Proton-neutron alignment in the yrast states of ⁶⁶Ge and ⁶⁸Ge

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The ⁶⁶Ge and ⁶⁸Ge nuclei are studied by means of the shell model with the extended P+QQ Hamiltonian, which succeeds in reproducing experimentally observed energy levels, moments of inertia, and other properties. The investigation using the reliable wave functions predicts T=0, J=9 one-proton-one-neutron $(1p_1n)$ alignment in the $g_{9/2}$ orbit, at high spins $(14_1^+, 16_1^+, \text{ and } 18_1^+)$ in these $N \approx Z$ even-even nuclei. It is shown that a series of the even-*J* positive-parity yrast states (observed up to 26_1^+ for ⁶⁸Ge) consists of the ground-state band and successive three bands with different types of particle alignments (two-neutron, $1p_1n$, two-proton-two-neutron) in the $g_{9/2}$ orbit.

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The study of $N \approx Z$ proton-rich nuclei calls much attention in the nuclear structure physics, and it is also interesting in a wider context. What nuclides exist at the proton drip line? Are there special states like isomers which contribute to nucleosynthesis? Proton-neutron (pn) pair correlations are considered to play a key role in those problems for $N \approx Z$ nuclei. A lot of effort has been devoted to the study of the $N \approx Z$ nuclei and the pn pair correlations. It has explored various aspects of structure such as shape coexistence and delayed alignment in proton-rich nuclei with A = 60 - 80. The $N \approx Z$ Ge isotopes at the gate to these proton-rich nuclei have been extensively studied. The recent development of experimental techniques accomplished detailed measurements of ⁶⁶Ge [1] and ⁶⁸Ge [2]. Our subject is explaining the observed data and clarifying the structure. Besides this subject, we aim to get a useful effective interaction for the shell model which is applicable to the exploration of the problems of heavier $N \approx Z$ nuclei. We have succeeded in reproducing a large number of energy levels observed in these nuclei. Using the wave functions, we have found a unique phenomenon of particle alignment which has not been expected in even-even nuclei. The particle alignments, which can be considered as breaking away from the collective T=1 or T=0 pair correlations caused by rapid rotation, reveal the features of the pn pair correlations as well as the like-nucleon pair correlations. The one-proton-one-neutron (1p1n) alignment with T=0, J=2jhas been discussed only in odd-odd nuclei. In this paper, dealing with *pn* interactions dynamically in the shell model, we show unexpected existence of the T=0 1p1n alignment at high-spin yrast states of the $N \approx Z$ even-even nuclei ⁶⁶Ge and 68 Ge. This is a unique appearance of the *pn* pair correlations.

The experiments for ⁶⁸Ge and ⁶⁶Ge [1,2] have found several bands with positive and negative parities up to high spins ($J \le 28$). The data which display changes in the structure with increasing spin call our attention to the particle alignments. The two-nucleon alignment at $J^{\pi}=8^+$ in ⁶⁸Ge and ⁶⁶Ge has been discussed by several authors [3–9]. The calculations based on the deformed mean field approximation in Ref. [1] predict simultaneous alignment of protons and neutrons just after the first band crossing. In a previous paper [10], we showed that the shell model with the extended P + QQ interaction in a restricted configuration space $(p_{3/2}, f_{5/2}, p_{1/2}, g_{9/2})$ successfully describes ⁶⁴Ge. The shell model has advantages that the nuclear deformation is dynamically determined through nuclear interactions and wave functions are strictly determined, which make it possible to calculate physical quantities and to discuss the structure of bands in detail. We carried out large-scale shell model calculations for ⁶⁶Ge and ⁶⁸Ge using the calculation code [11]. Results of the calculations explain well all the observed energy levels and other properties except for the superdeformed band. We analyze the wave functions obtained to investigate the structure of the even-*J* positive-parity yrast states.

We first employed the same single-particle energies as those used for ⁶⁴Ge in Ref. [10]. The parameters, however, cannot reproduce the relative energies of the positive and negative parity states in odd-mass Ge isotopes. We therefore lowered the $g_{9/2}$ orbit toward the pf shell so that our shell model can reproduce observed level schemes of odd-mass and even-mass Ge isotopes (and also ⁶⁶As) as a whole. This was linked with the search for force strengths. We thus obtained the following set of parameters for the Ge isotopes. The single-particle energies are $\varepsilon_{p3/2}=0.00$, $\varepsilon_{f5/2}=0.77$, $\varepsilon_{p1/2}=1.11$, and $\varepsilon_{g9/2}=2.50$ in MeV. The strengths of the J =0 and J=2 pairing, quadrupole-quadrupole, and octupole-octupole forces are $g_0=0.262$, $g_2=0.0$, $\chi_2=0.238$, and $\chi_3=0.047$ in MeV. The monopole corrections are $H_{mc}^{Te1}(p_{3/2}, f_{5/2})=-0.3$, $H_{mc}^{Te1}(p_{3/2}, p_{1/2})=-0.3$, $H_{mc}^{Te1}(f_{5/2}, p_{1/2})=-0.1$ in MeV.

In Fig. 1 we compare energy levels obtained for ⁶⁶Ge with the experimental ones in Ref. [1]. The calculations reproduce the several bands of the yrast states with positive and negative parities observed in ⁶⁶Ge. The agreement between the observed and calculated energy levels is excellent. The present model reproduces well observed energy levels of ⁶⁸Ge (which are more than twice as many as those of ⁶⁶Ge) and also satisfactorily describes energy levels observed in the odd-mass isotopes ⁶⁵Ge and ⁶⁷Ge. It reproduces the experimental Q moment of the 2⁺₁ state in ⁷⁰Ge. Such a consistent



FIG. 1. Experimental and calculated energy levels of ⁶⁶Ge.

description of both the even and odd Ge isotopes has not been reported previously.

The graph of spin J versus angular frequency $\omega(J) = [E(J) - E(J-2)]/2$ (we call it the " $J-\omega$ graph") is useful in seeing the variation of nuclear structure, because the moment of inertia $J/\omega(J)$ reflects the competition of various nuclear correlations. We illustrate the $J-\omega$ graph for the even-J positive-parity yrast states of ⁶⁶Ge, in Fig. 2. Our model reproduces well the variation of the experimental moments of inertia. The agreement with the experiment is better than that of the total Routhian surface (TRS) calculations [1]. This indicates that our wave functions are better than those of the TRS calculations. In Fig. 2, the $J-\omega$ graph displays a stable rotation in the ground-state (gs) band up to 8^+_1 and a sharp backbending toward 10^+_1 . The remarkable backbending from 8^+_1 to 10^+_1 indicates a structural change there. The straight line starting from the 14^+_1 state is also interesting.

To analyze the wave functions, we calculated expectation values of proton and neutron numbers in the four orbits for



FIG. 2. The $J-\omega$ graph for the positive-parity yrast states with even J of ⁶⁶Ge.



FIG. 3. Expectation values $\langle n_{g9/2}^{\nu} \rangle$ and $\langle n_{g9/2}^{\pi} \rangle$ in the upper panel, and $T_{g9/2}$ and $J_{g9/2}$ in the lower panel, for the yrast states (lines) and some other states (marks) of ⁶⁶Ge.

⁶⁶Ge. The results show that the nucleon-number expectation values $\langle n_a \rangle$ hardly change in the gs band up to 8^+_1 , which is consistent with the stable rotation expected from the $J-\omega$ graph. Above 8_1^+ , the most notable thing is characteristic changes in the numbers of protons and neutrons occupying the $g_{9/2}$ orbit, $\langle n_{g9/2}^{\pi} \rangle$ and $\langle n_{g9/2}^{\nu} \rangle$. We illustrate their variations for the yrast states and some other states in the upper panel of Fig. 3. In this figure, the neutron number in the $g_{9/2}$ orbit $(\langle n_{_{\rho}9/2}^{\nu}\rangle)$ increases abruptly at 10_1^+ . This change in the wave function explains the backbending of the experimental $J-\omega$ graph at 10^+_1 . However, the abrupt increase of $\langle n^{\nu}_{g9/2} \rangle$ is more remarkable in the 8^+_2 state, whereas the proton distribution to the four orbits remains almost the same as that in the states 0_1^+ to 8_1^+ . Since the expectation value $\langle n_{g9/2}^{\nu} \rangle$ is considered to be fractional at low energy, the value $\langle n_{g9/2}^{\nu} \rangle \approx 2$ (being about integer) in the 8^+_2 state suggests the alignment of two neutrons, $(g_{9/2}^{\nu})_{J=8,T=1}^2$. The large values of $\langle n_{g9/2}^{\nu} \rangle$ (~2)at 8_2^+ and 10_1^+ , and a strong E2 transition $10_1^+ \rightarrow 8_2^+$ in theory and experiment reveal a similar structure of the two states. The structural change from 8^+_1 to 10^+_1 is probably caused by the 2*n* alignment coupled to J=8, T=1 in the $g_{9/2}$ orbit. Figure 3 suggests a continuation from 8^+_2 to 10^+_1 . This situation can be called a "band crossing," where the 2n-aligned band crosses the gs band. The present explanation for the 8^+_1 and 8^+_2 states is in agreement with the assignment in the transfer reaction [6], the result in the IBM plus a pair treatment [9], and the discussion about the kinematic moment of inertia [1].

In Fig. 3, we can see a decrease of the neutron number $\langle n_{g9/2}^{\nu} \rangle$ and an increase of the proton number $\langle n_{g9/2}^{\pi} \rangle$ from 8_2^+ to 10_1^+ . The same trend is clear in the 12_1^+ state, and then the proton and neutron numbers become nearly equal to each other in the 14_1^+ state. The 14_1^+ , 16_1^+ , and 18_1^+ states keep nearly integral numbers $\langle n_{g9/2}^{\pi} \rangle \approx \langle n_{g9/2}^{\nu} \rangle \approx 1$. In our calculation for ⁶⁶As using the same Hamiltonian, we had also almost integral numbers $\langle n_{g9/2}^{\pi} \rangle \approx \langle n_{g9/2}^{\nu} \rangle \approx 1$ for the $J^{\pi} \ge 9^+$ states of the T=0 band. It is probable that ⁶⁶As has a T=0,



FIG. 4. Comparison of the calculated four bands with the experimental yrast states for 66 Ge.

J=9 aligned 1p1n pair in these states. Similarly, the nearly integral numbers $\langle n_{g9/2}^{\pi} \rangle \approx \langle n_{g9/2}^{\nu} \rangle \approx 1$ in ⁶⁶Ge are presumed to be the signature of the T=0, J=9 1p1n alignment at the 14⁺₁ states where the $J-\omega$ graph has a notable bend. Let us examine it by evaluating the expectation values of spin and isospin of nucleons in the $g_{9/2}$ orbit. The lower panel of Fig. 3 shows the values $J_{g9/2} = [\langle (\hat{j}_{g9/2})^2 \rangle + 1/4]^{1/2} - 1/2$ and $T_{g9/2}$ =[$\langle (\hat{t}_{g9/2})^2 \rangle$ +1/4]^{1/2}-1/2. This figure confirms our presumption, telling the following scenario: The two neutrons in the $g_{9/2}$ orbit outside the N=Z=32 central system align at the 8^+_2 state and produce the spin $J_{g9/2} \approx 8$ and the isospin $T_{g9/2} \approx 1$. During the competition between the J=8,T=1 2*n* pair and J=9,T=0 1p1n pair in the 10⁺₁ and 12⁺₁ states, the two nucleons in the $g_{9/2}$ orbit increase the spin and decrease the isospin. At last in the 14_1^+ state where $J_{g9/2} \approx 9$ and $T_{g9/2} \approx 0$, the J=9,T=0 1p1n pair overwhelms the J=8,T=1 2n pair. The superiority of the J=9,T=0 1p1n pair can be attributed to the condition that the T=0, J=9 pn interaction is stronger than the T=1, J=8 interaction (note that while the T=1, J=2j-1interaction is repulsive, the T=0, J=2j interaction is very attractive in ordinary effective interactions). If we set $\langle (g_{9/2})^2 | V | (g_{9/2})^2 : T = 0, J = 9 \rangle$ zero, the 1*p*1*n* aligned states do not become the yrast states, while the gs band is hardly disturbed.

To clarify the band crossing near J=12, we searched for the J=10 member of the 1p1n aligned band and the J=12member of the 2n aligned band in our calculations. Obtained candidates are 10_4^+ and 12_4^+ , for which the expectation values $\langle n_{g9/2}^{\pi} \rangle$, $\langle n_{g9/2}^{\nu} \rangle$, $J_{g9/2}$, and $T_{g9/2}$ are plotted in Fig. 3. Figure 3 indicates the band crossing between J=10 and J=12. The TRS calculations [1] suggested that the bend at 14_1^+ of the $J-\omega$ graph is caused by simultaneous alignment of 2p and 2n. However, the result presented above disagrees with this suggestion. As shown in Fig. 3, our model predicts that the simultaneous alignment of 2p and 2n takes place at the 18^+_2 state, and from 18^+_2 a band continues to the yrast states 20^+_1 , 22_1^+ , 24_1^+ , and 26_1^+ . Figure 3 shows that the 2p2n alignment in the $g_{9/2}$ orbit produces the spin $J_{g9/2} \approx 16$ and the isospin $T_{g9/2} \approx 0$, which indicates the aligned structure



FIG. 5. Comparison of the calculated four bands with the experimentally observed bands for ⁶⁸Ge.

 $[(g_{9/2}^{\mu})_{J=8,T=1}^{2}(g_{9/2}^{\nu})_{J=8,T=1}^{2}]_{J=16,T=0}$. The calculation yields the 20_{4}^{+} state as the J=20 member of the 1p1n aligned band. The third band crossing takes place between J=18 and J=20 in our model.

What conditions cause such a nearly pure 1p1n alignment? In Ref. [12], we investigated even-mass Ru isotopes around ⁹⁰Ru which is symmetrical to ⁶⁶Ge with respect to the particle-hole transformation in the $(p_{3/2}, f_{5/2}, p_{1/2}, g_{9/2})$ space. We did not find any sign of the T=0 1p1n alignment there, and could not see a pure 2n alignment at the backbending state 8^+_1 in ⁹⁰Ru. An important thing is that the Fermi level lies at the $g_{9/2}$ orbit itself in the Ru isotopes but considerably far from the $g_{9/2}$ orbit in the Ge isotopes. The appearance of the nearly pure 2n and 1p1n alignments in ⁶⁶Ge is based on the condition that the high-spin orbit $g_{9/2}$ is quite apart from the Fermi level and has the opposite parity to the pf shell. Only even-number nucleons are allowed to occupy the $g_{9/2}$ orbit after covering the cost of excitation energy from pf to $g_{9/2}$. We can expect the T=0 1p1n alignment in $N \approx Z$ eveneven nuclei near the Ge isotopes. It should be also noticed that the residual nucleons in the pf shell coupled with the aligned 1p1n pair with T=0, J=9 must have the isospin T =1 for the nucleus 66 Ge, while the residual nucleons coupled with the aligned 2n pair with T=1,J=8 can have the isospins T=0 and T=1. This is confirmed by calculating the isospin of nucleons in the pf shell. The different isospin couplings bring about different properties to the 1p1n and 2naligned bands. The problem is related to the competition between the T=1 and T=0 pair correlations in the central system which is represented by the *pf* shell in our shell model. We also calculated the spin of nucleons in the pf shell, " J_{pf} ." The calculated results indicate the approximate alignment of $J_{g9/2}$ and J_{pf} in the three aligned bands.

Thus, we have three bands which contain the three types of aligned nucleons in the $g_{9/2}$ orbit, in addition to the *gs* band, as shown in Fig. 4. The theoretical bands finely trace the experimentally observed footprints of the yrast states. The theory shows a slight deviation from the experiment near J=12, which suggests a stronger coupling between the 2n and 1p1n aligned bands.

Let us briefly discuss the structure of ⁶⁸Ge which has two more neutrons than ⁶⁶Ge. The present calculations show that the ⁶⁸Ge nucleus has the same structure in the $g_{9/2}$ orbit as that of ⁶⁶Ge. An important difference of ⁶⁸Ge from ⁶⁶Ge is the backbending at 8^+_1 in the $J-\omega$ graph. We obtained graphs similar to those of Fig. 3, which explain the band crossing at J=8 in terms of the 2n alignment in the $g_{9/2}$ orbit. The 2n aligned band starts from the 8_1^+ state, while the gs band continues to the 8^+_2 state. This explanation disagrees with the discussions in the particle-rotor model [3] and the VAMPIR calculation [5]. We do not have any sign of the two-proton alignment in our results for ⁶⁸Ge as well as ⁶⁶Ge. There is no significant difference above J=8 between ⁶⁸Ge and ⁶⁶Ge. Also in ⁶⁸Ge, we have the same three bands as those in ⁶⁶Ge, as shown in Fig. 5: the observed band on 8^+_1 corresponds to the 2n aligned band; the band on 12_4^+ to the 1p1n aligned band; the band on 18^+_2 to the 2p2n aligned band. The agreement between theory and experiment is good up to the 26^+_1 state where the 2p2n aligned band terminates. The theory has one deviation from the experiment with respect to the band PHYSICAL REVIEW C 70, 031301(R) (2004)

crossing at J=12. The 12_1^+ state is assigned as the continuation from 10_1^+ in the experiment [2], while the 12_1^+ state is the member of the 1p1n aligned band (mixed with the 12^+ state of the 2n aligned band) in our calculation. The slightly staggering curves in Fig. 5 show that the coupling between the different bands is stronger in ⁶⁸Ge than in ⁶⁶Ge. We close our discussions by pointing out that the prediction for the J>16states of ⁶⁶Ge in Fig. 4 is hopeful.

In conclusion, we have investigated the mechanism of angular momentum increase caused by the particle alignments, in the even-*J* positive-parity yrast states of ⁶⁶Ge and ⁶⁸Ge, using the reliable wave functions obtained by the successful shell model calculations. The investigation has revealed a new feature that the T=0 1p1n alignment in the $g_{9/2}$ orbit takes place at high spins $(14_1^+, 16_1^+ \text{ and } 18_1^+)$ in the $N \approx Z$ even-even Ge isotopes ⁶⁶Ge and ⁶⁸Ge. The three bands with different types of aligned nucleons in the $g_{9/2}$ orbit successively appear above the gs band as the spin increases, namely the 2n aligned band, the 1p1n aligned band and the 2p2n aligned band.

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