Proton-neutron alignment in the yrast states of $^{66}$Ge and $^{68}$Ge

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The $^{66}$Ge and $^{68}$Ge 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 $18^+_2$) 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 $^{66}$Ge) consists of the ground-state band and successive three bands with different types of particle alignments (two-neutron, $1p1n$, 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 $^{66}$Ge [1] and $^{68}$Ge [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 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 $T = 0$ $1p1n$ alignment at high-spin yrast states of the $N \approx Z$ even-even nuclei $^{66}$Ge and $^{68}$Ge. This is a unique appearance of the $pn$ pair correlations.

The new experiments for $^{66}$Ge and $^{68}$Ge [1, 2] have found several bands with positive and negative parities up to high spins ($J \leq 28$). The new 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 $^{68}$Ge and $^{66}$Ge has been discussed by several authors [3, 4, 5, 6, 7, 8]. 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 $^{64}$Ge. 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. [11]. 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 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 $H_{mc}^{T=1}(p_{3/2}, f_{5/2}) = -0.3$, $H_{mc}^{T=1}(p_{3/2}, p_{1/2}) = -0.3$, $H_{mc}^{T=1}(f_{5/2}, p_{1/2}) = -0.4$, $H_{mc}^{T=0}(g_{9/2}, g_{9/2}) = -0.2$ 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 $^{66}$Ge. 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 $^{70}$Ge. Such a consistent 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 “$J - \omega$ 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 $^{66}$Ge, 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 $^{66}$Ge. The results show that the nucleon-number expectation values $\langle n_\nu \rangle$ 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, $\langle n_{9/2}^g \rangle$ and $\langle n_{9/2}^\pi \rangle$. 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 $\langle n_{9/2}^\pi \rangle$ 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 $\langle n_{9/2}^g \rangle$ is more remarkable in the $8^+_2$ state, whereas

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**FIG. 1:** Experimental and calculated energy levels of $^{66}$Ge.

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

**FIG. 3:** The expectation values $\langle n_{9/2}^g \rangle$ and $\langle n_{9/2}^\pi \rangle$ in the upper panel, and $T_{9/2}$ and $J_{9/2}$ in the lower panel, for the yrast states (lines) and some other states (marks) of $^{66}$Ge.
the proton distribution to the four orbits remains almost the same as that in the states $0^+_1$ to $8^+_2$. Since the expectation value $\langle n'_{g9/2} \rangle$ is considered to be fractional at low energy, the value $\langle n'_{g9/2} \rangle \approx 2$ (being about integer) in the $8^+_2$ state suggests the alignment of two neutrons, $(g_{9/2})_j=8, T=1$. The large values of $\langle n'_{g9/2} \rangle \approx 2$ 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 $8^+_2$ to $10^+_1$ is probably caused by the $2n$ 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 $8^+_2$ and $8^+_1$ states is in agreement with the assignment in the transfer reaction, the result in the IBM plus a pair treatment, and the discussion about the kinematic moment of inertia.

In Fig. 3, we can see a decrease of the neutron number $\langle n_{g9/2} \rangle$ and an increase of the proton number $\langle n'_{g9/2} \rangle$ from $8^+_2$ to $10^+_1$. The same trend is clear in the $12^+_2$ 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 $\langle n_{g9/2} \rangle \approx \langle n'_{g9/2} \rangle \approx 1$. In our calculation for $^{66}$As using the same Hamiltonian, we had also almost integral numbers $\langle n_{g9/2} \rangle \approx \langle n'_{g9/2} \rangle \approx 1$ for the $J^x > 9^+$ states of the $T = 0$ band. It is probable that $^{66}$As has a $T = 0$, $J = 9$ aligned $1p1n$ pair in these states. Similarly, the nearly integral numbers $\langle n_{g9/2} \rangle \approx \langle n'_{g9/2} \rangle \approx 1$ in $^{66}$Ge 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 $J_{g9/2} = \frac{1}{2}(\langle (\hat{s}_{g9/2})^2 \rangle + 1/4)^{1/2} - 1/2$ and $T_{g9/2} = \frac{1}{2}(\langle (\hat{t}_{g9/2})^2 \rangle + 1/4)^{1/2} - 1/2$. 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 the spin $J_{g9/2} \approx 8$ and the isospin $T_{g9/2} \approx 1$. During the competition between the $J = 8, T = 1 2n$ 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 $T = 0$, $J = 9$ $pm$ 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 $\langle (g_{9/2})_j^2 \rangle : T = 0, J = 9$ zero, the $1p1n$ 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 $2n$ aligned band in our calculations. Obtained candidates are $10^+_2$ and $12^+_4$, for which the expectation values $\langle n_{g9/2} \rangle$, $\langle n'_{g9/2} \rangle$, $J$ and $T$ are plotted in Fig. 4. Figure 4 indicates the band crossing between $J = 10$ and $J = 12$. The TRS calculations suggested that the band at $14^+_2$ 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 4 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 $\langle (g_{9/2})_j^2 \rangle : T = 0, J = 16, T = 0$. The calculation yields the $20^+_1$ 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. 18, we investigated even-mass Ru isotopes around $^{90}$Ru which is symmetrical to $^{66}$Ge 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 $8^+_2$ 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 $^{66}$Ge 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 $N \approx Z$ even-even 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 2n 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 $g9/2$ 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 $^{68}$Ge which has two more neutrons than $^{66}$Ge. The present calculations show that the $^{68}$Ge nucleus has the same structure in the $g9/2$ orbit as that of $^{66}$Ge. An important difference of $^{68}$Ge from $^{66}$Ge is the backbending at $8^+$ 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 $g9/2$ orbit. The 2n aligned band starts from the $8^+$ state, while the $gs$ band continues to the $8^+_2$ state. This explanation disagrees with the discussions in the particle-rotor model [2] and the VAMPIR calculation [3]. 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 $^{68}$Ge and $^{66}$Ge. 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 2n aligned band; the band on $12^+_1$ to the 1p1n aligned band; the band on $18^+_1$ 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 crossing at $J = 12$. The $12^+_2$ state is assigned as the continuation from $10^+_2$ in the experiment [2], while the $12^+_1$ state is the member of the 1p1n aligned band (mixed with the $12^+_2$ 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 $^{68}$Ge than in $^{66}$Ge. We close our discussions by pointing out that the prediction for the $J > 16$ states of $^{68}$Ge in Fig. 5 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 $T = 0$ 1p1n alignment in the $g9/2$ orbit takes place at high spins ($14^+_1$, $16^+_1$ and $18^+_1$) in the $N = Z$ even-even Ge isotopes $^{66}$Ge and $^{68}$Ge. The three bands with different types of aligned nucleons in the $g9/2$ 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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