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Distinguishing a first order from a second order nuclear shape phase transition in the interacting boson model

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We study the characteristics of some quantities in the interacting boson model (IBM) that are sensitive to the nuclear shape phase transitions. By analyzing the variational features of the quantities with respect to the increasing of total boson number in the U(5)-SU(3) and U(5)-O(6) transitions, we find that the $B(E2)$ ratios, such as $B(E2; 4_1 \to 2_1)/B(E2; 2_1 \to 0_1)$ and $B(E2; 0_2 \to 2_1)/B(E2; 2_1 \to 0_1)$, can serve as the effective order parameters to distinguish a first order from a second order nuclear shape phase transition.

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Quantum phase transitions are of great interest in many areas of physics, and their manifestations vary significantly in different systems. For nuclear systems, the interacting boson model (IBM) reveals rich features of their shape phase transitions [1–10]. As an algebraic model [11], the IBM is closely related to the shell model as well as the geometry model [1,12,13]. Three dynamical symmetries in the IBM have been shown to correspond to three typical shape phases of nuclei, known as the spherical [vibrational with U(5) symmetry], axially deformed [rotational with SU(3) symmetry], and γ-soft deformed [rotational with O(6) symmetry] shapes. It has also been known that phase transitions coincide with transitions between dynamical symmetries, with a first order phase transition taking place in the U(5)-SU(3) transition, and a second order phase transition happening in the U(5)-O(6) transition [1]. In addition, two new symmetries, X(5) [14] and E(5) [15,16], have been introduced to describe the nuclei at the critical points corresponding to the first and second order transitions, respectively. And certain quantities sensitive to the phase transitions have been suggested as order parameters to characterize the phase transitions [5,17]. However, as shown in Ref. [17], some of the quantities that have been used as order parameters seem to fail in differentiating the two transitions when the boson number becomes large. It is therefore of interests to find physical quantities that can not only signify the occurrence of phase transitions but also distinguish the order of such transitions. The present paper reports our attempt along this line.

Our study starts with the well-known Hamiltonian [9]

$$\hat{H} = \epsilon\left[(1-\xi)\hat{n}_d - \frac{\xi}{4N}\hat{Q}^{\chi}\cdot\hat{Q}^{\chi}\right], \qquad (1)$$

where $\hat{n}_d = \sum_m d_m^\dagger d_m$ is the d-boson number operator, $\hat{Q}^{\chi} = (d^\dagger\tilde{s} + s^\dagger\tilde{d})^{(2)} + \chi(d^\dagger\tilde{d})^{(2)}$ with $-\sqrt{7}/2 \leqslant \chi \leqslant 0$ is the quadrupole operator, and $\xi \in [0, 1]$. In this paper, we focus on the U(5)-SU(3) and U(5)-O(6) transitions, corresponding to $\chi = -\sqrt{7}/2$ with $0 \leqslant \xi \leqslant 1$ and $\chi = 0$ with $0 \leqslant \xi \leqslant 1$, respectively.

To identify shape phase transitions and determine their orders, quantities sensitive to the phase transitions are definitely needed. Looking for such quantities and their characteristics, we first calculate the overlap of ground state wave functions of the Hamiltonian in Eq. (1) as a function of the control parameter ξ with those of the limit cases, $|\langle 0_g;\xi|0_g;\xi_0\rangle|$ with $\xi_0 = 0, 1$, along the line of thought of Refs. [5,17]. The results of the overlap $|\langle 0_g;\xi|0_g;\xi_0\rangle|$ are shown in Figs. 1 and 2, respectively, for the U(5)-SU(3) and the U(5)-O(6) transitions with total boson number $N = 10, 20, 50$.

It is seen from Fig. 1 that $|\langle 0_g;\xi|0_g;\xi_0 = 0\rangle|$ decreases and $|\langle 0_g;\xi|0_g;\xi_0 = 1\rangle|$ increases as ξ rises from 0 to 1. There is a crossover point with a nonzero amplitude around $\xi \sim 0.55$ for the overlaps $|\langle 0_g;\xi|0_g;\xi_0 = 0\rangle|$ and $|\langle 0_g;\xi|0_g;\xi_0 = 1\rangle|$, and the amplitude of the crossover point descends gradually as N increases. There is a drastic change in the overlap $|\langle 0_g;\xi|0_g;\xi_0 = 0\rangle|$ around $\xi \sim 0.5$, which indicates a critical point [6,7] of the phase transition. Such a characteristic becomes more significant with a larger N. At the same time, a similar feature is evident in Fig. 2 for the U(5)-O(6) transition. Such features are consistent with the results of Refs. [5,17]. These results show that the overlap of ground state wave functions is helpful in identifying phase transitions. However, the variational feature of the overlap behaves largely the same in the two different transitions when N becomes larger. Therefore, the overlap is seemingly unable to distinguish the first order phase transition of U(5) to SU(3) symmetries from the second order one of U(5) to O(6), although it does signal the transition and the critical point. There are other quantities, such as the fractional occupation probability of d bosons in the ground state, the reduced $E2$ transition rate $B(E2; 2_1 \to 0_1)$, and so on [5,17], all sharing the similar behavior and role.

To overcome such a limitation, people have looked into the difference between the expectation value of the d-boson number operator $\hat{n}_d$ of the first excited 0^+ state (0_2) and that of the ground state (0_1) $\nu_2 = \alpha_0(\langle 0_2|\hat{n}_d|0_2\rangle - \langle 0_1|\hat{n}_d|0_1\rangle)$ and that between the 2_1 state and the ground state $\nu_2' =$

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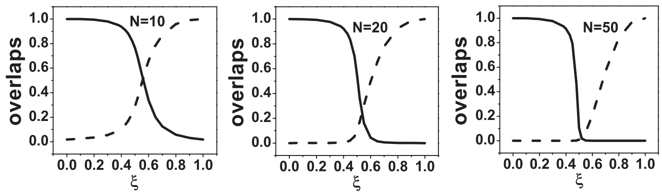

FIG. 1. Calculated variational behavior of the overlap of ground state wave functions in the U(5)-SU(3) transition with that in the limit cases. Solid curve for the overlap $|\langle 0_g;\xi|0_g;\xi_0=0\rangle|$, and dashed curve for the overlap $|\langle 0_g;\xi|0_g;\xi_0=1\rangle|$.

$\beta_0(\langle 2_1|\hat{n}_d|2_1\rangle - \langle 0_1|\hat{n}_d|0_1\rangle)$, which relate to the isomer shifts, as the order parameters to distinguish a first order from a second order phase transition in the IBM [5]. Reference [5] has shown that ν_2 displays a wiggling, sign-change behavior in the critical region due to the switching of the two coexisting phases, which is the characteristic of a first order phase transition, whereas ν_2 has a smoother variation in the second order phase transition. Furthermore ν_2' has characteristics similar to those of ν_2. However, Ref. [17] has shown that the above characteristics of these two quantities do not persist as the number of total bosons becomes large. Here we calculate with greater care the two quantities for the U(5)-SU(3) and the U(5)-O(6) transitions, as being done to the overlap of wave functions. The obtained results are shown in Fig. 3. From Fig. 3, we can see that both ν_2 and ν_2' involve a peak in the U(5)-SU(3) transition region, and both display a hump in the U(5)-O(6) transition region as the total boson number N gets large, which has been reported partially in Ref. [17]. Taking advantage of the fact that all the states in the U(5)-O(6) transition region are the common eigenstates of the Casimir operator of the group O(5) [because both the U(5) and the O(6) have a common maximal subgroup O(5)], one can easily calculate the energy spectra and wave functions of nuclei with very large boson numbers N in the U(5)-O(6) transition region [18,19]. Our calculations show that as the total boson number N gets very large (for instance, $N=1000$), the humps of ν_2 and ν_2' in the U(5)-O(6) transition region develop into very narrow and high peaks. From the obtained variational features of ν_2 and ν_2', one can notice that the peaks will also become very sharp in the transition of U(5)-SU(3). It seems that the wiggling behavior of ν_2 and ν_2' is not a mere result of the coexistence of two phases. These results indicate that, although ν_2 and ν_2' behave in different ways in the U(5)-SU(3) and the U(5)-O(6) transitions for small N, they involve quite similar characteristics as N becomes large.

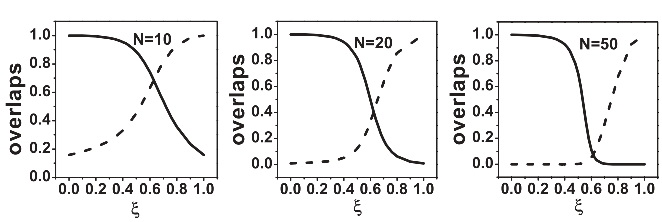

FIG. 2. Same as Fig. 1, but for the U(5)-O(6) transition.

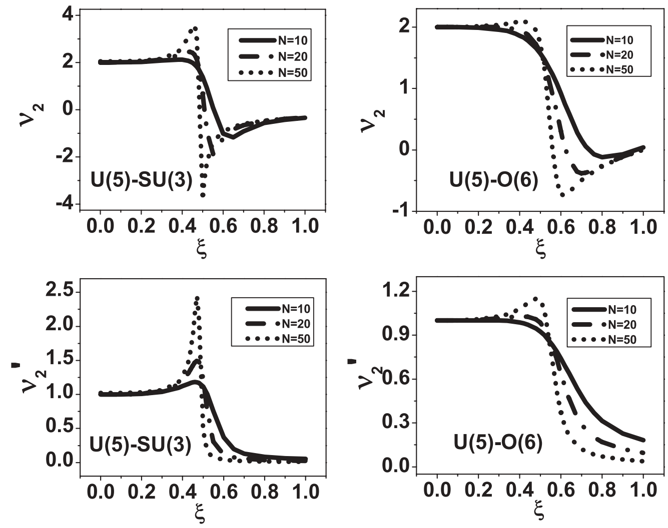

FIG. 3. Calculated variational behaviors of quantities ν_2 and ν_2' vs the control parameter ξ for systems with several values of N in the two transition regions (where the parameters α_0 and β_0 in ν_2 and ν_2' are both set to be unity).

As known, the order of a quantum phase transition should be well defined in the thermodynamic limit ($N\to\infty$), and an effective order parameter is better to exhibit different characteristics in transitions of different orders. The above analysis shows that ν_2 and ν_2' can be used to distinguish a first order from a second order phase transition in the system with a small boson number, but they cease to function so in the classical (thermodynamic) limit. It is then still necessary to find effective order parameters that are independent of the total boson number N and can determine the order of phase transitions. To that end, we explore two other quantities, $K_1 = B(E2;4_1\to 2_1)/B(E2;2_1\to 0_1)$ and $K_2 = B(E2;0_2\to 2_1)/B(E2;2_1\to 0_1)$, which can be measured experimentally. In the calculation, the $E2$ transition operator is taken as $\hat{T}(E2) = q_2[(d^\dagger\tilde{s} + s^\dagger\tilde{d})^{(2)} + \chi(d^\dagger\tilde{d})^2]$, where q_2 is the effective charge. The calculated variational behaviors of K_1 and K_2 with respect to the parameter ξ are shown in Fig. 4.

Figure 4 shows that (a) for small N, both K_1 and K_2 have a peak in the critical region of the U(5)-SU(3) transition, while K_1 and K_2 display bend slopes in the critical region of the U(5)-O(6) transition, (b) the prominence of both K_1 and K_2 develops into an obvious peak in the U(5)-SU(3) transition as N increases to quite a large value (such a feature has been pointed out in Ref. [7]), and (c) instead of developing into peaks, the bend slopes of K_1 and K_2 in the U(5)-O(6) transition become steeper with increasing N; however, the maxima of K_1 and K_2 locate always at the point with $\xi=0$ for any N. In short, both K_1 and K_2 display a completely different behavior in the critical region of the U(5)-SU(3) transition from that in the U(5)-O(6) transition, and this kind of difference becomes more apparent with increasing N.

The above analysis indicates that K_1 and K_2 are suitable effective order parameters, which are less dependent on the total boson number N. They can be used to distinguish

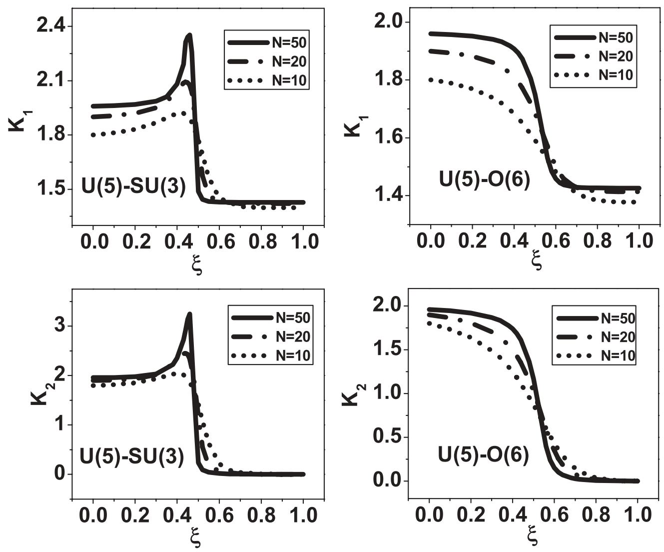

FIG. 4. Calculated variational behaviors of K_1 and K_2 vs the control parameter ξ for systems with several values of N in the two transition regions.

the first order from the second order nuclear shape phase transitions. To test the practicability of the proposed effective order parameters, we applied them to some well-established transitions. Figure 5 shows the variation of the experimentally observed $B(E2)$ ratio K_1 of Sm isotopes with respect to the neutron number, which has been known to be a transitional region between the spherical and the axially deformed nuclei [U(5)-SU(3) [27], and that of Ru isotopes which can be approximatively described with the U(5)-O(6) transition [29,30]. For comparison, we show also the theoretical variational feature of K_1 against the parameter ξ of the system with boson number $N = 20$ in the inset of Fig. 5 (which is similar to the case

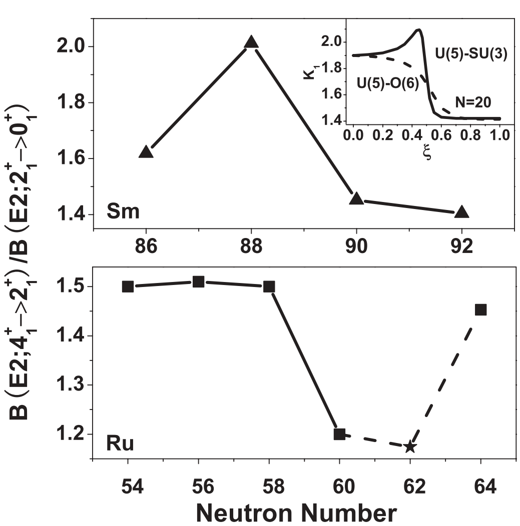

FIG. 5. Experimental data (from Refs. [20–27]) of the $E2$ transition ratio $B(E2; 4_1 \to 2_1)/B(E2; 2_1 \to 0_1)$ in Sm isotopes (filled triangles) and Ru isotopes (filled squares) vs neutron number and one theoretical datum (star) for ^{106}Ru taken from Ref. [28] (since the experimental one is lacking).

in Refs. [5] and [31] where N was taken as 15 and 10, respectively). It is worth mentioning that such a comparison is direct (although one is in terms of the neutron number, the other is with respect to the parameter ξ), since investigations [5,31] have shown that the parameter ξ is proportional to the boson number N (i.e., half of the number of valence nucleons in the original viewpoint of the IBM. In the present case, its variation comes only from half of the neutron number). From the upper panel of Fig. 5, one can recognize that the nucleus ^{152}Sm just locates at the critical point of the U(5)-SU(3) transition and has the X(5) symmetry, which is consistent with the result given in Refs. [32,33]. Meanwhile, nucleus ^{150}Sm also lies around the critical point, which coincides with the result that ^{150}Sm is very soft [34,35] and represents a common trait of the nuclei around the critical region of the transition U(5)-SU(3) [36]. Figure 5 (lower panel) also shows that ^{104}Ru locates apparently at the critical point of the second order phase transition U(5)-O(6). It indicates that ^{104}Ru might be a candidate of the E(5) symmetry, which is consistent with the result given in Ref. [37]. In addition, the deviation of ^{108}Ru from the U(5)-O(6) transition line hints that the U(5)-O(6) transition is only a crude approximation of the structure evolution of the even-even Ru isotopes [26,28,36]; rather, certain SU(3) components or more complicated interactions may be involved [26,28,36] in the extremely neutron-rich Ru nuclei.

In summary, we have restudied the variational behaviors of several physical quantities, such as the overlap of ground state wave functions and the ν_2 and ν_2' parameters introduced in Ref. [5], that are sensitive to nuclear shape phase transitions. We have also investigated the characteristics of two $B(E2)$ ratios, K_1 and K_2, in the U(5)-SU(3) and the U(5)-O(6) transitions. Such quantities are found to fall into three types depending on their variational behaviors. The first type, typified by the overlap of ground state wave functions, varies rapidly and behaves similarly in the U(5)-SU(3) and the U(5)-O(6) transition regions, when the boson number N is relatively small. As N gets larger, the variational behavior becomes more significant but retains the global similarity between the two transitions. This type of quantity also includes the fractional occupation probability of the d-boson number in ground states, the reduced $E2$ transition rate $B(E2; 2_1 \to 0_1)$, and others. The second type of quantity, represented by ν_2 and ν_2', displays different critical behavior in the U(5)-SU(3) and the U(5)-O(6) transitions when the boson number N is relatively small, and the general behavior of criticality becomes more similar as N increases, except that a U(5)-SU(3) transition experiences faster changes than U(5)-O(6). Such quantitative difference might be used to distinguish the first order from the second order shape phase transitions, although a qualitatively different characteristic would serve the purpose much better. To that end, we are fortunate to have the third type of quantity, typified by the $B(E2)$ ratios K_1 and K_2, which manifests marked differences in the U(5)-SU(3) and the U(5)-O(6) transitions throughout the range of N from small to large. Such completely different variational characteristics in the first and second order shape phase transitions indicate that the $B(E2)$ ratios K_1 and K_2 are appropriate for serving as effective order parameters to distinguish the two kind transitions. This type of effective order parameter also includes other $B(E2)$ ratios such as

$B(E2; L+2 \rightarrow L)/B(E2; 2_1 \rightarrow 0_1)$. Experimental data have provided some evidence, although more is needed, to establish such physical quantities. An effective order parameter is imperative to help people to find evidence of quantum phase transitions. However, a single order parameter by itself may not be able to determine the orders of all transitions. The analysis in this paper provides an example of how an effective order parameter may be identified in a specific system. The method may be extended to other systems such as molecules in the vibron model [38].

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