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Phys. Rev. C **93**, 044312 — Published 13 April 2016

DOI: [10.1103/PhysRevC.93.044312](https://doi.org/10.1103/PhysRevC.93.044312)

Quantum phase transition in the spherical mean-field plus the quadrupole-quadrupole and pairing model in a single- j shell

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The quantum phase transitional behavior of the spherical shell model mean-field plus the geometric quadrupole-quadrupole and standard pairing model within a single- j shell is analyzed in detail. Various quantities, such as low-lying energy levels, some typical energy ratios, the overlaps of the excited states with those of the corresponding limiting cases, $B(E2)$ values and electric quadrupole moments of some low-lying states and their ratios, as functions of the control parameter of the model in a $j = 15/2$ shell are calculated as an example, in which only a crossover occurs due to the Pauli exclusion. The results show that there are noticeable changes within the crossover region of the rotation-like to the pair-excitation (superconducting) phase transition, especially in the half-filling case. As application to realistic nuclear systems, a chain of isotones ^{212}Rn - ^{213}Fr - ^{214}Ra - ^{215}Ac is chosen to be described by the model with valence protons in the $1h_{9/2}$ shell. As far as the low-lying energy levels, the experimentally observed $B(E2)$ values, and the electric quadrupole moment within the yrast band are concerned, these nuclei seem fitted reasonably well. The results indicate that these nuclei are all within the rotation-like to the pair-excitation phase transition near to the crossover point.

Shell model; quantum phase transition; single- j shell

PACS numbers: 21.60.Ev, 21.60.Fw, 21.10.-k, 05.45.Mt, 21.10.Pc

I. INTRODUCTION

Quantum phase transition (QPT) has been attracting a lot of attention in many areas of physics [1, 2]. In a quantum many-body system, the QPT occurs when the interaction strengthes or called control parameters reach a critical point of different phases described by distinct types of ground or excited states of the system [1, 3]. In atomic nuclei, the QPTs have been studied extensively in either the Bohr-Mottelson model [4] (BMM) or the interacting Boson model [5] (IBM). It is now widely accepted that the three limiting cases of the IBM correspond to three different geometric shapes of nuclei, referred to as spherical (vibrational limit with $U(5)$ symmetry), axially deformed (rotational limit with $SU(3)$ symmetry) and γ -unstable (triaxial with $O(6)$ symmetry). More interesting scenarios occur when a system is in between two different phases, in which case a QPT occurs at the corresponding critical point with the distinct symmetry [6, 7], e. g., the critical point of the spherical to γ -unstable shape phase transition with the $E(5)$ symmetry [8], the critical point of the spherical to axially deformed shape phase transition with the $X(5)$ symmetry [9], and the critical point of the prolate to oblate shape phase transition with the $Z(5)$ symmetry [10], *etc.* in the BMM, which have been widely confirmed. Very recently, the critical point $T(5)$ symmetry for the spherical to triaxially deformed shape phase transition at a given γ deformation in the BMM has also been proposed [11].

On the other hand, it is commonly believed that the spherical shell model is fundamental in describing low-lying spectroscopy of nuclei when the most important residual interactions, such as the quadrupole-quadrupole and pairing interactions, are taken into consideration [12–15]. In [16, 17], the Hamiltonian with the Elliott's dynamic quadrupole-quadrupole and the standard pairing interaction restricted to a single spherical harmonic oscillator shell was studied, which sheds light on the nature of the QPT in the model. The analysis of the QPTs in the shell model restricted within the SD -pair subspace inspired by similar work in the IBM was also made [18, 19].

In this work, the QPT in the spherical shell model mean-field plus the quadrupole-quadrupole and standard pairing interaction in a single- j shell is analyzed, where the quadrupole operator used is the geometric one, with which behavior of excited states with larger angular momentum seem different from those of the model [16, 17] with the Elliott's dynamic quadrupole operator. Matrix elements of the model quantities in a single- j shell adapted to the $U(2j+1) \supset Sp(2j+1) \supset O(3)$ basis will be presented in Sec. II. As an example suitable to manifest the shape (phase) transition or the crossover of the model, low-lying level energies, $B(E2)$ values, quadrupole moments of some low-lying states, and their ratios as functions of the control parameter of the model for different number of valence particles within a single $j = 15/2$ shell will be analyzed in Sec. III. Some effective order parameters (physical observables)

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suitable to describe the crossover are discussed. In Sec. IV, as an application to realistic nuclear systems, the model within the $j = 9/2$ shell is used to describe a chain of isotones, ^{212}Rn - ^{213}Fr - ^{214}Ra - ^{215}Ac , which shows that these nuclei are all within the rotation-like to the pair-excitation (or called superconducting) phase transition region near to the crossover. A short summary is provided in the final section.

II. THE MODEL

In this work, the spherical shell model mean-field plus the geometric quadrupole-quadrupole and the standard pairing interaction within a single- j shell is adopted, of which the Hamiltonian is given by

$$\hat{H} = \epsilon_j \hat{n}_j - G S_+ S_- - \kappa \tilde{Q} \cdot \tilde{Q}, \quad (1)$$

where ϵ_j is the single-particle energy generated from the spherical shell model, $\hat{n}_j$ is the number operator for valence particles in the single- j shell, G and κ are the pairing and quadrupole-quadrupole interaction strength, respectively, $S_+ = \sum_{m>0} (-1)^{j-m} a_{jm}^\dagger a_{j-m}^\dagger$ ($S_- = (S_+)^\dagger$) are pair creation (annihilation) operator, in which $a_{jm}^\dagger$ is the creation operator of a particle in the single- j shell, and $\tilde{Q}_q = Q_q/r_0^2$ with $r_0^2 = \hbar/M_n\omega_0 = 1.012A^{1/3}\text{fm}^2$, in which M_n is the mass of a nucleon, ω_0 is the frequency of the harmonic oscillator potential. In the spherical shell model basis for a single- j shell, the geometric Q_q can be expressed as

$$Q_q = \frac{1}{\sqrt{5}} \langle Nl|r^2|Nl \rangle \langle (l\frac{1}{2})j \| Y^2 \| (l\frac{1}{2})j \rangle (a_j^\dagger \times \tilde{a}_j)_q^2, \quad (2)$$

where

$$\langle Nl|r^2|Nl \rangle = (N + \frac{3}{2})r_0^2 \quad (3)$$

due to the fact that it is restricted within the single- j shell, in which N is the principal quantum number, and l is the quantum number of the orbital angular momentum,

$$\langle (l\frac{1}{2})j \| Y^2 \| (l\frac{1}{2})j \rangle = (-1)^{j-\frac{1}{2}} \frac{2j+1}{2\sqrt{\pi}} \langle j\frac{1}{2}j - \frac{1}{2} | 20 \rangle, \quad (4)$$

and

$$(a_j^\dagger \times \tilde{a}_j)_q^2 = \sum_{m_1 m_2} \langle jm_1, jm_2 | 2q \rangle a_{jm_1}^\dagger \tilde{a}_{jm_2}, \quad (5)$$

in which $\tilde{a}_{jm} = (-)^{j+m} a_{j-m}$, and $\langle jm_1, jm_2 | 2q \rangle$ is the Clebsch-Gordan coefficient.

For a given number of valence particles in a single- j shell, the single-particle term in (1) is a constant, which is irrelevant to the QPT and will be omitted in the following. Furthermore, in order to investigate the QPT in the system, we set $G = cx$ and $\kappa = c(1-x)\xi$, in which $c > 0$ is a scale factor, x can be taken a value in the closed interval $[0, 1]$, and $\xi > 0$ is a dimensionless constant. Thus, x serves as the control parameter of the model. It is obvious that the system is in the rotation-like phase driven by $\tilde{Q} \cdot \tilde{Q}$ when $x = 0$ and in the pair-excitation phase driven by the pairing interaction $S_+ S_-$ when $x = 1$. It has been known from the QPT analysis in Bose systems [20, 21] that different parameter $\xi > 0$ only changes the position of the critical point, but does not alter the nature of the QPT. Therefore, in the following, the parameter ξ will be chosen with $0 < \xi < 1$ in order to keep the critical (or crossover) point not far from $x \sim 0.5$ according to the value of j . Since j is not large enough to accommodate large number of particles to show the QPT, only a crossover may be observed in this case.

Thus, for a given number of particles n , up to a constant, the model Hamiltonian is rewritten as

$$\hat{H}' = -c \left(x S_+ S_- + (1-x) \xi \tilde{Q} \cdot \tilde{Q} \right). \quad (6)$$

It should be emphasized that the results described by (6) with the geometric $\tilde{Q} \cdot \tilde{Q}$ seem different from those obtained from the model with the Elliott's dynamic quadrupole-quadrupole interaction shown in [16, 17], especially in higher

TABLE I: The multiplicity w of J for a given ν in the reduction $Sp(2j+1) \downarrow O(3)$ for $j = \frac{15}{2}$ and $n = 2, 3, \dots, 9$.

(a) $n = 2.$	(b) $n = 3.$	(c) $n = 4.$	(d) $n = 5.$	(e) $n = 6.$	(f) $n = 7.$	(g) $n = 8.$	(h) $n = 9.$
$\overline{\nu \ w \ J}$	$\overline{\nu \ w \ J}$	$\overline{\nu \ w \ J}$	$\overline{\nu \ w \ J}$	$\overline{\nu \ w \ J}$	$\overline{\nu \ w \ J}$	$\overline{\nu \ w \ J}$	$\overline{\nu \ w \ J}$
0 1 0	1 1 $\frac{15}{2}$	0 1 0	1 1 $\frac{15}{2}$	0 1 0	1 1 $\frac{15}{2}$	0 1 0	1 1 $\frac{15}{2}$
2 1 2	3 1 $\frac{15}{2}$	2 1 2	3 1 $\frac{15}{2}$	2 1 2	3 1 $\frac{15}{2}$	2 1 2	3 1 $\frac{15}{2}$
2 1 4	3 1 $\frac{15}{2}$	2 1 4	3 1 $\frac{15}{2}$	2 1 4	3 1 $\frac{15}{2}$	2 1 4	3 1 $\frac{15}{2}$
	3 1 $\frac{7}{2}$	4 2 0	3 1 $\frac{7}{2}$	4 2 0	3 1 $\frac{7}{2}$	4 2 0	3 1 $\frac{7}{2}$
		4 3 2	5 2 $\frac{7}{2}$	4 3 2	5 2 $\frac{7}{2}$	4 3 2	5 2 $\frac{7}{2}$
		4 2 3	5 3 $\frac{7}{2}$	4 2 3	5 3 $\frac{7}{2}$	4 2 3	5 3 $\frac{7}{2}$
		4 5 4	5 5 $\frac{7}{2}$	4 5 4	5 5 $\frac{7}{2}$	4 5 4	5 5 $\frac{7}{2}$
			5 7 $\frac{7}{2}$	6 3 0	5 7 $\frac{7}{2}$	6 3 0	5 7 $\frac{7}{2}$
				6 2 1	7 2 $\frac{7}{2}$	6 2 1	7 2 $\frac{7}{2}$
				6 7 2	7 6 $\frac{7}{2}$	6 7 2	7 6 $\frac{7}{2}$
				6 7 3	7 7 $\frac{7}{2}$	6 7 3	7 7 $\frac{7}{2}$
				6 11 4	7 9 $\frac{7}{2}$	6 11 4	7 9 $\frac{7}{2}$
						8 1 0	
						8 2 1	
						8 5 2	
						8 4 3	
						8 8 4	

excited states, of which the noticeable difference will be shown in the next section.

Practically, instead of the $SU(3)$ basis used in [16, 17], the Hamiltonian (6) is diagonalized in the $U(2j+1) \supset Sp(2j+1) \supset O(3)$ basis, of which the basis vectors are denoted as $[[1^n]\langle 1^\nu \rangle \alpha J M]$, where n is the number of valence particles in the single- j shell resulting in the totally anti-symmetric irreducible representation (irrep) $[1^n]$ of $U(2j+1)$, $\nu = n, n-2, \dots, 1$ or 0 , is the seniority quantum number, J and M are the quantum number of the total angular momentum and that of its third component, respectively, and α is the additional quantum number needed to distinguish different state with other quantum numbers the same because $Sp(2j+1) \downarrow O(3)$ is not branching multiplicity-free. The branching multiplicity of J in the reduction $Sp(2j+1) \downarrow O(3)$ for a given ν can be obtained by using the method shown in [22]. For $j = 15/2$ useful in the next section for example, the branching multiplicity w of J for a given ν is shown in Table I. Hence, the eigenstates of (6) are expressed as

$$|n, \zeta, JM\rangle = \sum_{\nu \alpha} C_{\nu \alpha J}^{(\zeta)} [[1^n]\langle 1^\nu \rangle \alpha J M], \quad (7)$$

where ζ labels the ζ -th excited state with the total angular momentum J , and $C_{\nu \alpha J}^{(\zeta)}$ is the corresponding expansion coefficient, namely,

$$\hat{H}'|n, \zeta, JM\rangle = E(J_\zeta)|n, \zeta, JM\rangle, \quad (8)$$

where $E(J_\zeta)$ is the corresponding excitation energy.

Since $\{a_{jm}^\dagger\}$ is the rank- $[1]$, $\langle 1 \rangle$ and j irreducible tensor of $U(2j+1)$, $Sp(2j+1)$, and $O(3)$, simultaneously, according to the generalized Wigner-Eckart theorem, the $O(3)$ -reduced matrix elements of $a_j^\dagger$ can be written as

$$\langle [1^n]\langle 1^\nu \rangle \alpha J \| a_j^\dagger \| [1^{n'}]\langle 1^{\nu'} \rangle \alpha' J' \rangle = (-1)^{2j} \sqrt{2J+1} \begin{bmatrix} [1^{n'}] & [1] \\ \langle 1^{\nu'} \rangle & \langle 1 \rangle \end{bmatrix} \begin{bmatrix} [1^n] \\ \langle 1^\nu \rangle \end{bmatrix} \left\langle \begin{matrix} \langle 1^{\nu'} \rangle & \langle 1 \rangle \\ \alpha' J' & j \end{matrix} \middle| \begin{matrix} \langle 1^\nu \rangle \\ \alpha J \end{matrix} \right\rangle \langle [1^n] \| a^\dagger \| [1^{n'}] \rangle, \quad (9)$$

which satisfies the conjugation relation

$$\langle [1^{n'}]\langle 1^{\nu'} \rangle \alpha' J' \| \tilde{a}_j \| [1^n]\langle 1^\nu \rangle \alpha J \rangle = (-1)^{J-j-J'} \langle [1^n]\langle 1^\nu \rangle \alpha J \| a_j^\dagger \| [1^{n'}]\langle 1^{\nu'} \rangle \alpha' J' \rangle. \quad (10)$$

In (9),

$$\langle [1^n] \| a^\dagger \| [1^{n'}] \rangle = \sqrt{n} \delta_{n, n'+1} \quad (11)$$

is the $U(2j+1)$ -reduced matrix element, $\begin{bmatrix} [1^{n'}] & [1] \\ \langle 1^{\nu'} \rangle & \langle 1 \rangle \end{bmatrix} \begin{bmatrix} [1^n] \\ \langle 1^\nu \rangle \end{bmatrix}$ and $\left\langle \begin{matrix} \langle 1^{\nu'} \rangle & \langle 1 \rangle \\ \alpha' J' & j \end{matrix} \middle| \begin{matrix} \langle 1^\nu \rangle \\ \alpha J \end{matrix} \right\rangle$ are the isoscalar factors (ISFs) of $U(2j+1) \supset Sp(2j+1)$ and $Sp(2j+1) \supset O(3)$, respectively. The ISFs of $U(2j+1) \supset Sp(2j+1)$ useful in this

case are given by [23]

$$\left[\begin{array}{c} [1^{n-1}] \\ \langle 1^{\nu-1} \rangle \end{array} \begin{array}{c} [1] \\ \langle 1 \rangle \end{array} \middle| \begin{array}{c} [1^n] \\ \langle 1^\nu \rangle \end{array} \right] = \left(\frac{\nu(2j-n-\nu+3)}{n(2j-2\nu+3)} \right)^{\frac{1}{2}}, \quad \left[\begin{array}{c} [1^{n-1}] \\ \langle 1^{\nu+1} \rangle \end{array} \begin{array}{c} [1] \\ \langle 1 \rangle \end{array} \middle| \begin{array}{c} [1^n] \\ \langle 1^\nu \rangle \end{array} \right] = - \left(\frac{(n-\nu)(2j-\nu+3)}{n(2j-2\nu+3)} \right)^{\frac{1}{2}}, \quad (12)$$

which satisfy the orthonormal relation

$$\sum_{\nu'} \left[\begin{array}{c} [1^{n'}] \\ \langle 1^{\nu'} \rangle \end{array} \begin{array}{c} [1] \\ \langle 1 \rangle \end{array} \middle| \begin{array}{c} [1^n] \\ \langle 1^\nu \rangle \end{array} \right]^2 = 1. \quad (13)$$

The algorithm for calculating the ISFs of $Sp(2j+1) \supset O(3)$ according to the algebraic angular momentum projection method outlined in [22] will be provided in the Appendix A. By using (9) and (10), the $O(3)$ -reduced matrix elements of coupled tensor operators can be derived by using the angular momentum coupling and recoupling techniques. For example, the $O(3)$ -reduced matrix element of the quadrupole operator $\tilde{Q}$ can be expressed as

$$\begin{aligned} & \langle [1^{n_1}] \langle 1^{\nu_1} \rangle_{\alpha_1 J_1} \| \tilde{Q} \| [1^{n_2}] \langle 1^{\nu_2} \rangle_{\alpha_2 J_2} \rangle \\ &= \sum_{\nu' \alpha' J'} (-1)^{J_1+2J_2-J'-\frac{1}{2}} \frac{(2j+1)n_1}{2} \left\{ \frac{(2J_1+1)(2J_2+1)}{\pi} \right\}^{\frac{1}{2}} (N+\frac{3}{2}) (j\frac{1}{2}j-\frac{1}{2}|20) \\ & \times \left\{ \begin{array}{ccc} j & j & 2 \\ J_2 & J_1 & J' \end{array} \right\} \left[\begin{array}{c} [1^{n_1-1}] \\ \langle 1^{\nu'} \rangle \end{array} \begin{array}{c} [1] \\ \langle 1 \rangle \end{array} \middle| \begin{array}{c} [1^{n_1}] \\ \langle 1^{\nu_1} \rangle \end{array} \right] \left[\begin{array}{c} [1^{n_1-1}] \\ \langle 1^{\nu'} \rangle \end{array} \begin{array}{c} [1] \\ \langle 1 \rangle \end{array} \middle| \begin{array}{c} [1^{n_1}] \\ \langle 1^{\nu_2} \rangle \end{array} \right] \left\langle \begin{array}{c} \langle 1^{\nu'} \rangle \\ \alpha' J' \end{array} \begin{array}{c} \langle 1 \rangle \\ j \end{array} \middle| \begin{array}{c} \langle 1^{\nu_1} \rangle \\ \alpha_1 J_1 \end{array} \right\rangle \left\langle \begin{array}{c} \langle 1^{\nu'} \rangle \\ \alpha' J' \end{array} \begin{array}{c} \langle 1 \rangle \\ j \end{array} \middle| \begin{array}{c} \langle 1^{\nu_2} \rangle \\ \alpha_2 J_2 \end{array} \right\rangle, \quad (14) \end{aligned}$$

with which we have

$$\begin{aligned} & \langle [1^n] \langle 1^\nu \rangle_{\alpha J M} | \tilde{Q} \cdot \tilde{Q} | [1^n] \langle 1^{\nu'} \rangle_{\alpha' J M} \rangle = \frac{1}{2J+1} \sum_{n'' \nu'' \alpha'' J''} (-1)^{J''-J} \\ & \times \langle [1^n] \langle 1^\nu \rangle_{\alpha J} \| \tilde{Q} \| [1^{n''}] \langle 1^{\nu''} \rangle_{\alpha'' J''} \rangle \langle [1^{n''}] \langle 1^{\nu''} \rangle_{\alpha'' J''} \| \tilde{Q} \| [1^n] \langle 1^{\nu'} \rangle_{\alpha' J} \rangle. \quad (15) \end{aligned}$$

While the matrix elements for $S_+ S_-$ are simply given by

$$\langle [1^{n_1}] \langle 1^{\nu_1} \rangle_{\alpha_1 J_1 M_1} | S_+ S_- | [1^{n_1}] \langle 1^{\nu_2} \rangle_{\alpha_2 J_1 M_1} \rangle = \frac{1}{4} (n_1 - \nu_1) (2j - n_1 - \nu_1 + 3) \delta_{\nu_1, \nu_2} \delta_{\alpha_1, \alpha_2}. \quad (16)$$

Once the Hamiltonian (1) in the $U(2j+1) \supset Sp(2j+1) \supset O(3)$ basis with entries provided in (15) and (16) is diagonalized for a given number of particles n and the total angular momentum J , the eigen-energies $E(J_\zeta)$ and the corresponding expansion coefficients $C_{\nu\alpha J}^{(\zeta)}$ in (7) are thus determined. The $E2$ transition operator is simply chosen as

$$T_q(E2) = e_{\text{eff}} Q_q, \quad (17)$$

where e_{eff} is the effective charge, with which $B(E2)$ values and the electric quadrupole moment $Q(J_\zeta)$ are given by

$$B(E2; J_\zeta \rightarrow J'_{\zeta'}) = \frac{e_{\text{eff}}^2 r_0^4}{2J+1} \left| \sum_{\nu\nu'\alpha\alpha'} C_{\nu\alpha J}^{(\zeta)} C_{\nu'\alpha' J'}^{(\zeta')} \langle [1^n] \langle 1^{\nu'} \rangle_{\alpha' J'} \| \tilde{Q} \| [1^n] \langle 1^\nu \rangle_{\alpha J} \rangle \right|^2 \quad (18)$$

and

$$Q(J_\zeta) = e_{\text{eff}} r_0^2 \sqrt{\frac{16\pi J(2J-1)}{5(J+1)(2J+1)(2J+3)}} \sum_{\nu\nu'\alpha\alpha'} C_{\nu\alpha J}^{(\zeta)} C_{\nu'\alpha' J}^{(\zeta)} \langle [1^n] \langle 1^{\nu'} \rangle_{\alpha' J} \| \tilde{Q} \| [1^n] \langle 1^\nu \rangle_{\alpha J} \rangle, \quad (19)$$

respectively.

III. THE QPT BEHAVIORS

In order to investigate the QPT in the model, we take $j = 15/2$ in the $N = 7$ major shell as an example, which is the largest single- j shell suitable to describe some experimentally reachable heavy nuclei. To show how the energy

FIG. 1: Some low-lying energy levels with $j = \frac{15}{2}$ across the transitional region for $n = 2, \dots, 9$, where $x = 0$ corresponds to the rotation-like phase and $x = 1$ to the pair-excitation (superconducting) phase.

levels change as functions of the control parameter x and the total number of particles n , low-lying energy levels as functions of x for the system with the number of particles $n = 2, \dots, 9$ are shown in Fig. 1, for which $\xi = 0.22$ is taken to keep that $x \sim 0.5$ is at or near the crossover of the phase transition, and the $n = 8$ case corresponds to the half-filling.

It can be observed from Fig. 1 that, for even n cases, the energy ratios $R_{4/2} = E(4_1)/E(2_1)$ and $R_{6/2} = E(6_1)/E(2_1)$ decrease with the increasing of x . However, for any even n , the ratios $R_{4/2}$ and $R_{6/2}$ for $x = 0$ are always smaller than

FIG. 2: Some low-lying energy ratios of the model for $n = 4, \dots, 9$ in the $j = 15/2$ shell, where curve a represents $E(4_1)/E(2_1)$, b represents $E(4_2)/E(2_1)$, c represents $E(4_2)/E(4_1)$, d represents $E(6_1)/E(2_1)$, the solid curve represents $E(\frac{3}{2}_3)/E(\frac{7}{2}_3)$, and the dotted curve represents $E(\frac{5}{2}_1)/E(\frac{7}{2}_2)$, respectively, for odd n cases.

the corresponding values of the typical rotational spectrum except $R_{6/2}$ when $n = 6$, which becomes far smaller with increasing of the number of particles for $n > 6$, of which the exact values are provided in Table II. It seems that $R_{4/2}$ and $R_{6/2}$ with $n = 4$ are most close to the corresponding values of the typical rotational spectrum with $R_{4/2} = 3.23$ and $R_{6/2} = 6.56$. Therefore, the system with $x = 0$ is called in the rotation-like phase. With the increasing of x from 0 to 1, the system is driven from the rotation-like phase toward the crossover point with $x \sim 0.5$ because sharp change in level energy never happens due to the fact that the number of particles is always small and finite, and then is driven away from the crossover point toward the pair-excitation (superconducting) phase. Actually, there is no obvious crossover when $n = 2$ due to the fact that the number of particles is too small. However, with the increasing of the number of particles n toward the half-filling, the level pattern when $x < 0.5$ or $x > 0.5$ are noticeably different from that when $x \sim 0.5$. It can be clearly observed from Fig. 1 that there are many level-crossings when $x < 0.5$ or $x > 0.5$, which are typical for a quasi-integrable system because the model in such cases is either driven by the quadrupole-quadrupole or driven by the pairing interaction. The situation for $x \sim 0.5$, however, is quite different, in which no level-crossing happens, but, instead, there is an obvious level-repulsion for the 4_1 and 4_2 levels around $x = 0.5$ as clearly shown in Fig. 1 for $n = 4, 6$, and 8 . For both even and odd n cases, the common feature of the spectra when $x = 1$ is that there are many energy levels with different total angular momentum become degenerate due to the fact that the level energies in the pair-excitation phase, which is seniority conserving, only depend on the number of particles and the seniority quantum number ν , but irrelevant with J . The energy spectrum of odd n cases near the crossover is somewhat different, in which no level repulsion occurs. Similar to the even n case, there is no obvious crossover when $n \leq 3$. Moreover, the total angular momentum of the ground state for odd $3 \leq n \leq 9$ cases is always $J_\zeta = 7/2_1$ with $J_\zeta = 5/2_1$ or $7/2_2$ the first excited state. Even when $x = 0$, the energy levels in the yrast band do not follow the rotational pattern though the results vary with j . Nevertheless, with the increasing of n , it can be seen from Fig. 1 that there is a minimum in the low-lying excitation energy when the control parameter $x \sim 0.5$, with the minimum growing sharper as the total number of particles increases though the minimum position of excited states is a little different from one another. Hence, $x \sim 0.5$ in this case may be recognized as the crossover point of the rotation-like to pair-excitation phase transition. To the left of the crossover point, $0 < x < 0.5$, there are many level crossings that gradually split with increasing x non-degenerate levels around $x = 0.5$. Similarly, beyond the critical region, $0.5 < x \leq 1.0$, there are also many level-crossings. These levels finally coalesce into two groups of degenerate levels when $x = 1.0$. It should be noted that the levels near $x = 0.5$ are truly non-degenerate, and that the level density grows noticeably near the crossover point with increasing of the number of particles n .

To search for energy ratios suitable to identify the crossover, several energy ratios as functions of x for the number of particles $n = 4, \dots, 9$ in the $j = 15/2$ shell are shown in Fig. 2. As shown in the upper panel of Fig. 2, though all the four energy ratios for the even n cases decrease monotonically with the increasing of x , with increasing of the number of particles n , there is a minimum in $E(4_2)/E(4_1)$ near the crossover point $x \sim 0.46$ due to the level-repulsion, while there is a maximum in $E(4_1)/E(2_1)$ near $x = 0.48$ due to a sudden energy increase of the 4_1 level.

TABLE II: Some low-lying energy ratios of the model at several x points for $n = 2$, and $n = 4, \dots, 9$ in the $j = 15/2$ shell.

		$x = 0$	$x = 0.3$	$x = 0.5$	$x = 0.7$	$x = 1$
$n = 2$	$E(4_1)/E(2_1)$	3.14	1.24	1.11	1.05	1
	$E(6_1)/E(2_1)$	5.98	1.56	1.26	1.11	1
$n = 4$	$E(4_1)/E(2_1)$	3.23	1.83	1.51	1.22	1
	$E(6_1)/E(2_1)$	6.56	2.25	1.65	1.25	1
$n = 6$	$E(4_1)/E(2_1)$	3.06	1.93	1.74	1.30	1
	$E(6_1)/E(2_1)$	12.38	2.87	1.79	1.31	1
$n = 8$	$E(4_1)/E(2_1)$	1.92	1.87	1.70	1.32	1
	$E(6_1)/E(2_1)$	2.95	2.45	1.74	1.32	1
$n = 5$	$E(\frac{5}{2}_1)/E(\frac{7}{2}_2)$	1.12	1.49	0.64	0.10	0
	$E(\frac{3}{2}_3)/E(\frac{7}{2}_3)$	2.05	2.20	1.94	1.44	1
$n = 7$	$E(\frac{5}{2}_1)/E(\frac{7}{2}_2)$	0.60	0.86	0.24	0.004	0
	$E(\frac{3}{2}_3)/E(\frac{7}{2}_3)$	1.42	1.33	2.46	1.50	1
$n = 9$	$E(\frac{5}{2}_1)/E(\frac{7}{2}_2)$	0.60	0.86	0.24	0.004	0
	$E(\frac{3}{2}_3)/E(\frac{7}{2}_3)$	1.42	1.33	2.46	1.50	1

For odd n cases, two low-lying energy ratios $E(3/2_3)/E(7/2_3)$ and $E(5/2_1)/E(7/2_2)$ seem suitable to be the order parameters to identify the crossover. Specifically, near the half-filling, the crossover region seems within the range of $x = 0.45 - 0.53$, in which the ratio $E(5/2_1)/E(7/2_2)$ decreases to its minimum, while the ratio $E(3/2_3)/E(7/2_3)$ increases to its maximum. Therefore, in the $j = 15/2$ shell, the energy ratios $E(4_1)/E(2_1)$ and $E(6_1)/E(2_1)$ for even n cases, and $E(3/2_3)/E(7/2_3)$ and $E(5/2_1)/E(7/2_2)$ for odd n cases seem suitable to identify the crossover.

In addition, as pointed out previously, within a single finite j shell, spectrum of the geometric quadrupole-quadrupole interaction adopted in this work does not follow the rotational pattern as that generated by the Elliott's dynamic quadrupole-quadrupole interaction, especially in the higher J levels. In order to show the level pattern of the geometric quadrupole-quadrupole interaction, we diagonalize the $-\kappa\tilde{Q} \cdot \tilde{Q}$ term in the $n = 2$ subspace, of which the eigen-energy $E(J)$ for an allowed total angular momentum J is given by

$$E(J) = -h_0 \frac{(2j+1)^2}{\pi} \langle j \frac{1}{2} j - \frac{1}{2} | 20 \rangle^2 \sum_{J'} (2J' + 1) \left\{ \begin{matrix} j & j & 2 \\ J & J' & j \end{matrix} \right\}^2, \quad (20)$$

where $h_0 = \kappa(N + \frac{3}{2})^2$. We have calculated $E(J)$ with $J = 0, 2, \dots, 2j - 1$ from $j = 3/2$ to $j = 103/2$, of which the results are shown in the panel (a) and (b) of Fig. 3. As clearly shown in panel (a) and (b) of Fig. 3 for $n = 2$, except the two smallest $j = 3/2$ and $j = 5/2$ cases, of which the excitation energies increase with the increasing of the total angular momentum J , the excitation energies decrease with the increasing of J when J surpasses a specific value as the result of the sum rule involving the $6j$ symbol used in (20) though it can not be expressed analytically. The situation seems improved with the increasing of particles n . As shown in panel (c) of Fig. 3, the excitation energies become increasing with the increasing of the total angular momentum J for finite j cases from $j = 5/2$ to $j = 15/2$ though the energy ratios still away from the corresponding values of a rotational spectrum. Nevertheless, for a sufficiently large j shell, which may be regarded as a single- j approximation to the actual situation in nuclear system with multi- j shells, the low-lying level energies of the $-\kappa\tilde{Q} \cdot \tilde{Q}$ term indeed gradually follow the rotational pattern with the energy ratios $E(4)/E(2) \approx 3.33$, $E(6)/E(2) \approx 7.00$, $E(8)/E(2) \approx 12.00$, and $E(10)/E(2) \approx 18.33$ when $j \geq 477/2$. Our conclusion is that only low-lying energy levels generated from the geometric quadrupole-quadrupole interaction follow the pattern of a rotational spectrum in a single- j shell when j is sufficiently large, while these energy ratios for small j cases generally are away from the corresponding values of a rotational spectrum mainly due to the fact the geometric quadrupole operator is less collective as compared to the Elliott's dynamic counterpart.

In order to reveal the crossover region more precisely, similar to the analysis [20, 21] for the Bose systems, overlaps of the excited states of Hamiltonian (6) for given n and J as functions of the control parameter x with those of the corresponding limiting cases $|\langle nJ_\zeta; x = x_0 | nJ_\zeta; x \rangle|$ with $x_0 = 0$ and $x_0 = 1$ for several J_1 values including that corresponding to the ground state and different total number of particles n in the $j = 15/2$ shell are calculated, of which the results for $n = 4, \dots, 8$ cases are shown in Figs. 4. It can be seen from Figs. 4 that there is a crossover point x_c for each J . The position of the crossover point differ with J but all within the $x \sim 0.4$ - 0.55 region, except the $n = 7$ case, in which the crossover region becomes a little wider within $x \sim 0.31$ - 0.5 . These overlaps varying with x are rather

FIG. 3: Low-lying energy levels generated from the $-\kappa\hat{Q}\cdot\hat{Q}$ term, where panel (a) and (b) provide the results with $n = 2$, and panel (c) with $n = 4$.

FIG. 4: The overlaps $|\langle nJ_{\zeta}; x = x_0 | nJ_{\zeta}; x \rangle|$ with $x_0 = 0$ and $x_0 = 1$ for several J_1 values for $n=4, \dots, 8$ in the $j = 15/2$ shell, where the solid line is the overlap $|\langle nJ_{\zeta}; x = 0 | nJ_{\zeta}; x \rangle|$, and the dotted line is the overlap $|\langle nJ_{\zeta}; x = 1 | nJ_{\zeta}; x \rangle|$.

smooth for small n cases. The exception is the 4_1 case, for which there is a sharp change in $|\langle nJ_\zeta; x = x_0 | nJ_\zeta; x \rangle|$ with $x_0 = 0$ or $x_0 = 1$ around $x_c = 0.44$. Therefore, generally speaking, the actual crossover point in excited states differs from that of the ground state, which was also noticed in the Bose systems [20] previously. Hence, there is only a crossover region within which the overlaps, energy ratios, and other quantities may change noticeably. In the following, we take x_c deduced from the ground state overlaps as the crossover point of the QPT though the crossover point in other quantities may be different.

As is well known from the analysis of the QPT in Bose systems [20, 21], some $B(E2)$ ratios may be sensitive to the shape phase transitions. Several $B(E2)$ ratios of the model as functions of x for $n = 4, 6$, and 8 in the $j = 15/2$ shell are presented in the upper panel of Fig. 5, which show that these quantities undergo noticeable change within the crossover region. Specifically, $B(E2; 4_1 \rightarrow 2_1)/B(E2; 2_1 \rightarrow 0_g)$ gradually increases with the increasing of x when $x < 0.4$ and then becomes decreasing with the increasing of x when $x > 0.4$. Its change is smooth when n is small, and becomes sharper towards the half-filling. On the contrary, there is a sudden increasing in both the ratios $B(E2; 4_2 \rightarrow 2_1)/B(E2; 2_1 \rightarrow 0_g)$ and $B(E2; 3_1 \rightarrow 4_1)/B(E2; 2_1 \rightarrow 0_g)$ within the crossover region. There are also similar changes in $B(E2)$ values shown in the lower panel of Fig. 5 for $B(E2; 4_1 \rightarrow 2_1)$ and $B(E2; 4_2 \rightarrow 2_1)$. With the increasing of the number of particles, there are more $B(E2)$ values and their ratios undergo noticeable change though other $B(E2)$ values and ratios are not provided in Fig. 5. The situation for odd n cases is quite similar though only $B(E2; 5/2_1 \rightarrow 7/2_1)$ as a function of x is shown in Fig. 6. Since the E2 transition is related with two different excited states, generally, the crossover region recognized from $B(E2)$ values may differ from that identified from the overlaps shown previously. Moreover, the crossover region in the $B(E2)$ values or their ratios becomes rather narrower when the number of particles reaches to the half-filling when n is even. As clearly shown in Fig. 5 for the even n cases, the crossover region becomes a point around $x_c \sim 0.43$, at which both the $B(E2)$ values and the ratios undergo a sudden change.

Besides $B(E2)$ values, electric quadrupole moments $Q(J_{\zeta})$ and their ratios may also be used to identify the crossover.

FIG. 5: Several B(E2) ratios (the upper panel) and B(E2) values (the lower panel) as functions of x for $n = 4, 6$, and 8 particles in the $j = 15/2$ shell. In the upper panel, the curve a represents $B(E2; 4_1 \rightarrow 2_1)/B(E2; 2_1 \rightarrow 0_g)$, the curve b represents $B(E2; 4_2 \rightarrow 2_1)/B(E2; 2_1 \rightarrow 0_g)$, and the curve c represents $B(E2; 3_1 \rightarrow 4_1)/B(E2; 2_1 \rightarrow 0_g)$. In the lower panel, the solid line a represents $B(E2; 4_1 \rightarrow 2_1)/e_{\text{eff}}^2 r_0^4$, and the dashed line b represents $B(E2; 4_2 \rightarrow 2_1)/e_{\text{eff}}^2 r_0^4$.

FIG. 6: The B(E2) value $B(E2; 5/2_1 \rightarrow 7/2_1)/e_{\text{eff}}^2 r_0^4$ as a function of x for $n = 5$ and $n = 7$ particles in the $j = 15/2$ shell.

Similar to the B(E2) ratios, there are many quadrupole moment ratios of low-lying states may undergo noticeable change within the crossover region though only three quadrupole moment ratios of low-lying states for $n = 6$ and $Q(5/2_1)/Q(7/2_1)$ for $n = 7$ as functions of x for $j = 15/2$ are shown in Fig. 7. The divergence in $Q(5/2_1)/Q(7/2_1)$ for $n = 7$ occurs because the $Q(7/2_1)$ is almost zero at $x \sim 0.42$ and $x \sim 0.49$. It should be pointed out that the quadrupole moment at the half-filling case is always zero and independent of the control parameter x , which is unique. Since the $O(3)$ -reduced matrix elements of the geometric quadrupole operator $\langle [1^n] \langle 1^{\nu'} \rangle \alpha' J_f \| Q \| [1^n] \langle 1^{\nu} \rangle \alpha J_i \rangle$ with $\nu' = \nu$ can be expressed as

$$\langle [1^n] \langle 1^{\nu} \rangle \alpha' J_f \| Q \| [1^n] \langle 1^{\nu} \rangle \alpha J_i \rangle = \left(n - \frac{2j+1}{2} \right) f(\nu, j, \alpha', \alpha, J_f, J_i) \quad (21)$$

as observed by Talmi [15], it is obviously zero at the half-filling when $n = j+1/2$. While $\langle [1^n] \langle 1^{\nu'} \rangle \alpha' J_f \| Q \| [1^n] \langle 1^{\nu} \rangle \alpha J_i \rangle$ is nonzero when $\nu' \neq \nu$, which still leads to the nonzero contribution of $\tilde{Q} \cdot \tilde{Q}$ to the Hamiltonian in the half-filling case.

FIG. 7: Several electric quadrupole moment ratios of low-lying states for $n = 6$ (the left panel) and $Q(5/2_1)/Q(7/2_1)$ for $n = 7$ (the right panel) in the $j = 15/2$ shell as functions of x . In the left panel, the curve a represents $Q(2_3)/Q(2_1)$, the curve b represents $Q(4_1)/Q(2_1)$, and the curve c represents $Q(4_2)/Q(2_1)$. In the right panel, the curve represents $Q(5/2_1)/Q(7/2_1)$.

IV. APPLICATIONS

In this section, we try to describe some nuclei using the single- j model, of which the spectra should be in between the rotation-like and the pair-excitation phase. As shown in [15] and [24], most nuclei that can be described within a single- j shell are those with a few particles outside a closed shell mainly driven by the pairing interaction with some other seniority conserving interaction terms. These seniority conserving interaction terms can also be added to the Hamiltonian (6) contributing to the diagonal part of the matrix elements only, which, however, are not included in this work for simplicity. We found that a chain of isotones ^{212}Rn - ^{213}Fr - ^{214}Ra - ^{215}Ac with equal neutron number $N_\nu = 126$ seem suitable to be described by the current model, of which the spectra seem always somewhat rotation-like. The valence protons in these nuclei are regarded as confined in the $1h_{9/2}$ shell. There are $n = 4$ protons in ^{212}Rn , $n = 5$ protons (the half-filling case) in ^{213}Fr , $n = 6$ protons in ^{214}Ra , and $n = 7$ protons in ^{215}Ac outside the sixth closed shell with $N_\pi = 82$, respectively. Since the parameter ξ only affects the position of the crossover region, we simply set $\xi = r_0^4/40\text{fm}^4$, of which the value is slightly different from nucleus to nucleus because r_0 is mass number dependent. Once the dimensionless constant ξ is chosen, other parameters are obtained by a best fit to the energy spectrum of each nucleus provided in Table III, in which x_c is the crossover point deduced from the ground state overlaps defined in the previous section. The calculated low-lying energy levels in the yrast band of these nuclei are shown in Fig. 8. Accordingly, some calculated $B(E2)$ values and the electric quadrupole moment $Q(J_1)$ within the yrast band are shown in Table IV. The experimental data seem fitted reasonably well by the model with two effective parameters x and c .

TABLE III: The parameters of (6) and the effective charge e_π used to describe ^{212}Rn , ^{213}Fr , ^{214}Ra , and ^{215}Ac , where c is in MeV. The crossover point $x_c = 0.71$ is deduced from the ground state overlaps.

Parameter	^{212}Rn	^{213}Fr	^{214}Ra	^{215}Ac
ξ	0.910	0.913	0.916	0.919
c	0.24	0.26	0.26	0.33
x	0.56	0.63	0.58	0.76
e_π	$0.91e$	$0.50e$	$0.51e$	$0.50e$

FIG. 8: Some low-lying energy levels (in MeV) in the yrast band obtained from the model with parameters shown in Table III and compared with the corresponding experimental data [25–31], where the spin and parity in the parentheses indicate they are not confirmed experimentally.

TABLE IV: Several $B(E2)$ values (in W. u.) and electric quadrupole moment $Q(J_\zeta)$ (in $e \cdot b$) within the yrast band calculated from the model (Cal.) with parameters shown in Table III and compared with the corresponding experimental data (Exp.).

	$J_i^\pi \rightarrow J_f^\pi$	Exp. [25–31]	Cal.
^{212}Rn	$4_1^+ \rightarrow 2_1^+$	1.04	2.52
	$6_1^+ \rightarrow 4_1^+$	0.4	0.9
	$8_1^+ \rightarrow 6_1^+$	0.115	0.219
	$12_1^+ \rightarrow 10_1^+$	4.4	1.1
	$Q(8_1^+)$	(–)0.17	–0.10
^{213}Fr	$\frac{13}{2}_1^- \rightarrow \frac{9}{2}_1^-$	0.0014928	0.66
	$\frac{17}{2}_1^- \rightarrow \frac{13}{2}_1^-$	0.55	0.71
	$\frac{21}{2}_1^- \rightarrow \frac{17}{2}_1^-$	0.0439	0.59
	$Q(9/2_1^-)$	–0.14	0.00
^{214}Ra	$4_1^+ \rightarrow 2_1^+$	0.152	0.785
	$6_1^+ \rightarrow 4_1^+$	0.178	0.268
	$8_1^+ \rightarrow 6_1^+$	0.00137	0.06658
^{215}Ac	$\frac{17}{2}_1^- \rightarrow \frac{13}{2}_1^-$	0.08	0.42
	$\frac{21}{2}_1^- \rightarrow \frac{17}{2}_1^-$	0.119	0.244

TABLE V: Several energy and B(E2) ratios obtained from the model (Cal.) and compared with the corresponding experimental data, in which the corresponding value in the limiting cases and that at the crossover point determined by the overlaps is also shown, where “—” denotes that the corresponding experimental value is not available.

	^{212}Rn	Cal.	$x = 0$	$x = x_c$	$x = 1$	^{214}Ra	Cal.	$x = 0$	$x = x_c$	$x = 1$
$E(2_1^+)/E(4_1^+)$	0.85	0.59	0.51	0.64	1.00	0.84	0.59	0.51	0.64	1.00
$E(12_1^+)/E(4_1^+)$	1.92	2.08	4.44	1.74	1.60	1.99	2.02	4.44	1.74	1.60
$B(E2; 8_1^+ \rightarrow 6_1^+)$	0.29	0.25	1.08	0.95	0.40	0.008	0.25	1.08	0.95	0.40
$B(E2; 6_1^+ \rightarrow 4_1^+)$										
$B(E2; 12_1^+ \rightarrow 10_1^+)$	11.00	1.32	0.73	6.31	9.79	—	1.32	0.73	6.30	9.79
$B(E2; 6_1^+ \rightarrow 4_1^+)$										
	^{213}Fr	Cal.	$x = 0$	$x = x_c$	$x = 1$	^{215}Ac	Cal.	$x = 0$	$x = x_c$	$x = 1$
$E(7/2_1^-)/E(17/2_1^-)$	0.35	0.33	0.21	0.41	1.00	—	0.50	0.24	0.42	1.00
$E(13/2_1^-)/E(17/2_1^-)$	0.84	0.58	0.44	0.59	1.00	0.81	0.80	0.51	0.77	1.00

It can be seen from Table IV that the B(E2) values and the electric quadrupole moments observed from these nuclei seems fitted reasonably well except $Q(9/2^-)$ of ^{213}Fr , which is zero obtained from the model because the number of valence protons in ^{213}Fr is at the half-filling. Moreover, the effective charges of valence protons in these nuclei used in the fits are smaller with $0.5 \leq e_\pi < 1$ as shown in Table III, which may be due to the fact that the model with the single- j shell is too simple. It may be improved in a multi- j extension of the model. Several energy and B(E2) ratios obtained from the model in comparison with the corresponding experimental data are provided in Table V, in which the corresponding value in the limiting cases and that at the crossover point determined by the ground state overlaps is also shown. One can observe that these ratios are near the corresponding values at the crossover point determined from the theory, which indicate these nuclei are near to the crossover point of the shape phase transition, though the crossover point determined from the ground state overlaps is a little different from that determined by these ratios, and changes in these ratios with x are not monotonic, especially near the crossover point.

V. SUMMARY

In this paper, the QPT behavior of the spherical shell model mean-field plus the geometric quadrupole-quadrupole and standard pairing model within a single- j shell is analyzed in detail. Our analysis shows that the spectrum generated by the geometric quadrupole-quadrupole interaction does not follow the $J(J+1)$ -law, especially in the higher lying states of the yrast band when the number of particles and the value of j is small, which may be due to the fact that the geometric quadrupole operator is less collective in comparison to the Elliott’s dynamic counterpart. Only when j is sufficiently large, does the low-lying part of the spectrum generated by the geometric quadrupole-quadrupole interaction follow the $J(J+1)$ -law even when there are only a few particles. Due to the Pauli exclusion, only a crossover occurs in the model because j is small and finite. Various quantities, such as low-lying energy levels, some typical energy ratios, the overlaps of the excited states with those of the corresponding limiting cases, B(E2) values and electric quadrupole moments of some low-lying states and their ratios, as functions of the control parameter of the model in the $j = 15/2$ shell are calculated. The results show that there are noticeable changes within the crossover region of the rotation-like to the pair-excitation (superconducting) phase transition, especially in the half-filling case. The crossover region becomes narrower with the increasing of the number of particles toward the half-filling, especially in the even j cases. Though the crossover is most noticeable at the half-filling, the quadrupole moments in this case, however, are always zero as observed by Talmi [15]. As application to realistic nuclear systems, a chain of isotones ^{212}Rn - ^{213}Fr - ^{214}Ra - ^{215}Ac is chosen to be described by the model with valence protons confined in the $1h_{9/2}$ shell. As far as the low-lying energy levels in the yrast band, and the experimentally observed $B(E2)$ values and the electric quadrupole moment within the yrast band are concerned, these nuclei seem fitted reasonably well. The results indicate that these nuclei are all within the rotation-like to the pair-excitation phase transition near to the crossover.

In order to study the QPT in the spherical shell model mean-field plus the geometric quadrupole-quadrupole and standard pairing model more precisely, multi- j extension of the current model is necessary, in which other seniority conserving interaction terms introduced in [15, 24] may also be considered. These extensions will be a part of our future work.

Acknowledgments

Support from the U. S. National Science Foundation (OCI-0904874, ACI-1516338), U. S. Department of Energy (DE-SC0005248), the Southeastern Universities Research Association, the China-U.S. Theory Institute for Physics with Exotic Nuclei (CUSTIPEN) (DE-FG02-13ER42025), the National Natural Science Foundation of China (11375080, 11405080), and the LSU-LNNU joint research program (9961) is acknowledged.

Appendix A: An algorithm for evaluating the one-particle ISFs of $Sp(2j+1) \supset O(3)$

The ISFs of $Sp(2j+1) \supset O(3)$ were studied in many different ways [23, 32–34]. Especially, in [33], the fractional parentage coefficients, which are related to the ISF of $Sp(2j+1) \supset O(3)$, are tabulated for n up to the half-filling and $j \leq 11/2$, and $n \leq 5$ for $j = 13/2$ and $j = 15/2$. In [34], the algorithm for calculating the ISFs of $Sp(2j+1) \supset O(3)$ is provided based on a recursive method. In the following, we provide the improved angular momentum projection method for identical fermions in a single- j shell proposed in [22].

Let $\{J_\mu^\beta; \mu = +, -, 0\}$, where $\beta = 1, 2, \dots, n$, be generators of the β -th copy of the $SU(2)$ algebra, and $|j_\beta, m_\beta\rangle$ be the corresponding orthonormal basis vectors with angular momentum quantum number j_β and quantum number m_β of its third component. According to the angular momentum projection method [22], one can write n -coupled state with total angular momentum $J = J_{\max} - k$ and $M = J$ as

$$|\eta; J, M = J\rangle = \mathcal{N} J_-(x_1^{(\eta)}) J_-(x_2^{(\eta)}) \cdots J_-(x_k^{(\eta)}) |\text{h.w.}\rangle, \quad (\text{A1})$$

where $\mathcal{N}$ is the normalization constant, and $|\text{h.w.}\rangle$ is the $SU(2)$ highest weight state satisfying $J_+^\beta |\text{h.w.}\rangle = 0$ for any β ,

$$J_-(x_i^{(\eta)}) = \sum_{\beta=1}^n \frac{1}{x_i^{(\eta)} - \varepsilon_\beta} J_-^\beta, \quad (\text{A2})$$

in which the parameters $\{\varepsilon_\beta\}$ are a set of arbitrary parameters chosen to resolve the multiplicity, and η is used to distinguish different n -coupled states with the same angular momentum J , and $\{x_i^{(\eta)}\}$ should satisfy

$$\sum_{\beta=1}^n \frac{2m_\beta^{\max}}{x_i^{(\eta)} - \varepsilon_\beta} - \sum_{t=1(\neq i)}^k \frac{2}{x_i^{(\eta)} - x_t^{(\eta)}} = 0 \quad (\text{A3})$$

for $i = 1, 2, \dots, k$, where $m_\beta^{\max}$ is the quantum number m_β in the highest weight state. It is clear that the multiplicity label η in (A1) is taken to be the label of different solutions $\{x^{(\eta)}\}$ of Eq. (A3).

For n identical fermions in a single- j shell, the creation operators are denoted simply as $a_{jm}^\dagger \equiv a_m^\dagger$ ($m = j, j-1, \dots, -j$). Due to the Pauli exclusion, the highest weight state is $|\text{h.w.}\rangle = a_j^\dagger a_{j-1}^\dagger \cdots a_{j-n+1}^\dagger |0\rangle$ for $1 \leq n \leq 2j+1$, where $|0\rangle$ is the vacuum state. Thus, in this case, the β -th copy of the angular momentum operator J_μ^β are only effective to the β -th creation operator $a_{j-\beta+1}^\dagger$ and keep other creation operators in the highest weight state $|\text{h.w.}\rangle$ unchanged. Thus, $m_\beta^{\max} = j - \beta + 1$ and $J_{\max} = n(2j - n + 1)/2$ for this case. Since the state (A1) of n identical fermions is always totally antisymmetric, it is also a basis vector of $U(2j+1) \supset O(3)$ with the irrep $[1^n]$ of $U(2j+1)$.

The number of linearly independent states obtained from (A1), $D_F(n, k)$, can be calculated as follows: Let $Q_n(k)$ be number of different n -partitions of the integer k with $k = \sum_{i=1}^n k_i$, where k_i ($i = 1, 2, \dots, n$) are non-negative integers satisfying $2j+1-n \geq k_n \geq \dots \geq k_2 \geq k_1 \geq 0$. Then, the number of linearly independent states obtained from (A1), $D_F(n, k) = Q_n(k) - Q_n(k-1)$, which gives the multiplicity of given $J = J_{\max} - k$ in the reduction $U(2j+1) \downarrow O(3)$ for the irrep $[1^n]$ of $U(2j+1)$. As shown in [22], $D_F(n, k)$ is far less than the number of independent solutions obtained from (A3). Therefore, generally (A1) obtained from solutions of (A3) are over-complete and non-orthonormal. One only needs to choose $D_F(n, k)$ solutions of (A3) with the quantum number $\tilde{\eta}$ as the multiplicity label after the Gram-Schmidt orthonormalization. Therefore, the parameters $\{\varepsilon_\beta\}$ are chosen with as fewer number of different values as possible to simplify (A3).

Once all orthonormalized states (A1) are obtained, one can expand (A1) in terms of the n single-particle product states with

$$|[1^n]\tilde{\eta}; J = J_{\max} - k, M = J\rangle = \sum_{k_1 \cdots k_n} F_{k_1 \cdots k_n}^{\tilde{\eta}} |[k_n k_{n-1} \cdots k_1]\rangle. \quad (\text{A4})$$

where $|[k_n k_{n-1} \cdots k_1]\rangle \equiv a_{j-k_1}^\dagger a_{j-1-k_1}^\dagger \cdots a_{j-n+1-k_n}^\dagger |0\rangle$. The expansion coefficients $F_{k_1 \cdots k_n}^{\tilde{\eta}}$ in (A4) can be obtained from (A1) after the expansion accordingly. Then, the state with any M can be expressed in the standard way as

$$|[1^n]\tilde{\eta}; J, M\rangle = \sqrt{\frac{(J+M)!}{(2J)!(J-M)!}} J_-^{J-M} |[1^n]\tilde{\eta}; J, J\rangle. \quad (\text{A5})$$

In order to get the basis vectors of $U(2j+1) \supset Sp(2j+1) \supset O(3)$ with definite seniority number for fixed J , we choose a linear combination of (A4) with

$$|[1^\nu]\langle 1^\nu \rangle \tilde{\alpha} J = J_{\max} - k, M = J\rangle = \sum_{\tilde{\eta}} \Phi_{\tilde{\eta}}^{\tilde{\alpha}} |[1^\nu]\tilde{\eta}; J, M = J\rangle, \quad (\text{A6})$$

which must satisfy the condition:

$$S_- |[1^\nu]\langle 1^\nu \rangle \tilde{\alpha} J\rangle = 0. \quad (\text{A7})$$

Using (A4) with $n = \nu$ and $S_- = \sum_{m>0} (-1)^{j-m} a_{-m} a_m$, we have

$$S_- |[1^\nu]\tilde{\eta}; J, M = J\rangle = \sum_{k_1 \cdots k_n} F_{k_1 \cdots k_n}^{\tilde{\eta}} S_- |[k_n k_{n-1} \cdots k_1]\rangle = \sum_{k_1 \cdots k_{n-2}} \tilde{F}_{k_1 \cdots k_{n-2}}^{\tilde{\eta}} |[k_{n-2} k_{n-3} \cdots k_1]\rangle, \quad (\text{A8})$$

where $|[k_{n-2} k_{n-3} \cdots k_1]\rangle$ is the single-particle product state of the remaining $n-2$ particles, and $\tilde{F}_{k_1 \cdots k_{n-2}}^{\tilde{\eta}}$ is the corresponding coefficient after S_- is applied accordingly. Thus, (A7) leads to

$$\sum_{\tilde{\eta}} \tilde{F}_{k_1 \cdots k_{n-2}}^{\tilde{\eta}} \Phi_{\tilde{\eta}}^{\tilde{\alpha}} = 0. \quad (\text{A9})$$

Thus, generally, $\tilde{\mathbf{F}}_{n-2}$ is a non-symmetric matrix. The coefficients $\{\Phi_{\tilde{\eta}}^{\tilde{\alpha}}\}$ ($\tilde{\eta} = 1, 2, \dots, D_F(n, k)$) are components of the $\tilde{\alpha}$ -th null space vectors of $\tilde{\mathbf{F}}_{n-2}$. Therefore, the null space vectors of $\tilde{\mathbf{F}}_{n-2}$ provide the expansion coefficients $\{\Phi_{\tilde{\eta}}^{\tilde{\alpha}}\}$, for which there are many simple algorithms for the purpose. It should be noted that $\{\Phi_{\tilde{\eta}}^{\tilde{\alpha}}\}$ obtained in this way are also non-orthogonal with respect to $\tilde{\alpha}$, namely $\Phi^{\tilde{\alpha}} \cdot \Phi^{\tilde{\alpha}'} \neq \delta_{\tilde{\alpha}\tilde{\alpha}'}$. After the Gram-Schmidt orthonormalization, the multiplicity label in the reduction $Sp(2j+1) \downarrow O(3)$ is denoted as α , of which the corresponding expansion coefficients are denoted as $\{\Phi_{\tilde{\eta}}^{\alpha}\}$.

Once the expansion coefficients $\{\Phi_{\tilde{\eta}}^{\alpha}\}$ are obtained, using (A4), one can get the single-particle ISF of $Sp(2j+1) \supset O(3)$ from the matrix element directly:

$$\langle [1^{\nu+1}]\langle 1^{\nu+1} \rangle \alpha' J' J' | a_m^\dagger | [1^\nu]\langle 1^\nu \rangle \alpha J J \rangle = \left\langle \begin{matrix} \langle 1^\nu \rangle & \langle 1 \rangle \\ \alpha J & j \end{matrix} \middle| \begin{matrix} \langle 1^{\nu+1} \rangle \\ \alpha' J' \end{matrix} \right\rangle \langle [1^{\nu+1}] | a^\dagger | [1^\nu] \rangle \langle J J, j m | J' J' \rangle, \quad (\text{A10})$$

where we always choose $m = J' - J$ to ensure the CG coefficient $\langle J J, j m | J' J' \rangle$ nonzero. The left-hand-side of (A10) can further be expressed as

$$\langle [1^{\nu+1}] \langle 1^{\nu+1} \rangle_{\alpha' J' J'} | a_m^\dagger | [1^\nu] \langle 1^\nu \rangle_{\alpha J J} \rangle = \sum_{\tilde{\eta} \tilde{\eta}'} \Phi_{\tilde{\eta}}^{\alpha'} \Phi_{\tilde{\eta}}^\alpha \sum_{k_1 \dots k_{\nu+1}} F_{k_1 \dots k_{\nu+1}}^{\tilde{\eta}'} \tilde{F}_{k_1 \dots k_{\nu+1}}^{\tilde{\eta}}, \quad (\text{A11})$$

where $\tilde{F}_{k_1 \dots k_{\nu+1}}^{\tilde{\eta}}$ is determined from the expansion

$$a_m^\dagger | [1^\nu] \langle 1^\nu \rangle_{\alpha J J} \rangle = \sum_{\tilde{\eta}} \Phi_{\tilde{\eta}}^\alpha \sum_{k_1 \dots k_{\nu+1}} \tilde{F}_{k_1 \dots k_{\nu+1}}^{\tilde{\eta}} | [k_{\nu+1} k_\nu \dots k_1] \rangle. \quad (\text{A12})$$

By using (11) and (A11), (A10) can be rewritten as

$$\left\langle \begin{matrix} \langle 1^\nu \rangle \\ \alpha J \end{matrix} \begin{matrix} \langle 1 \rangle \\ j \end{matrix} \middle| \begin{matrix} \langle 1^{\nu+1} \rangle \\ \alpha' J' \end{matrix} \right\rangle = \frac{1}{\sqrt{\nu+1} \langle J J, j m | J' J' \rangle} \sum_{\tilde{\eta} \tilde{\eta}'} \Phi_{\tilde{\eta}'}^{\alpha'} \Phi_{\tilde{\eta}}^\alpha \sum_{k_1 \dots k_{\nu+1}} F_{k_1 \dots k_{\nu+1}}^{\tilde{\eta}'} \tilde{F}_{k_1 \dots k_{\nu+1}}^{\tilde{\eta}}, \quad (\text{A13})$$

which satisfies the conjugation relation

$$\left\langle \begin{matrix} \langle 1^{\nu+1} \rangle \\ \alpha' J' \end{matrix} \begin{matrix} \langle 1 \rangle \\ j \end{matrix} \middle| \begin{matrix} \langle 1^\nu \rangle \\ \alpha J \end{matrix} \right\rangle = (-1)^{J'+j-J} \sqrt{\frac{(2J'+1)(\nu+1)(2j-2\nu+3)}{(2J+1)(2j-\nu+3)(2j-2\nu+1)}} \left\langle \begin{matrix} \langle 1^\nu \rangle \\ \alpha J \end{matrix} \begin{matrix} \langle 1 \rangle \\ j \end{matrix} \middle| \begin{matrix} \langle 1^{\nu+1} \rangle \\ \alpha' J' \end{matrix} \right\rangle \quad (\text{A14})$$

and the orthonormality relation:

$$\sum_{\zeta J} \left\langle \begin{matrix} \langle 1^\nu \rangle \\ \alpha J \end{matrix} \begin{matrix} \langle 1 \rangle \\ j \end{matrix} \middle| \begin{matrix} \langle 1^{\nu+1} \rangle \\ \alpha' J' \end{matrix} \right\rangle \left\langle \begin{matrix} \langle 1^\nu \rangle \\ \alpha J \end{matrix} \begin{matrix} \langle 1 \rangle \\ j \end{matrix} \middle| \begin{matrix} \langle 1^{\nu+1} \rangle \\ \alpha'' J' \end{matrix} \right\rangle = \delta_{\alpha' \alpha''}. \quad (\text{A15})$$

In the following, we take $n = 4$ with $J = M = 6$ in a $j = 9/2$ shell as an example, of which the multiplicity is three. (A1) in this case may be expressed as

$$|[1^4] \eta; M = J = 6 \rangle = \mathcal{N} J_-(x_1^{(\eta)}) J_-(x_2^{(\eta)}) \dots J_-(x_6^{(\eta)}) a_j^\dagger a_{j-1}^\dagger a_{j-2}^\dagger a_{j-3}^\dagger | 0 \rangle \quad (\text{A16})$$

with the conditions

$$\frac{16}{x_i^{(\eta)} - 1} + \frac{5}{x_i^{(\eta)}} + \frac{3}{x_i^{(\eta)} + 1} - \sum_{t(\neq i)} \frac{2}{x_i^{(\eta)} - x_t^{(\eta)}} = 0 \quad (\text{A17})$$

for $i = 1, 2, \dots, 6$, where $\varepsilon_1 = \varepsilon_2 = 1$, $\varepsilon_3 = 0$, and $\varepsilon_4 = -1$ are chosen since the multiplicity is only 3 in the reduction $U(10) \downarrow O(3)$ for this case, in which there are three linearly independent states with $\nu = 2$ and $\nu = 4$ mixed. There are many sets of roots, but we only need to choose three from them. The three sets of linearly independent roots of Eq. (A17) are obtained by using the algorithm proposed in [35] in the limit $G \rightarrow \infty$, from which we get

$$\begin{aligned} x_1^{(\eta=1)} &= -0.13393 - 0.18212I, \quad x_2^{(\eta=1)} = -0.13393 + 0.18212I, \quad x_3^{(\eta=1)} = 0.050073 - 0.13133328I, \\ x_4^{(\eta=1)} &= 0.050073 + 0.13133328I, \quad x_5^{(\eta=1)} = 0.107467 - 0.04432751I, \quad x_6^{(\eta=1)} = 0.107467 + 0.04432751I; \\ x_1^{(\eta=2)} &= -0.8921340 - 0.227694I, \quad x_2^{(\eta=2)} = -0.8921340 + 0.227694I, \quad x_3^{(\eta=2)} = -0.8001246, \\ x_4^{(\eta=2)} &= 0.17201701, \quad x_5^{(\eta=2)} = 0.13759373 - 0.139707I, \quad x_6^{(\eta=2)} = 0.13759373 + 0.139707I; \\ x_1^{(\eta=3)} &= 0.08145 - 0.18376I, \quad x_2^{(\eta=3)} = 0.08145 + 0.18376I, \quad x_3^{(\eta=3)} = 0.148008 - 0.057837I, \\ x_4^{(\eta=3)} &= 0.148008 + 0.057837I, \quad x_5^{(\eta=3)} = -0.684475 - 0.1948886I, \quad x_6^{(\eta=3)} = -0.684475 + 0.1948886I. \end{aligned} \quad (\text{A18})$$

The states (A16) obtained in this way is non-orthonormal with respect to η . After the Gram-Schmidt orthonormal-

ization, we have the following expansion:

$$|[1^4]\tilde{\eta}; M = J = 6\rangle = \sum_{k_1 \dots k_4} F_{k_1 \dots k_4}^{\tilde{\eta}} |[k_4 \dots k_1]\rangle \quad (\text{A19})$$

with $\tilde{\eta} = 1, 2, 3$, where the corresponding expansion coefficients $F_{k_1 \dots k_4}^{\tilde{\eta}}$ are given in Table VI.

TABLE VI: The expansion coefficients $F_{k_1 \dots k_4}^{\tilde{\eta}}$ used in (A19).

$\tilde{\eta}$	[6000]	[5100]	[4200]	[4110]	[3300]	[3210]	[3111]	[2220]	[2211]
1	0.0322	-0.0211	-0.3478	0.4471	0.4199	-0.1264	-0.4765	-0.1768	0.4765
2	0.5085	-0.3329	0.0510	0.2704	0.2512	-0.3725	0.1953	0.5261	-0.1953
3	-0.5760	0.3770	-0.3188	0.0133	0.4198	-0.1595	0.2401	0.3277	-0.2401

Then, according to (A6), we have

$$|[1^4]\langle 1^4 \rangle \tilde{\alpha}; J = M = 6\rangle = \sum_{\tilde{\eta}} \Phi_{\tilde{\eta}}^{\tilde{\alpha}} |[1^4]\tilde{\eta}; J = M = 6\rangle, \quad (\text{A20})$$

where the coefficients $\Phi_{\tilde{\eta}}^{\tilde{\alpha}}$ should satisfy the condition (A8) with

$$\begin{aligned} S_- |[1^4]\tilde{\eta} = 1; J = M = 6\rangle &= -0.6450|[20]\rangle - 0.6450u|[11]\rangle, \\ S_- |[1^4]\tilde{\eta} = 2; J = M = 6\rangle &= -0.0772|[20]\rangle - 0.0772u|[11]\rangle, \\ S_- |[1^4]\tilde{\eta} = 3; J = M = 6\rangle &= 0.6914|[20]\rangle + 0.6914u|[11]\rangle, \end{aligned} \quad (\text{A21})$$

where $[20]\rangle \equiv a_{9/2}^\dagger a_{3/2}^\dagger |0\rangle$ and $[11]\rangle \equiv a_{7/2}^\dagger a_{5/2}^\dagger |0\rangle$. Thus, we get the corresponding 2×3 matrix $\tilde{\mathbf{F}}_2$ of the following form

$$\tilde{\mathbf{F}}_2 = \begin{pmatrix} -0.6450 & -0.0772 & 0.6914 \\ -0.6450u & -0.0772u & 0.6914u \end{pmatrix} \quad (\text{A22})$$

with $u = -1.52744$. The null space vectors $\Phi_{\tilde{\eta}}^\alpha$ of $\tilde{\mathbf{F}}_2$ after the Gram-Schmidt orthonormalization are shown in Table VII.

TABLE VII: $\Phi_{\tilde{\eta}}^\alpha$ for $\nu = 4$ and $J = 6$.

$\alpha \setminus \tilde{\eta}$	1	2	3
1	0.6883	-0.41384	0.5958
2	0.2531	0.9067	0.3374

It should be stated that the coefficients $\{\Phi_{\tilde{\eta}}^\alpha\}$ are not unique. Any rotation of the vector $\Phi_{\tilde{\eta}}$ within the multiplicity space gives equivalent results, but the values will be different. For example, one can make a rotation

$$\begin{pmatrix} \Phi_{\tilde{\eta}}^{\alpha'=1} \\ \Phi_{\tilde{\eta}}^{\alpha'=2} \end{pmatrix} = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \Phi_{\tilde{\eta}}^{\alpha=1} \\ \Phi_{\tilde{\eta}}^{\alpha=2} \end{pmatrix} \quad (\text{A23})$$

with any θ , of which the results are equivalent but different [36].

Similarly, for example, we can construct the basis vector of $Sp(10) \supset O(3)$ with $n=\nu=3$ and $J = M=17/2$ as

$$|[1^3]\langle 1^3 \rangle; J = M = 17/2\rangle = -0.6325|[200]\rangle + 0.7746|[110]\rangle, \quad (\text{A24})$$

which is multiplicity-free. By acting $a_{m=-5/2}^\dagger$ on (A24), we get

$$a_{-5/2}^\dagger |[1^3]\langle 1^3 \rangle; J = M = 17/2\rangle = 0.6325|[4200]\rangle - 0.7746|[4110]\rangle. \quad (\text{A25})$$

According to (A11), (A20), and the results shown in Tables VI and VII, we finally get

$$\left\langle \begin{array}{cc} \langle 1^3 \rangle & \langle 1 \rangle \\ 17/2 & 9/2 \end{array} \middle| \begin{array}{c} \langle 1^4 \rangle \\ \alpha = 1, 6 \end{array} \right\rangle = -0.4419, \quad \left\langle \begin{array}{cc} \langle 1^3 \rangle & \langle 1 \rangle \\ 17/2 & 9/2 \end{array} \middle| \begin{array}{c} \langle 1^4 \rangle \\ \alpha = 2, 6 \end{array} \right\rangle = -0.3748. \quad (\text{A26})$$

The ISFs of $Sp(2j+1) \supset O(3)$ needed in this paper are thus obtained.

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