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 $(1p1n)$ alignment in the $g_{9/2}$ orbit, at high spins $(14^+_1, 16^+_1,$ 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 $26₁⁺$ for ⁶⁸Ge) consists of the ground-state band and successive three bands with different types of particle alignments (two-neutron, 1*p*1*n*, two-proton–twoneutron) 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 66 Ge [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 $T=0, J=2j$ has 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 $T=0$ 1p1*n* alignment at high-spin yrast states of the $N \approx Z$ even-even nuclei ⁶⁶Ge and 68Ge. This is a unique appearance of the *pn* pair correlations.

The experiments for 68 Ge and 66 Ge [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 66 Ge 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 66 Ge and 68 Ge 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 64 Ge 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 ${}^{66}As$) 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 octupoleoctupole forces are $g_0 = 0.262$, $g_2 = 0.0$, $\chi_2 = 0.238$, and χ_3 =0.047 in MeV. The monopole corrections are $H_{mc}^{T=1}(p_{3/2}, f_{5/2}) = -0.3$, $H_{mc}^{T=1}(p_{3/2}, p_{1/2}) = -0.3$, $H_{mc}^{T=1}(f_{5/2}, p_{1/2})$ $T_{mc}^{T=0}(g_{9/2}, g_{9/2}) = -0.2$, and $H_{mc}^{T=0}(g_{9/2}, g_{9/2}) = -0.1$ in MeV.

In Fig. 1 we compare energy levels obtained for 66 Ge 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 68 Ge (which are more than twice as many as those of 66 Ge) and also satisfactorily describes energy levels observed in the odd-mass isotopes 65 Ge and 67 Ge. 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*−ω 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 $8₁²$ and a sharp backbending toward $10₁⁺$. The remarkable backbending from $8₁⁺$ to $10₁⁺$ indicates a structural change there. The straight line starting from the $14₁⁺$ 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 66 Ge.

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 $(\langle n_{g9/2}^{\nu} \rangle)$ increases abruptly at 10⁺₁. This change in the wave function explains the backbending of the experimental $J-\omega$ graph at $10^{\frac{1}{1}}$. However, the abrupt increase of $\langle n_{g9/2}^{\nu} \rangle$ 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^{\pm}_2 and 10_1^+ , and a strong *E*2 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 2*n*-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 $10₁⁺$. The same trend is clear in the $12₁⁺$ state, and then the proton and neutron numbers become nearly equal to each other in the $14₁⁺$ state. The $14₁⁺$, $16₁⁺$, and $18₁⁺$ 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 $J^{\pi} \geq 9^+$ 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 ⁶⁶Ge.

 $J=9$ 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 $T=0, J=9$ 1p1*n* alignment at the 14⁺ states where the *J*− ω 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 $J=9, T=0$ 1*p*1*n* pair in the 10⁺ and 12⁺ states, the two nucleons in the $g_{9/2}$ orbit increase the spin and decrease the isospin. At last in the 14^{\dagger}_{1} state where $\hat{J}_{g9/2} \approx 9$ and $T_{g9/2} \approx 0$, the *J*=9,*T*=0 1*p*1*n* pair overwhelms the *J*=8,*T*=1 2*n* pair. The superiority of the $J=9$, $T=0$ 1*p*1*n* 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 $T=1, J=2j-1$ interaction 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 $J=12$ member of the 2*n* 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*−ω graph is caused by simultaneous alignment of 2*p* and 2*n*. 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 $18^{\frac{1}{2}}$ state, and from 18^{\dagger}_{2} a band continues to the yrast states 20^{\dagger}_{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.

 $[(g_{9/2}^{\pi})_{J=8,T=1}^2 (g_{9/2}^{\nu})_{J=8,T=1}^2]_{J=16,T=0}$. 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 1*p*1*n* 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 $T=0$ 1p1*n* alignment there, and could not see a pure 2*n* alignment at the backbending state 8_1^+ in 90 Ru. 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 1*p*1*n* 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 ⁶⁶Ge, while the residual nucleons coupled with the aligned 2*n* 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 1*p*1*n* and 2*n* aligned 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 2*n* and 1*p*1*n* aligned bands.

Let us briefly discuss the structure of 68 Ge 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 66 Ge. An important difference of 68 Ge from 66 Ge is the backbending at $8⁺₁$ in the *J*− ω graph. We obtained graphs similar to those of Fig. 3, which explain the band crossing at $J=8$ in terms of the 2*n* alignment in the $g_{9/2}$ orbit. The 2*n* aligned band starts from the $8₁⁺$ 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 68 Ge as well as 66 Ge. There is no significant difference above $J=8$ between ⁶⁸Ge and ⁶⁶Ge. Also in 68 Ge, we have the same three bands as those in 66 Ge, as shown in Fig. 5: the observed band on 8^+_1 corresponds to the 2*n* aligned band; the band on 12^+_4 to the 1*p1n* aligned band; the band on 18°_2 to the $2p2n$ aligned band. The agreement between theory and experiment is good up to the $26₁⁺$ state where the 2*p*2*n* aligned band terminates. The theory has one deviation from the experiment with respect to the band

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crossing at $J=12$. The $12₁⁺$ state is assigned as the continuation from $10₁⁺$ in the experiment [2], while the $12₁⁺$ state is the member of the $1p1n$ aligned band (mixed with the 12^+ state of the 2*n* aligned band) in our calculation. The slightly staggering curves in Fig. 5 show that the coupling between the different bands is stronger in 68 Ge than in 66 Ge. We close our discussions by pointing out that the prediction for the *J*.16 states 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 66 Ge and 68 Ge, using the reliable wave functions obtained by the successful shell model calculations. The investigation has revealed a new feature that the $T=0$ 1p1*n* alignment in the $g_{9/2}$ orbit takes place at high spins $(14^+_1, 16^+_1, 18^+_1)$ 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 2*n* aligned band, the 1*p*1*n* aligned band and the 2*p*2*n* aligned band.

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