus, in general there exist three critical points, which is illustrated in Fig. 2 for \( N=10 \) bosons for the limiting case of \( \chi = -\sqrt{7}/2 \). The thick lines in Fig. 2 give points in the \( (\zeta, \beta) \) plane, which are local minima of the energy functional (2). The shaded area is the parameter range of \( \zeta \), where two local minima of the energy functional coexist. The lower dashed line gives the critical \( \zeta \) value where a deformed minimum appears, while the upper dashed line gives the critical point in \( \zeta \) where the spherical minimum disappears and only the deformed minimum is left. The dotted line gives the critical \( \zeta \) value where two coexisting minima are equally deep. The parameter region in between is small for any boson number.
Thus, as it is the aim of this work to identify the critical points in observables, and we do not expect to be able to distinguish between these three points (close lying in $\zeta$) in real nuclei, we restrict ourselves to the critical point given by condition (3) where the spherical minimum disappears, and which is given by

$$\zeta_c = \frac{4N}{8N - 8 + \chi^2} \xrightarrow{N \to \infty} 0.5 .$$ (4)

The $\chi$ dependence is just a finite $N$ effect, and thus it is convenient to vary only the parameter $\zeta$ for the investigation of phase transitions between vibrational and rotational nuclei. Additionally we note that the choice of our parametrization has the convenient feature that in the large $N$ limit we get $\zeta_c = 0.5$.

While, due to their physical meaning, the endpoints of the line of critical points between $\chi = 0$ and $\chi = -\sqrt{7}/2$ in Fig. 1 can be approximately related to the non-IBA symmetries $E(5)$ and $X(5)$, we see that a much richer structure shows up in the IBA, where critical points occur over the whole transitional region between these legs of the symmetry triangle.

Since we are interested in obtaining signatures for critical points in observables including matrix elements, we now survey the behavior of Q-invariants [18,19] in the transition regions. Recently, the concept of Q-invariants has been re-investigated in the framework of the IBA model and the Q-phonon approach [20,21], and the behavior of these moments across the gamut of nuclear collective structures has been elucidated [22–24]. These invariants represent quadratic and higher order moments of the quadrupole operator. The invariants are denoted $q_n$ and $K_n \equiv q_n/q_{2n/2}$, and are defined by expressions of the generic type

$$q_n \sim \langle \Psi_0 | Q_1 \cdot Q_2 \cdots Q_n | \Psi_0 \rangle$$ (5)

where $\Psi_0$ is the ground state wave function, and where intermediate angular momentum couplings in the operator are omitted for simplicity.

For the IBA [8], the Q-invariants have been evaluated over the entire symmetry triangle of Fig. 1. To show the extreme cases, we first focus on the two transition paths $U(5) \leftrightarrow SU(3)$ ($\chi = -\sqrt{7}/2$) and $U(5) \leftrightarrow O(6)$ ($\chi = 0$). We note that the invariants $q_2$, $K_3$, $K_4$, and $\sigma_\gamma \equiv K_6 - K_3^2$ represent, respectively, the quadrupole deformation, the triaxiality, the softness of the nuclear shape in $\beta$, and in $\gamma$.

We first study the $U(5) \leftrightarrow SU(3)$ transition and obtain the results shown for $N=10$ in the top row of Fig. 3 for $q_2$, $K_4$ and $\sigma_\gamma$. Each of these exhibits a rapidly changing behavior which has a turning point $\zeta_t$ near $\zeta = 0.5$. To investigate this
in more detail, the second row of Fig. 3 shows the first derivatives with respect
to $\zeta$. Again there is a striking consistency of behavior: the first derivative has
an extremum at essentially the same point for each invariant.

Specifically, the turning points (the zeros of the second derivatives) are: $\zeta_t = 0.54$ for $q_2$; $\zeta_t = 0.53$ for $K_4$; and $\zeta_t = 0.52$ for $\sigma_\gamma$. In the coherent state
formalism, for $N=10$, one obtains $\zeta_c = 0.54$ for the $U(5)\leftrightarrow SU(3)$ case. This
is very close to the turning points in $q_2, K_4$ and $\sigma_\gamma$: that is $\zeta_t \sim \zeta_c$. This
correspondence between the turning points and the critical points is the main
result of this work. The small differences probably represent a finite boson
number effect.

This identification of a special point along the structural evolution from vi-
brator to rotor is apparent even in the simplest observables as well. In Fig. 4
we show the behavior of the structural observables $R_{4/2} \equiv E(4^+_1)/E(2^+_1)$ and
$B(E2) : 2^+_1 \rightarrow 0^+_1$ for the $U(5)\leftrightarrow SU(3)$ transition, again for $N=10$. Clearly,
as seen in the first derivative plots in the second row, both quantities exhibit
their steepest rates of change near the critical points. Here, the first derivative
has an extremum at $\zeta_t = 0.54$ for both $R_{4/2}$ and the $B(E2)$ value. In this lat-
ter case, this result is not surprising since this $B(E2)$ value and $q_2$ are directly
related.

The existence of three critical points on the $U(5)\leftrightarrow SU(3)$ transition path seems
not to be reflected in the $Q$-invariants, which may be explained by the very
compact parameter region in $\zeta$ where these critical points occur, while the
peaks in the derivatives have a certain width. Also note that fluctuations,
resulting from the limited numerical accuracy of the PHINT code used for
these calculations, have been smoothed by the use of splines. Thus, perhaps
the three critical points just cannot be resolved in the observables due to
numerical truncations.

Returning to the $Q$-invariants, similar results apply in the $U(5)\rightarrow O(6)$ region.
Fig. 5 (left panels) shows this for $q_2$ and $K_4$. In this case the turning points
(determined from the rates of change), are: $\zeta_t = 0.60$ for $q_2$ and $\zeta_t = 0.56$
for $K_4$. From Eq. (2), the coherent state formalism gives $\zeta_c = 0.56$ for $N=10$.
Again the $\zeta_t$ and $\zeta_c$ values obtained from the behavior of the $Q$-invariants and
from the coherent state formalism are quite close. Lastly, we note that the
rate of change of $q_2$ and $K_4$ in the $U(5)\leftrightarrow O(6)$ case is much less than in the
first order $U(5)\rightarrow SU(3)$ transition region. For example $(dq_2/d\zeta)_{\text{max}} \sim 800$ for
$U(5)\leftrightarrow SU(3)$ while it is only $\sim 200$ for $U(5)\leftrightarrow O(6)$. Also, the widths of the first
derivative curves are much wider (corresponding to a more gradual structural
evolution) in the $U(5)\leftrightarrow O(6)$ case.

Using the IBA, it is also possible to investigate internal paths in the symmetry
triangle. In particular internal straight line trajectories, starting from $U(5)$,
will correspond to $\chi$ values between 0 and $-\sqrt{7}/2$, allowing a full mapping of transitional trajectories. We illustrate such results by showing the change of the first derivative of the shape invariant $K_4$ for various values of $\chi$ in Fig. 6. The minima of the derivatives follow the line of critical points that is also given in the coherent state formalism, with only a small $\chi$ dependence.

Finally, in regard to Q-invariants, we look at the $O(6)\leftrightarrow SU(3)$ transitional region. The right panels of Fig. 5 show the behavior of $q_2$ and its derivative. Note that the shape is qualitatively different than in the other transition regions, showing a gradually asymptotic curve and a first derivative against $\chi$ (the appropriate variable for this region) which is monotonic. No critical point is definable in this region of $\chi$ values, except when $O(6)$ itself is reached (see ref. [11]).

Another theme in nuclear structure recently has been the study of order and chaos for different structures. It was shown in ref. [25] that nuclear systems display ordered spectra at and near the three symmetry limits of the IBA, but that there is a rapid onset of chaotic behavior away from these benchmark regions. (See Fig. 1 of ref. [25] but note that the symmetry triangle is differently defined therein.) Recently, Cejnar and Jolie [26,27] have developed the concept of wave function entropy as an alternate (and physically intuitive) way of studying the relative complexity of nuclear wave functions. Basically, the entropy of a state is a measure of its spreading within a given basis. Note that this is not the same as the chaoticity (which is basis invariant) since a wave function may have high entropy in one basis [e.g., U(5)] and low entropy in another [e.g., SU(3)].

Now that we showed a visible effect of critical points in various observables, it is interesting to see whether effects of a phase transition can also be seen in the wave functions and thus the wave function entropy. A rise of the wave function entropy can be expected in moving from one limit to another, but the question is whether it also appears in a close region with turning points which coincide with the turning points of the previously mentioned observables. Thus, we define [26] a quantity, called $W_\Psi^B$, for a state $\Psi$, that can be written in the basis $B$ as $\Psi = \sum_{i_B} a_{i_B}^B |\Psi_B^B>$, as

$$W_\Psi^B \equiv - \sum_{i_B=1}^n |a_{i_B}^B|^2 \ln |a_{i_B}^B|^2$$

(6)

where $n$ is the number of basis vectors. If $\Psi$ coincides with a basis vector, then $W_\Psi^B = 0$. If $\Psi$ is uniformly spread out over the basis $B$, then $W_\Psi^B \approx \ln n$.

A physically intuitive expression of the entropy is the quantity [27]

$$n_{eff,\Psi}^B \equiv \exp W_\Psi^B$$

(7)
which expresses a kind of "effective number" of wave function components. For a "pure" state $\Psi$, $n_{\text{eff}}^{B} = 1$ and for a fully de-localized state $n_{\text{eff}}^{B} \approx n$.

To properly normalize the entropies we define the entropy ratio

$$r^{B} \equiv \frac{\exp W_{B}^{\Psi} - 1}{\exp \langle W_{\text{GOE}} \rangle - 1}$$

(8)

relative to that for the Gaussian Orthogonal Ensemble [27]. The ratio $r_{\Psi}^{B}$ varies from 0 for a pure (localized in the basis $B$) state to $\sim 1$ for a highly mixed state (see ref. [27] for a more detailed discussion of this normalization).

We show the results in Fig. 7 for $r_{B}^{\Psi}$ and its derivative as a function of the order parameter $\zeta$ for the U(5)$\leftrightarrow$SU(3) and U(5)$\leftrightarrow$O(6) transition regions (all for $N=10$). The entropy ratio for the ground state undergoes a very rapid change near $\zeta_{c}$ for both transition regions. We note that for larger boson numbers $N$ the transition becomes much sharper (see Fig. 6 in [11]). For the U(5)$\leftrightarrow$SU(3) and U(5)$\leftrightarrow$O(6) phase transitions, it is easy to read the turning points, $\zeta_{t}$, values from the derivative plots, obtaining $\zeta_{t} = 0.52$ and $\zeta_{t} = 0.59$ [in a U(5) basis], respectively, compared to values of $\zeta_{c} = 0.54$ and $\zeta_{c} = 0.56$ from the coherent state formalism. We note that the steepness of the entropy functions against $\zeta$ increases with boson number $N$, as pointed out in ref. [28]. This also holds true for the observables studied above.

To conclude, from the behavior of several rather different quantities, the Q-invariants, the simple observables $R_{4/2}$ and $B(E2 : 2_{1}^{+} \rightarrow 0_{1}^{+})$, and the wave function entropy, we have shown that critical points of the phase transitional regions U(5)$\leftrightarrow$SU(3) and U(5)$\leftrightarrow$O(6) are reflected in the behavior of these observables along these evolutionary trajectories. This result was obtained for finite boson numbers, making it possible to investigate effects of valence particle number on the singularities.

We are grateful to N.V. Zamfir, F. Iachello, J. Eberth and K. Heyde for useful discussions, and to P. Cejnar for the entropy calculations. Work supported by the U.S.DOE under Grant number DE-FG02-91ER40609 and by the DFG under Project number Br 799/10-1 and by NATO Research Grant no. 950668. One of us [RFC] is grateful to the Institut für Kernphysik in Köln for support.

References

[1] A. Wolf et al., Phys. Rev. C49 (1994) 802.

[2] R.F. Casten, N.V. Zamfir, and D.S. Brenner, Phys. Rev. Lett. 71 (1993) 227.
[3] F. Iachello, N.V. Zamfir, and R. F. Casten, Phys. Rev. Lett. 81 (1998) 1191.

[4] R. F. Casten, Dimitri Kusnezov, and N.V. Zamfir, Phys. Rev. Lett. 82 (1999) 5000.

[5] Jan Jolie, Pavel Cejnar, and Jan Dobes, Phys. Rev. C60 (1999) 061303.

[6] A.E.L. Dieperink, O. Scholten, and F. Iachello, Phys. Rev. Lett. 44 (1980) 1747.

[7] J.N. Ginocchio and M.W. Kirson, Phys. Rev. Lett. 44 (1980) 1744.

[8] F. Iachello and A. Arima, The Interacting Boson Model (Cambridge University Press, Cambridge, 1987).

[9] F. Iachello, Phys. Rev. Lett. 87 (2001) 052502.

[10] F. Iachello, Phys. Rev. Lett. 85 (2000) 3580.

[11] J. Jolie, R.F. Casten, P. von Brentano, V. Werner, Phys. Rev. Lett. 87 (2001) 162501.

[12] R.F. Casten and N.V. Zamfir, Phys. Rev. Lett. 87 (2001) 052503.

[13] R.F. Casten and N.V. Zamfir, Phys. Rev. Lett. 85 (2000) 3584.

[14] E. Lopez-Moreno and O. Castanos, Phys. Rev. C 54 (1996) 2374.

[15] E. Lopez-Moreno and O. Castanos, Rev. Mex. Fis. 44 (1998) 48.

[16] D.D. Warner, and R.F. Casten, Phys. Rev. Lett. 48 (1982) 1385.

[17] P.O. Lipas, B.P. Toivonen, and D.D. Warner, Phys. Lett. B155 (1985) 295.

[18] D. Cline, Ann. Rev. Nucl. Part. Sci. 36 (1986) 683.

[19] K. Kumar, Phys. Rev. Lett. 28 (1972) 249.

[20] G. Siems, et al., Phys. Lett. B320 (1994) 1.

[21] T. Otsuka and K.-H. Kim, Phys. Rev. C50 (1994) 1768.

[22] R.V. Jolos, et al., Nucl. Phys. A618 (1997) 126.

[23] Yu.V. Palchikov, P. von Brentano, and R.V. Jolos, Phys. Rev. C57 (1998) 3026.

[24] V. Werner, et al., Phys. Rev. C61 (2000) 021301.

[25] Y. Al-hassid and N. Whelan, Phys Rev Lett. 67 (1991) 816.

[26] Pavel Cejnar and Jan Jolie, Phys. Lett. B420 (1998) 241.

[27] Pavel Cejnar and Jan Jolie, Phys. Rev. E58 (1998) 387.

[28] Pavel Cejnar and Jan Jolie, Phys. Rev. E61 (2000) 6237.
Fig. 1. Symmetry triangle of the IBA model. The U(5)→O(6) leg is characterized by \( \chi = 0 \) and varying \( \zeta \), while the U(5)→SU(3) transition region has \( \chi = -\sqrt{7}/2 \) and \( \zeta \) is varied. The dashed line indicates the phase transitional region where critical points are found.

Fig. 2. The thick lines represent the locus in the \((\zeta, \beta)\) parameter space where the energy functional of the coherent state formalism has a local minimum. The thick line at \( \beta = 0 \) extends downwards to \( \zeta = 0 \). The results are shown for the case of \( N=10 \) bosons. Dashed lines mark critical \( \zeta \) values where one minimum disappears (the spherical one at and above the larger value, the deformed one at and below the lower value). Only in the shaded area two minima coexist. The dotted line marks the critical \( \zeta \) value where these two minima are equally deep.
Fig. 3. Behavior of $q_2$, $K_4$ and $\sigma_\gamma$, and their first derivatives with respect to $\zeta$, for the $U(5)\leftrightarrow SU(3)$ transition region, calculated for $N=10$ bosons.

Fig. 4. Similar to Fig. 3 (for $N=10$) for the observables $R_{4/2}$ and $B(E2; 2_1^+ \rightarrow 0_1^+)$ for the $U(5)\leftrightarrow SU(3)$ transition region.
Fig. 5. Similar to Fig. 3 (for N=10), for $q_2$ and $K_4$, for the $U(5)\leftrightarrow O(6)$ transition region (left panels), and for $q_2$ in the $O(6)\leftrightarrow SU(3)$ (note here with respect to $\chi$) transition region (right).

Fig. 6. First derivative of $K_4$ (for N=10), but for various values of the parameter $\chi$. A peak indicating a phase transition occurs for every value of $\chi$. The dependence of its position on $\chi$ is a finite N effect.
Fig. 7. The entropy ratio (for N=10) for the $0^+_1$ state (top row) in the three transition regions, plotted against $\zeta$ and given, for each region, in two bases as indicated [e.g., U(5) and SU(3) for the U(5)$\leftrightarrow$SU(3) transition]. The lower panels give the derivative of the entropy ratio against $\zeta$ in the appropriate basis.