Band crossing in the odd-particle system

S. Tazaki
Department of Applied Physics, Fukuoka University, Fukuoka, 814-01, Japan

M. Hasegawa
Laboratory of Physics, Fukuoka Dental College, Fukuoka, 814-01, Japan
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The interaction between the yrast and yrare bands is discussed in the case of five particles in the single-j shell model space with $j=\frac{13}{2}$. Comparison between the case of four and five particles in the same model space is made and it is shown that the interaction between the yrast and yrare bands in the five-particle system is stronger than that in the four-particle system. The results of the Hartree-Fock-Bogoliubov cranking (HFBC) method are compared with those obtained from the diagonalization of the cranking model Hamiltonian and it is shown that the HFBC method is insufficient for describing the band crossing in the five-particle system.

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I. INTRODUCTION

The study of the backbending phenomena has been one of the central subjects in the study of rotating nuclei. Backbending phenomena are known to be caused by the crossing of two bands. Hence, the study of the backbending phenomena is to investigate the mechanism of the band crossings. In order to investigate the band crossings, we have to take into account the effects of the nuclear deformation, the pairing correlations and the Coriolis force which is caused by the nuclear rotation. The cranking model has been used by many authors to study the interweaving of these effects and the BCS approximation is commonly used to treat the pairing interaction. The Hartree-Fock-Bogoliubov cranking (HFBC) method is now extensively used in the study of the nuclear high spin states. In spite of its success, as the BCS treatment of the pairing interaction is known to have some drawbacks, some authors have tried to examine how good approximations the BCS treatment of the pairing interaction gives for its diagonalization in the cranking model Hamiltonian making use of the single-j shell model space [1–3].

The interaction between the crossing bands has been studied [4] and it has been shown, in terms of the HFBC method, that the strength of the interaction between the two bands is an oscillatory function of the position of the chemical potential. Rowley, Pál, and Nagarajan [5] have studied the strength of the interaction between the yrast and yrare bands with their particle-number-conserving method and have shown that the interaction is smaller in the odd-particle systems than in the even-particle systems. However, they have cast doubts on the correctness of the HFBC approach where both even and odd cases are calculated from the same universal curve as a function of the Fermi energy λ.

The strength of the interaction between crossing bands is discussed in terms of the energy difference between them at the crossing point [4]. Wu *et al.* [6] have studied the interaction between the yrast and yrare bands in the cases of even particles in the single-j shell model space with $j=\frac{13}{2}$ and they have shown that the interaction is much larger than that obtained by the HFBC method in all cases they have examined.

The interaction between the yrast and yrare bands can, however, also be known from the behavior of the spin alignments at the crossing region. Rowley and Pál [7] have shown for the four-particle system in $j=\frac{13}{2}$ that the HFBC method reproduces the behavior of the spin alignment of the yrast band obtained by the diagonalization; this shows that the BCS treatment of the pairing interaction gives good approximations to its diagonalization in the four-particle system. The present authors also have obtained the same results as those obtained by Rowley and Pál [7] and corroborated their results.

In this paper, we want to discuss the different situations between the band crossings in the even-particle system and that in the odd-particle system, and to compare the results obtained with the diagonalization of the cranking model Hamiltonian and those obtained with the HFBC method.

II. MODEL AND TREATMENTS

We employ the single-j shell model space with $j=\frac{13}{2}$ in the axially symmetric Nilsson potential. The single-particle energies are given as

$$\varepsilon_k=\kappa\frac{3k^2-j(j+1)}{j(j+1)} \quad . \tag{1}$$

Here k is the z component of the angular momentum of the particle. As we are using the axially symmetric Nilsson potential, the quantum numbers which specify the single-particle states are the absolute value of k and the signature. The parameter κ is usually treated as the energy unit [1–3,7]. As a matter of fact, we have two independent parameters in the Hamiltonian (2) below, i.e.,

G/κ and ω/κ. The parameter κ, however, stands for the deformation of the mean field [8,9], and in the case of the many-j shell model space, it is independent of the strength of the pairing interaction and of the angular frequency of the nuclear rotation. In the discussion in Sec. III, we will see the results which were obtained with the values of κ different from unity.

The cranking Hamiltonian is

$$H=H_{\rm intr}-\omega J_x \ , \tag{2}$$

where

$$H_{\rm intr}=\sum_{k\sigma}\varepsilon_k c^\dagger_{k\sigma}c_{k\sigma}-G\sum_{kk'}c^\dagger_{k+}c^\dagger_{k-}c_{k'-}c_{k'+} \ , \tag{3}$$

$$J_x=\sum_{kk'}\langle k|j_x|k'\rangle(c^\dagger_{k+}c_{k'+}-c^\dagger_{k-}c_{k'-}) \ . \tag{4}$$

The signs + and − correspond to the states of signature $-i$ and $+i$, respectively, and G is the strength of the pairing interaction. The basis states with which we diagonalize the Hamiltonian (2) are as follows. For the $N=5$ system,

$$c^\dagger_{k_1\sigma_1}S^\dagger_{k_2}S^\dagger_{k_3}|0\rangle \ , \tag{5}$$

$$c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}c^\dagger_{k_3\sigma_3}S^\dagger_{k_4}|0\rangle \ , \tag{6}$$

$$c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}c^\dagger_{k_3\sigma_3}c^\dagger_{k_3\sigma_3}c^\dagger_{k_4\sigma_4}c^\dagger_{k_5\sigma_5}|0\rangle \ , \tag{7}$$

and for the $N=4$ system,

$$S^\dagger_{k_1}S^\dagger_{k_2}|0\rangle \ , \tag{8}$$

$$c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}S^\dagger_{k_3}|0\rangle \ , \tag{9}$$

$$c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}c^\dagger_{k_3\sigma_3}c^\dagger_{k_4\sigma_4}|0\rangle \ , \tag{10}$$

with

$$S^\dagger_k=c^\dagger_{k+}c^\dagger_{k-} \ , \tag{11}$$

where σ stands for the sign of the signature exponent ($\sigma=+$ or $-$). We took the states with signature $-i$ for the $N=5$ system and took the states with signature 1 for the $N=4$ system. We call the states (5), (6), and (7) the states with seniority $v=1$, 3, and 5 states, respectively, according to the number of unpaired nucleons. Likewise, we call (8), (9), and (10) $v=0$, 2, and 4 states, respectively, in the $N=4$ system.

The eigenstates of (2) for each value of ω are written as

$$\begin{aligned}|N=5;\omega,\alpha\rangle=&\sum_{k_1\sigma_1,k_2,k_3}g^{v=1}_\alpha(k_1\sigma_1,k_2,k_3;\omega)c^\dagger_{k_1\sigma_1}S^\dagger_{k_2}S^\dagger_{k_3}|0\rangle\\&+\sum_{k_1\sigma_1,k_2\sigma_2,k_3\sigma_3,k_4}g^{v=3}_\alpha(k_1\sigma_1,k_2\sigma_2,k_3\sigma_3,k_4;\omega)c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}c^\dagger_{k_3\sigma_3}S^\dagger_{k_4}|0\rangle\\&+\sum_{k_1\sigma_1,k_2\sigma_2,k_3\sigma_3,k_4\sigma_4,k_5\sigma_5}g^{v=5}_\alpha(k_1\sigma_1,k_2\sigma_2,k_3\sigma_3,k_4\sigma_4,k_5\sigma_5;\omega)c^\dagger_{k_1\sigma_1}c^\dagger_{k_2\sigma_2}c^\dagger_{k_3\sigma_3}c^\dagger_{k_4\sigma_4}c^\dagger_{k_5\sigma_5}|0\rangle \ ,\end{aligned} \tag{12}$$

for the $N=5$ system, where α is the label of the order in energy. The eigenstates for the $N=4$ system are defined in the same way as for the $N=5$ system.

In order to compare the results obtained by the diagonalization of the Hamiltonian (2) and those by the HFBC method, we performed the HFBC calculations in the same model space. The HFBC Hamiltonian is given by

$$\begin{aligned}H_{\rm HFBC}=&\sum_k(\varepsilon_k-\lambda)c^\dagger_{k\sigma}c_{k\sigma}\\&+\tfrac{1}{2}\Delta\sum_k(c^\dagger_{k+}c^\dagger_{k-}+c_{k-}c_{k+})-\omega J_x \ ,\end{aligned} \tag{13}$$

where λ is the chemical potential and Δ is the pairing gap.

When we diagonalized the Hamiltonian (2), we took $G=0.207$ in our case for $N=5$ so as to correspond to our previous work for the $N=4$ system [3]. The values for the parameters λ and Δ in (13) were obtained by the BCS calculations for each value of κ, G, and N.

III. DISCUSSION AND CONCLUSIONS

It is instructive to see the case in which single-particle energies are degenerate, i.e., $\kappa=0$. In this case, we do not have the deformed single-particle energy term. As the pairing Hamiltonian commutes with the cranking term, we have no interaction between bands, and when the deformed single-particle energy term exists ($\kappa\neq0$), as the cranking term does not commute with the single-particle energy term, the interaction between bands comes out.

The ω dependence of the expectation value of the x component of the angular momentum operator with respect to the ground-state band $\langle J_x\rangle$ in the $N=5$ system is shown in Fig. 1 for each value of κ. In the case of $\kappa=0$, spin alignments occur sharply at $\omega=0.125$ and 0.139. This shows the following situations. From $\omega=0$ to 0.125, the value of $\langle J_x\rangle$ is $\frac{13}{2}$, which represents the alignment of the last odd particle added to the even system of aligned spin 0, and one pair dissociates at $\omega=0.125$ and aligns its spins to give $\langle J_x\rangle=\frac{33}{2}$, and at $\omega=0.139$, all pairs dissociate. As the value of κ increases, the increase of $\langle J_x\rangle$ becomes more gradual as seen in the case of $\kappa=0.2$, and in the case of $\kappa=1.0$, the increase of the value $\langle J_x\rangle$ becomes almost monotonous.

In the case of the $N=4$, we had a rapid increase of the value $\langle J_x\rangle$ in the yrast band even in the case of $\kappa=1.0$ (see the solid line in Fig. 3 of Ref. [3]). This suggests that the interaction between the yrast and yrare bands is stronger in the case of $N=5$ than in the case of $N=4$.

In order to see the difference between the $N=4$ and 5

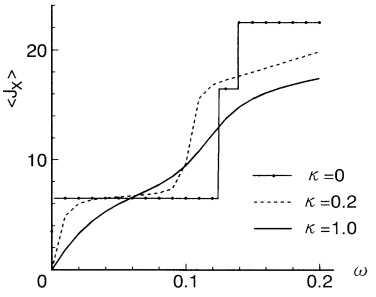

FIG. 1. ω dependence of the expectation value of J_x with respect to the yrast state $\langle J_x \rangle$ for each value of κ in Eq. (1).

systems, we go back to the case of $\kappa=0$ once more. In Fig. 2, the two energy diagrams obtained with $\kappa=0$ are shown. The upper graph shows the energy eigenvalues of the $N=4$ system obtained by the diagonalization of Hamiltonian (2), while the lower graph shows those of the $N=5$ system. Qualitatively, situations are as follows. In the case of $N=4$, there is one state with $v=0$ and there are several degenerate levels with $v=2$ above this $v=0$ state when $\omega=0$. As the angular frequency increases, one of the $v=2$ states comes down and it crosses the $v=0$ state at a certain value of the angular frequency. In this case, the sharp increase of the spin alignment is caused by the crossing of the $v=0$ state and $v=2$. As a matter of fact, even in the case of $\kappa=1.0$, one of these crossing levels is mainly composed of the $v=0$ state and the other is mainly composed of the $v=2$ state. In the case of the $N=5$ system, however, the situation is more complicated. There are some degenerate $v=1$ states and there are some $v=3$ degenerate states above them at $\omega=0$. As ω increases, one of the $v=3$ state comes down and it crosses some $v=1$ states before it crosses the lowest $v=1$ state. The successive crossings make this state a well mixed state of $v=1$ and 3, and, when this state crosses the lowest state, it becomes an almost equally mixed state of $v=1$ and 3. Therefore, the band crossing in this case is the crossing of the two states, one of

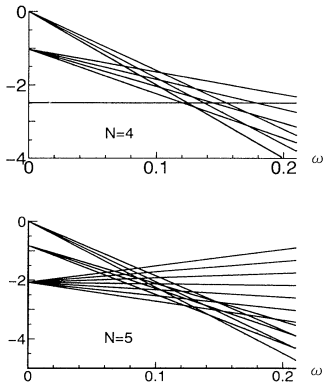

FIG. 2. Energy eigenvalues of the Hamiltonian (2) for $\kappa=0$. The upper part shows that $N=4$ and the lower part shows that $N=5$.

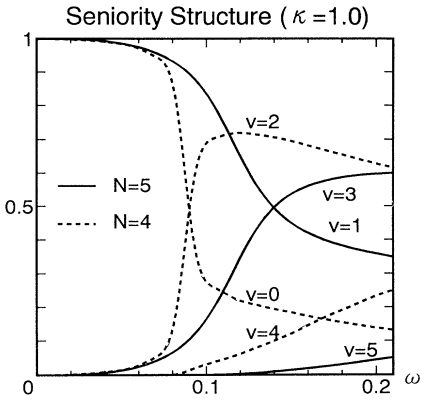

FIG. 3. The seniority structures [the values $\sum_{k,\sigma}|g^{v}_{\alpha=1}((k,\sigma);\omega)|^2$; the definition of g^{v}_{α} can be found in (12)] of the yrast bands of the $N=5$ and 4 systems for $\kappa=1.0$.

which is mainly composed of $v=1$ while the other state is the highly mixed state of $v=1$ and 3. In the case of $\kappa=1.0$, some $v=1$ states lie higher than the lowest $v=3$ state at $\omega=0$. But there are still some lower-lying $v=1$ states with which the lowest $v=3$ state crosses.

In Fig. 3, where seniority structures

$$\sum_{(k,\sigma)} |g^{v}_{\alpha=1}((k,\sigma);\omega)|^2$$

of the yrast bands of the $N=5$ and 4 systems are shown for $\kappa=1.0$, we can see the difference between the cases of $N=4$ and 5. In the case of $N=4$, the $v=2$ component dominates after the crossing, while the components $v=3$ and 1 are comparable in the $N=5$ after the crossing. This figure also shows that the change of the seniority structure is rapid in $N=4$ while it is gradual in the $N=5$ system, which indicates that the interaction between the yrast and yrare bands is stronger in the $N=5$ system than in the $N=4$.

In Fig. 4, five low-lying energy eigenvalues of (2) with $\kappa=1.0$ are plotted against the angular frequency ω. In the $N=4$ system, band crossing occurs at $\omega\simeq 0.9$ and the energy difference between the yrast and yrare bands is not so large at this point. In $N=5$, however, this figure

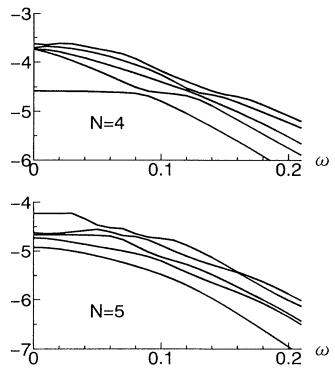

FIG. 4. The energy eigenvalues of (2) with $\kappa=1.0$ plotted against the angular frequency ω.

does not clearly indicate where the band crossing occurs. In addition, the energy difference between them is quite large around $\omega \simeq 0.13$ in comparison with that in the $N=4$. This figure suggests that the band crossing in the $N=5$ system does not occur sharply as in the $N=4$ because the interaction between the yrast and yrare bands is much stronger than in the $N=4$.

Next we discuss how the HFBC describes these situations. In Fig. 7 of Ref. [7], Rowley and Pál showed that the HFBC method gives a fairly good approximation to the diagonalization of the cranking model Hamiltonian in the case of $N=4$. As seen from the dotted lines in Fig. 3, the $v=2$ component dominates the yrast state after the band crossing. However, the mixing of $v=0$ and 4 components plays very important role to increase the spin alignment of the yrast band in this region. The fact that the HFBC method gives the fairly good approximation to the diagonalization means that the mixing of these components into the yrast state is properly taken into account by the HFBC method in the $N=4$ system.

In Fig. 5, the same comparison is made for the $N=5$ system. The dashed line shows the ω dependence of the value $\langle J_x \rangle$ of the yrast band which was obtained by the HFBC method, while the solid line shows that by the diagonalization of the Hamiltonian (2) (the same curve as the solid line in Fig. 1 is reinserted for comparison). As seen from this figure, the value $\langle J_x \rangle$ obtained by the HFBC method varies like a step function as ω increases; it does not behave smoothly as in the diagonalization. Especially, the variation of $\langle J_x \rangle$ between $\omega=0.10$ and 0.16 is considered to correspond to the first backbending in the $N=4$ system where the spin alignment of the yrast band varies rapidly. The results of the $N=5$ system obtained by the diagonalization are quite different from those of the $N=4$ system, while the results of $N=4$ and 5 systems obtained by the HFBC are similar. We have checked the HFBC method in the following way. Setting $G=0.207$ and $\kappa=1.0$, we solved the BCS equations for $N=4$ and 5. We got $\Delta=0.42$ and $\lambda=-0.83$ for $N=4$ and $\Delta=0.41$ and $\lambda=-0.68$ for $N=5$. Using these two sets of parameters, we calculated the values $\langle J_x \rangle$ in some low-lying bands by the HFBC method, one of which is the dashed line in Fig. 4, but we could not find any significant difference in ω dependence between these two sets of parameters.

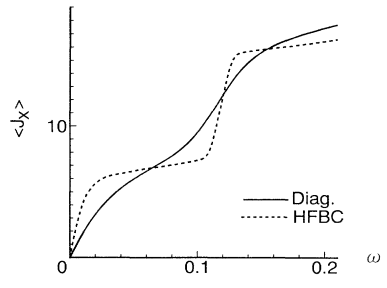

FIG. 5. ω dependence of the value $\langle J_x \rangle$ obtained by the HFBC method is compared to that obtained by the diagonalization. See also Fig. 1.

Some improvements of the HFBC method can be considered. The self-consistent HFBC method is one of the candidates. We tried to find the self-consistent solution of our cranking Hamiltonian (2) for each value of ω in our model space. Although we could not confirm mathematically that no self-consistent solution of it exists in a certain region of ω, we could not find the solution from a value of ω which was smaller than the crossing frequency in our model space. The self-consistent solution may be found in a realistic model space even after the first band crossing. However, it should be noted that, after the first band crossing, pairs dissociate next to next and the pairing gap decreases rapidly [3]. In this situation, where the pairing correlations are weak, BCS treatment of the pairing correlations does not necessarily give good approximations. This is more crucial in the odd-particle system than in the even-particle system. The number projection method is also one of the candidates. As Rowley *et al.* showed in their article, the interaction between the yrast and yrare bands became smaller in the odd-particle system than that in the even-particle system in their number projection method. Hence, it is not clear at the present if the number projection method brings about the suitable difference between the four- and five-particle systems. The difference between the band crossings in these systems, which we have discussed above in terms of the diagonalization method, comes mainly from the dynamical interweaving of the states with different seniorities. Hence, it seems to be difficult to describe it by the HFBC method even if the blocking effect is taken into account.

From the above discussion, we can say that the interaction between the yrast and yrare bands is stronger in the system of $N=5$ than in $N=4$. In the odd-particle system, the backbending in the yrast band is not as simple as that in the even-particle system. The first backbending in the yrast band of the odd-particle system corresponds to the second or higher backbending in the even-particle system because the band which crosses the yrast band is a highly mixed state due to some crossings which have occurred in advance of its crossing with the yrast band. This brings about the stronger interaction between these bands and, consequently, result in the smooth behavior in the ω dependence of the spin alignment of the yrast band.

The HFBC method seems insufficient for describing this situation, i.e., the different situations of the crossing bands in the odd- and even-particle systems. As it is impossible to diagonalize the cranking Hamiltonian in the realistic model space, proper approximation method is desirable for the analysis of the band crossing in odd-particle systems.

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