

Quantum phase transitional patterns in the SD -pair shell modelYanan Luo,^{1,*} Yu Zhang,² Xiangfei Meng,¹ Feng Pan,^{3,4} and Jerry P. Draayer⁴¹*School of Physics, Nankai University, Tianjin 300071, People's Republic of China*²*Department of Physics and State Key Laboratory of Nuclear Physics and Technology, Peking University, Beijing 100871, People's Republic of China*³*Department of Physics, Liaoning Normal University, Dalian 116029, People's Republic of China*⁴*Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, USA*

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Patterns of shape-phase transition in the proton-neutron coupled systems are studied within the SD -pair shell model. The results show that some transitional patterns in the SD -pair shell model are similar to the $U(5)$ - $SU(3)$ and $U(5)$ - $SO(6)$ transitions with signatures of the critical point symmetry of the interacting boson model.

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I. INTRODUCTION

Recently, based on the generalized Wick theorem [1], a nucleon-pair shell model (NPSM) was proposed [2], in which nucleon pairs with various angular momenta are used as building blocks. Since modern computing facilities fail for the calculation in the full shell-model space for the medium-weight and heavy nuclei, some truncation schemes need to be used. The tremendous success of the interacting boson model (IBM) [3] suggests that S and D pairs play a dominant role in the spectroscopy of low-lying modes [4–6]. Therefore, one normally truncates the full shell-model space to the collective SD -pair subspace in the NPSM. The latter is called the SD -pair shell model (SDPSM) [2,7,8].

A crucial point in the SDPSM is the validity of the SD -pair truncation. Shell-model foundations of the IBM were summarized by Iachello and Talmi [9], from which the results seem to indicate that the SD -pair truncation is a reasonable approximation to the full shell-model space. This problem was also studied in Refs. [10–12] with the conclusion that the SD -pair subspace works well in the vibrational region, but in the deformed region, the inclusion of G pairs may be also necessary. So far the rotational motion has not yet been well studied along the lines of the microscopic foundation of the IBM. In Ref. [13], a comparison between calculations in the full shell-model space and in the SD -pair subspace was discussed. It is found that in the single- j shell case, when the model Hamiltonian consists of monopole and quadrupole pairing plus quadrupole-quadrupole interactions, the SD -pair subspace satisfactorily reproduces the low-lying levels of the shell model and $E2$ transitions between them. This means that the SD -pair truncation for a single- j shell is reasonable when the Hamiltonian consists of pairing and quadrupole-quadrupole interactions. In the multi- j case, if a pure quadrupole-quadrupole interaction and a reasonable collective SD pairs are considered, the essential properties of Elliott's $SU(3)$ model are well produced within the SD -pair subspace. This is very important since it shows that the SD -pair truncation is a good approximation of the shell model for

rotational motion. The pair approximation of applying SDG pairs to deformed nuclei has not yet been done so far. In Ref. [14], the general pairing interaction and pair truncation approximations were studied for fermions in a single- j shell. It was shown that an attractive J th pairing interaction favors pairs with angular momentum J in low-lying states. Therefore, one may use pairs with angular momentum J as building blocks of wave functions of low-lying states. In the low-energy region, monopole and quadrupole correlations dominate in residual two-body interactions. Hence, the configurations of low-lying levels favor SD -pair structure. This provides a very simple picture that supports schematic calculations by using (only) S and D pairs. The fact that the SDPSM can describe the collectivity of low-lying states for nuclei around $A = 130$ implies that the SD -pair truncation is reasonable for low-lying states of transitional nuclei [15–20].

Nuclei, as a mesoscopic system, have been found to possess interesting geometric shapes, such as spherical vibrational [$U(5)$], axially deformed [$SU(3)$], and γ -soft [$O(6)$], which are usually described in terms of the Casten triangle in the IBM [21]. The search for signatures of transitions among various shapes (phases) of atomic nuclei is an interesting subject in nuclear structure theory. An understanding of such shape (phase) transitions may provide insight into quantum phase transitions in other mesoscopic systems [3]. Theoretical study of shape phase transitions and critical point symmetries in nuclei has mainly been carried out [3,22–38] in the interacting boson model for identical systems (IBM-I) [3]. Investigations on nuclear shape phase transition and critical point symmetry for identical nucleon systems have also been carried out with fermionic degrees of freedom in Refs. [39–44]. Recently, investigations of the shape phase transitions and critical point symmetries in nuclei have also been carried out [45,46] in the proton-neutron interaction boson model (IBM-II) [3].

Since the SDPSM is also built up from SD pairs, it is expected that the SDPSM can produce results similar to those from the IBM. Our previous work shows that the vibrational, rotational, and γ -soft spectra can be well reproduced [47] similar to the $U(5)$, $SU(3)$, and $SO(6)$ limiting spectra in the IBM. The vibrational-rotational phase transition for identical systems can also be produced within the framework of the SDPSM with fermionic degrees of freedom [48]. Since nuclei

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are neutron-proton coupled systems, and a rich phase structure can be obtained in the IBM-II, it is interesting to see whether the phase transitional patterns in the neutron-proton coupled system also show up in the SDPSM with fermionic degrees of freedom. This is the main objective of this paper.

II. MODEL

In the shell-model description, the pairing and quadrupole-quadrupole interactions are the most important short-range and long-range correlations. Given that the Hamiltonian used to study the shape phase transition in the IBM is mainly composed of monopole pairing and quadrupole-quadrupole interaction (e.g., Refs. [45,46]), a schematic Hamiltonian is adopted in the SDPSM that is a combination of monopole pairing and quadrupole-quadrupole interaction with

$$\begin{aligned}
 H_X &= \sum_{\sigma=\pi,\nu} (-G_\sigma S_\sigma^\dagger S_\sigma - \kappa_\sigma Q_\sigma^{(2)} \cdot Q_\sigma^{(2)}) - \kappa Q_\pi^{(2)} \cdot Q_\nu^{(2)}, \\
 S^\dagger &= \sum_a \frac{\hat{a}}{2} (C_a^\dagger \times C_a^\dagger), \\
 Q^{(2)} &= \sqrt{16\pi/5} \sum_i r_i^2 Y^2(\theta_i, \phi_i),
 \end{aligned} \tag{1}$$

where X in H_X is denoted as U(5), SU(3), or SO(6) corresponding to vibrational, rotational, or γ -soft limiting case in the model, G_σ and κ_σ are the pairing and quadrupole-quadrupole interaction strength between identical nucleons, respectively, and κ is the quadrupole-quadrupole interaction strength between proton and neutrons. In this paper, we set $G_\pi = G_\nu$ and $\kappa_\pi = \kappa_\nu$. $Q_\sigma^{(2)}$ is the quadrupole operator, for which the second quantized form is given by

$$\begin{aligned}
 Q_\mu^{(2)} &= \sum_{cd} q(cd2) P_\mu^2(cd), \\
 q(cd2) &= (-)^{c-\frac{1}{2}} \frac{2}{5} \widehat{cd} C_{c\frac{1}{2},d-\frac{1}{2}}^{20} \Delta_{cd2} \langle Nl_c | r^2 | Nl_d \rangle, \\
 \Delta_{cd2} &= \frac{1}{2} [1 + (-)^{l_c+l_d+2}], \\
 P_\mu^t(cd) &= (C_c^\dagger \times \tilde{C}_d)_\mu^t,
 \end{aligned}$$

where $\widehat{l} \equiv \sqrt{2l+1}$, $C_{c\frac{1}{2},d-\frac{1}{2}}^{20}$ is the corresponding CG coefficient, and N is the principal quantum number of the harmonic oscillator wave function with energy eigenvalue $(N+3/2)\hbar\omega_0$. The matrix elements for r^2 are

$$\langle Nl_c | r^2 | Nl_d \rangle = \begin{cases} (N+3/2)r_0^2, & l_c = l_d, \\ \varphi[(N+l_d+2 \pm 1)(N-l_d+1 \mp 1)]^{1/2} r_0^2, & l_c = l_d \pm 2, \end{cases}$$

where the phase factor φ can be taken either as -1 or $+1$, and $r_0^2 = \hbar/M_N\omega_0 = 1.012A^{1/3} \text{ fm}^2$, M_N is the mass of a nucleon, and ω_0 is the frequency of the harmonic oscillator.

To study the phase transitional patterns, the Hamiltonian for the proton-neutron coupled system is written as

$$H = (1 - \alpha)H_{U(5)} + \alpha H_X, \tag{2}$$

where $0 \leq \alpha \leq 1$ is a control parameter and H_X is taken as $H_{SU(3)}$ when we study vibration-rotation transitional patterns and is taken as $H_{SO(6)}$ when we study vibration to γ -soft transitional patterns.

The $E2$ transition operator adopted is

$$T(E2) = e_\pi Q_\pi^{(2)} + e_\nu Q_\nu^{(2)}, \tag{3}$$

where e_π (e_ν) is the effective charge for the proton (neutron).

The collective S pair is defined as

$$S^\dagger = \sum_a y(aa0) (C_a^\dagger \times C_a^\dagger)^0. \tag{4}$$

By solving the BCS equation, we obtain u_a and v_a , the empty and occupied amplitudes for orbit a for a certain pairing interaction, respectively. Because we use the degenerate single-particle levels, u_a and v_a are independent of the pairing strengths. Therefore, the S -pair structure coefficient is fixed to be $y(aa0) = \widehat{a} \frac{v_a}{u_a} = \widehat{a} \sqrt{\frac{N}{\Omega_a - N}}$, where Ω_a is defined as $\Omega_a = a + 1/2$ and N is the number of pairs for like nucleons. A commonly used prescription for the D pair [49] is by using

the commutator

$$D^\dagger = \frac{1}{2} [Q^{(2)}, S^\dagger] = \sum_{ab} y(ab2) (C_a^\dagger \times C_b^\dagger)^2. \tag{5}$$

After symmetrization, it is easy to obtain that

$$y(ab2) = -\frac{1}{2} q(ab2) \left[\frac{y(aa0)}{\hat{a}} + \frac{y(bb0)}{\hat{b}} \right]. \tag{6}$$

In this method, the many-body effect on the structure of the building block is included.

III. RESULTS

To identify shape phase transitions and determine the corresponding patterns, Iachello *et al.* initiated a study on effective order parameters, which should display different critical behaviors for the phase transitions with different order. Specifically, the quantities related to isomer shifts, defined as $v_2 = (\langle 0_2^+ | \hat{n}_d | 0_2^+ \rangle - \langle 0_1^+ | \hat{n}_d | 0_1^+ \rangle) / N$ and $v_2' = (\langle 2_1^+ | \hat{n}_d | 2_1^+ \rangle - \langle 0_1^+ | \hat{n}_d | 0_1^+ \rangle) / N$, were proposed as effective-order parameters in Ref. [31]. Consequently, some other quantities, such as the $B(E2)$ ratios $K_1 = B(E2; 4_1^+ \rightarrow 2_1^+) / B(E2; 2_1^+ \rightarrow 0_1^+)$ and $K_2 = B(E2; 0_2^+ \rightarrow 2_1^+) / B(E2; 2_1^+ \rightarrow 0_1^+)$ [38], as well as the energy ratio $R_{60} = E_{6_1^+} / E_{0_2^+}$, were also suggested as the effective order parameters to identify phase transitions and the corresponding orders. Therefore, to study the shape phase transition in the SD -pair fermion model space, v_2, v_2' ,

TABLE I. The parameters used to produce the vibrational, rotational, and γ -soft spectra. G_σ is in units of MeV; κ_σ and κ are in units of MeV/r_0^4 .

	Limit	G_π	G_ν	κ_π	κ_ν	κ
Vibration-rotation	Vibration	0.5	0.5	0	0	0.01
	Rotation	0	0	0.1	0.1	0.2
Vibration- γ -soft	Vibration	0.5	0.5	0	0	-0.01
	γ -soft	0.15	0.15	0	0	-0.015

in which the d -boson number operator \hat{n}_d is replaced by D -pair number operator \hat{N}_D in the SDPSM, K_1 , K_2 , and R_{60} will be studied in this paper. Because of the importance of $R_{42} = E_{4_1^+}/E_{2_1^+}$ in determining the limiting cases and shape phase transitions [50], R_{42} is also presented.

A. Vibration-rotation transitional patterns

We begin by considering the vibration-rotation phase transition. A system with $N_\pi = N_\nu = 3$ in the gds shell was studied. By fitting $R_{42} \equiv E_{4_1^+}/E_{2_1^+} = 2$ for the vibrational case, the parameters used to produce the vibrational spectra were obtained, and these are presented in Table I. A detailed discussion of the vibrational spectra can be found in Ref. [47]. In the SDPSM, the full shell-model space was truncated to the SD -pair subspace. The investigation on the validity of the SD -pair truncation in Refs. [10–12] shows that the SD -pair truncation cannot produce the rotational spectra. But Zhao's work [13] and our previous work [47] show that if a reasonable Hamiltonian and a suitable collective SD -pair structure were considered, the rotational behaviors can be produced very well. It is found that with $2\kappa_\pi = 2\kappa_\nu = \kappa = 0.2 \text{ MeV}/r_0^4$, results similar to those found in the $SU(3)_\pi \times SU(3)_\nu$ limit of the IBM can be reproduced, in which the typical energy ratios $E_{4_1^+}/E_{2_1^+}$ and $E_{6_1^+}/E_{2_1^+}$ are 3.33 and 6.96, close to the IBM results of 3.33 and 7, respectively. A detailed discussion can be found in Refs. [13,47].

Energy ratios R_{42} and R_{60} against control parameter α are shown in Fig. 1. Figure 1(a) shows that the energy ratio R_{42} is 2 (when $\alpha = 0$) and 3.3 (when $\alpha = 1$), which are typical values of vibrational and rotational spectra, respectively, in the IBM [3]. It is also shown that the rapid change occurs

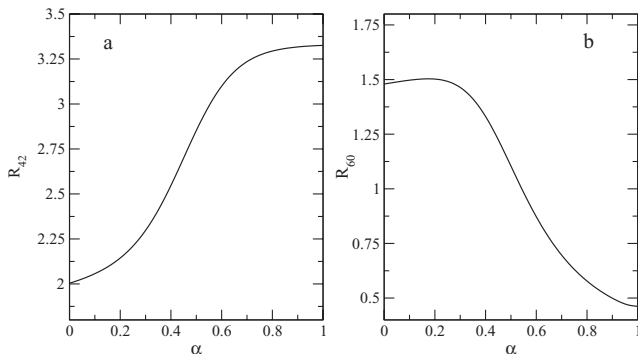


FIG. 1. Energy ratios R_{42} and R_{60} vs α for the vibration-rotation transition.

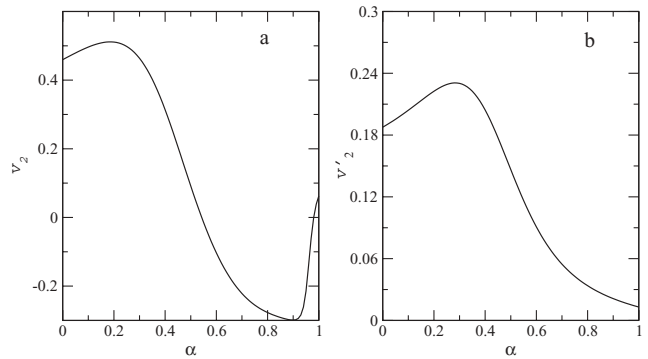


FIG. 2. v_2 and v'_2 vs α in the vibration-rotation transition.

when $0.3 \leq \alpha \leq 0.6$, which indicates that the phase transition occurs within this region.

The energy ratio R_{60} given in Fig. 1(b) shows that a behavior similar to that of the IBM for a finite number of bosons, N_B , is reproduced. It exhibits a modest peak followed by a sharp decrease across the phase transition, a typical signature of the first-order quantum phase transition [51].

The SDPSM results of v_2 , v'_2 , K_1 , and K_2 are given in Figs. 2 and 3. The effective charges were fixed with $e_\pi = 3e_\nu = 1.5e$. As argued in Ref. [31], v_2 , v'_2 should have wiggling behaviors in the region of the critical point owing to the switching of the two coexisting phases for the first-order phase transition. Indeed, the obvious wiggling behaviors shown by v_2 , v'_2 in Fig. 2 further confirm that the transition is first order. The results for the $B(E2)$ ratio K_1 is also consistent with those of other effective quantities [31,38]. The critical behavior of K_2 seems to deviate from the character of the first-order phase transition.

In the IBM, the critical point symmetry [27] between U(5) and SU(3) is X(5). Since the shape phase transition between vibrational and rotational limits can be reproduced in the SDPSM, it is interesting to see whether the properties of the X(5)-like symmetry also occur within the SDPSM. We found that there is indeed a signature with $\alpha = 0.54$ in the SDPSM similar to that of the X(5) in the IBM. A few typical values are given in Table II, from which one can see that the typical feature of the X(5) symmetry stated in Refs. [51,52] indeed occurs in the SDPSM. For example, R_{42} , R_{60} , and $E_{0_2^+}/E_{2_1^+}$ are

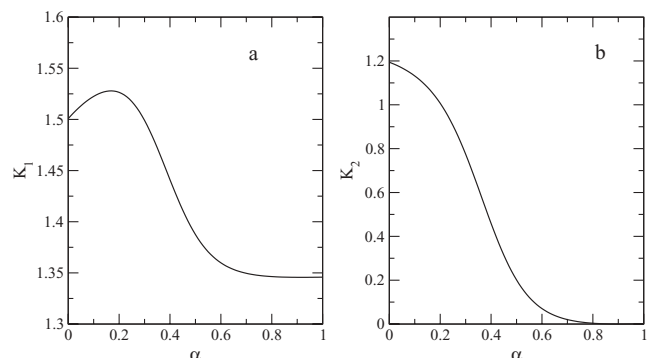


FIG. 3. $B(E2)$ ratios vs α in the vibration-rotation transition.

TABLE II. Energy and $B(E2)$ ratios at vibrational and rotational limits and the X(5)-like critical point calculated in the SDPSM.

Limit	$E_{4_1^+}/E_{2_1^+}$	$E_{6_1^+}/E_{2_1^+}$	$E_{6_1^+}/E_{0_2^+}$	$\frac{4_1^+ \rightarrow 2_1^+}{2_1^+ \rightarrow 0_1^+}$	$\frac{6_1^+ \rightarrow 4_1^+}{2_1^+ \rightarrow 0_1^+}$
Vibrational limit	1.99	2.97	1.47	1.49	1.48
X(5)-like point	2.91	5.60	1.05	1.38	1.38
Rotational limit	3.33	6.96	0.46	1.34	1.32
	$E_{0_2^+}/E_{2_1^+}$	$\frac{E_{2_2^+} - E_{0_2^+}}{E_{2_1^+}}$	$\frac{E_{4_2^+} - E_{0_2^+}}{E_{2_1^+}}$	$\frac{2_2^+ \rightarrow 0_2^+}{2_1^+ \rightarrow 0_1^+}$	$\frac{4_2^+ \rightarrow 2_2^+}{2_1^+ \rightarrow 0_1^+}$
X(5)-like point (0_2^+ band)	5.32	2.30	5.33	0.37	0.43

2.91, 1.05, and 5.32, respectively, in the SDPSM calculation, close to the IBM results of 2.91, 1.0, and 5.67, respectively.

B. Vibration- γ -soft transitional patterns

The investigation of the vibration- γ -soft shape phase transition in the IBM has been studied in Ref. [53], in which the corresponding quantum phase transition was suggested to be of second order. Recently, a similar phase transition within the fermion model for identical-nucleon systems has also been indicated [43,44].

From the periodic chart, one can deduce that nuclei with SO(6) character lie close to the end of the shell, at least in the neutron sector. Therefore, to explore whether the transitional patterns between vibration and γ -soft spectrum can be realized in the SDPSM, we considered a system with $N_\pi = \tilde{N}_\nu = 3$ in the gds shell. Namely, neutron pairs in this case were treated as three neutron-hole pairs and a negative κ was used, as shown in Ref. [47]. By fitting $R_{42} = 2$ and 2.5 for vibrational and γ -soft limiting cases, the parameters were fixed, and the results are listed in Table I. The detailed discussion of the two limiting cases in the SDPSM can be found in Ref. [47].

The IBM calculations show that the level crossing–repulsion behavior of 0_2^+ and 0_3^+ states occurs [54] in the critical region of the U(5)-SO(6) transition. The SDPSM results of

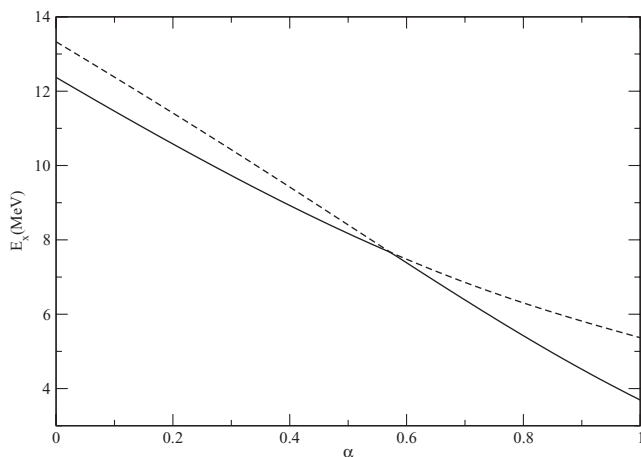


FIG. 4. Energy levels of 0_2^+ and 0_3^+ states vs α in the vibration- γ -soft transitional region.

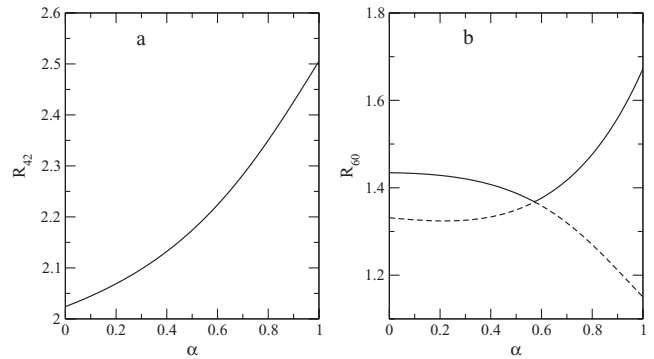


FIG. 5. Energy ratios R_{42} and R_{60} vs α in the vibration- γ -soft transitional region. Dashed and solid lines are the results for the 0_3^+ and 0_2^+ states, respectively.

0_2^+ and 0_3^+ states, given in Fig. 4, show a similar behavior of level crossing–repulsion when $\alpha = 0.58$. Therefore, to see the behavior of effective order parameters against the control parameters clearly, the quantities related to the 0_2^+ state were also calculated for the 0_3^+ state.

The results for R_{42} (R_{60}), K_1 (K_2), and v_2 (v_2') are given in Figs. 5, 6, and 7, respectively. The effective charges were fixed as $e_\pi = -3e_\nu = 1.5e$ since the neutron pairs were treated as holes.

Figure 5(a) shows that the typical ratios, $R_{42} = 2$ (when $\alpha = 0$) and 2.47 (when $\alpha = 1$), of vibration and γ -soft spectra were produced. Interestingly, we found that in comparison with that of the rotation-vibration transitional results, R_{42} in the vibration- γ -soft transitional region increases with α smoothly.

From Fig. 6 and R_{42} given in Fig. 5(a), and in comparison with the IBM results [38], one can see that the wiggling behavior in K_1 is smoothed out in the vibration- γ -soft transition. One can also see that because the structure of 0_2^+ and 0_3^+ exchange at $\alpha \sim 0.58$, the amplitudes of $B(E2; 0_2^+ \rightarrow 2_1^+)$ and $B(E2; 0_3^+ \rightarrow 2_1^+)$ also exchange at this point.

In Ref. [51], the experimental data of Xe and Ba isotopes were analyzed. For smaller neutron numbers, $^{134,136}\text{Ba}$ and ^{128}Xe , the 0_3^+ state was taken in the R_{60} if its $B(E2)$ decay was consistent with $\sigma = N - 2$. It was also shown that [54] $B(E2; 0_2^+ \rightarrow 2_1^+)/B(E2; 2_1^+ \rightarrow 0_1^+) = 0.07$ for ^{196}Pt ,

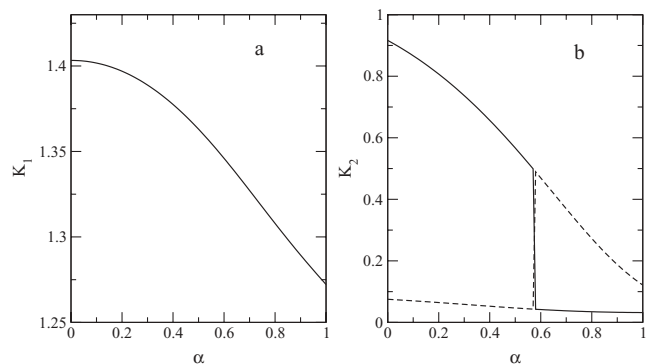


FIG. 6. $B(E2)$ ratios vs α in the vibration- γ -soft transitional region. Dashed and solid lines are the results for the 0_3^+ and 0_2^+ states, respectively.

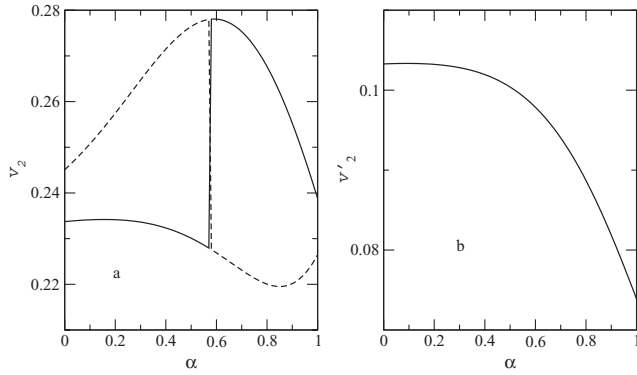


FIG. 7. v_2 and v'_2 vs α in the vibration- γ -soft transitional region. Dashed and solid lines are the results for 0_3^+ and 0_2^+ states, respectively.

whereas it is 0.81 for ^{198}Pt . By considering these results, the 0_3^+ state were taken in the R_{60} , K_2 , and v'_2 when $\alpha > 0.58$. In comparison with those in the vibration-rotation transition, Fig. 5(b) and Fig. 6(a) show that R_{60} , K_1 , and K_2 change smoothly with α , which are typical features of a second-order phase transition [38,51].

Figure 7 shows that as predicted in the IBM and shell-model calculation for identical systems, the vibration- γ -soft phase transition takes place and it is a second order phase transition, for which v_2 and v'_2 change smoothly with α , and the wiggling behavior with sign change in the region of the critical point are smoothed out.

In the U(5)-SO(6) transitional region in the IBM, E(5) is the critical point symmetry [53,55]. It is interesting to see whether the signature of the E(5)-like symmetry can be realized in the SDPSM for the proton-neutron coupled system. We found that $E_{4^+}/E_{2^+} = 2.19$ when $\alpha = 0.54$, corresponding to the typical value of E(5) symmetry in the IBM. Other typical results are listed in Table III, in which the IBM results for $N = 5$ are also given [53]. It is seen that except for $E_{0_2^+}/E_{2^+} = 2.59$, which is smaller than that of the IBM result for $N = 5$, the characters of E(5) symmetry in the IBM indeed shows up in the SDPSM.

TABLE III. The SDPSM results for E(5)-like symmetry. The corresponding results with $N = 5$ in the IBM are also given [53].

Limit	E_{4^+}/E_{2^+}	$E_{0_2^+}/E_{0_3^+}$	$E_{0_2^+}/E_{2^+}$
SDPSM	2.19	0.99	2.59
IBM	2.19	1.04	3.68
	$\frac{4_1^+ \rightarrow 2_1^+}{2_1^+ \rightarrow 0_1^+}$	$\frac{2_2^+ \rightarrow 2_1^+}{2_1^+ \rightarrow 0_1^+}$	$\frac{0_2^+ \rightarrow 2_1^+}{2_1^+ \rightarrow 0_1^+}$
SDPSM	1.36	1.29	0.53
IBM	1.38	1.39	0.51
	$\frac{0_2^+ \rightarrow 2_2^+}{0_2^+ \rightarrow 2_1^+}$	$\frac{0_3^+ \rightarrow 2_1^+}{0_3^+ \rightarrow 2_2^+}$	
SDPSM	0.06	0.03	
IBM	0	0	

IV. SUMMARY

In summary, the shape phase transition patterns for the roton-neutron coupled system have been studied within the framework of the SD -pair shell model. The results show that patterns of vibration-rotation and vibration- γ -soft shape phase transitions are indeed similar to the corresponding results obtained from the IBM previously. The signatures of the critical point symmetry in the SD -pair shell model are also close to those shown in the IBM. This work also confirms in yet another way that the truncation scheme adopted in the SD -pair shell model seems reasonable as long as the Hamiltonian is reasonably chosen.

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