Competition between isoscalar and isovector pairing correlations in $N = Z$ nuclei

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We study the isoscalar ($T = 0$) and isovector ($T = 1$) pairing correlations in $N = Z$ nuclei. They are estimated from the double difference of binding energies for odd-odd $N = Z$ nuclei and the odd-even mass difference for the neighboring odd-mass nuclei, respectively. The empirical and BCS calculations based on a $T = 0$ and $T = 1$ pairing model reproduce well the almost degeneracy of the lowest $T = 0$ and $T = 1$ states over a wide range of even-even and odd-odd $N = Z$ nuclei. It is shown that this degeneracy is attributed to competition between the isoscalar and isovector pairing correlations in $N = Z$ nuclei. The calculations give an interesting prediction that the odd-odd $N = Z$ nucleus $^{82}$Nb has possibly the ground state with $T = 0$.

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There is a current topic with increasing interests in studying isovector ($T = 1$) and isoscalar ($T = 0$) proton-neutron (pn) pairing correlations in $N = Z$ nuclei. At present, it is not clear whether pn pairing correlations are strong enough to form a static condensate. It is well known that an experimental signature of like-nucleon proton-proton (pp) and neutron-neutron (nn) $J = 0$ pairing correlations in nuclei with neutron excess is the odd-even mass difference, which is extra binding energy of even-even nuclei relative to that of odd-mass nuclei. However, the odd-even mass differences for even-even $N = Z$ nuclei are larger than those of the neighboring even-even $N = Z + 2$ nuclei, and it reflects the gain in pairing due to stronger pn correlations. It has recently been shown that the three-point odd-even mass difference for an odd-mass nucleus with neutron excess is an excellent measure of pp and nn pairing correlations in neighboring even-even nuclei, although it is still controversial. This conclusion suggests that the pp and nn pairing correlations in $N = Z$ even-even nuclei also can be estimated from the odd-even mass difference of neighboring odd-mass nuclei with $N = Z + 1$. On the other hand, the pn pairing can be estimated from the double difference of binding energies. When we assume isospin symmetry in $N \approx Z$ nuclei, the $T = 1$ pn pairing and like-nucleon (pp and nn) pairing are classified in the same $T = 1$ pairing correlations, and the former correlation energy should be the same as the latter one.

Odd-odd $N = Z$ nuclei are an ideal experimental laboratory for the study of pn pairing correlations. It is well known that the lowest $T = 0$ and $T = 1$ states in odd-odd $N = Z$ nuclei are almost degenerate and exhibit the inversion of the sign of the energy difference $E_{T=1} - E_{T=0}$, while all even-even $N = Z$ nuclei have the $T = 0$ ground states and the $T = 1$ excited states with large excitation energies. Several authors already pointed out that this degeneracy in odd-odd $N = Z$ nuclei reflects the delicate balance between the symmetry energy and the pairing correlations. The $T = 0$ and $T = 1$ ground-state binding energies of $N = Z$ nuclei were calculated by using an algebraic model based on IBM-4. In this paper, we study the $T = 0$ and $T = 1$ pairing correlations from a phenomenological point of view, and analyze them in the BCS calculations within a schematic model that includes $T = 1$ and $T = 0$ pairing interactions.

We begin with the estimation of $T = 1$ pairing correlations in $N = Z$ nuclei. A typical indicator for $T = 1$ pairing correlations is the following three-point odd-even mass difference:

$$\Delta^{(3)}_{n}(Z, N) = \frac{(-1)^{N}}{2}[B(Z, N + 1) - 2B(Z, N) + B(Z, N - 1)],$$

where $B(Z, N)$ is the negative binding energy of a system. Since $B(Z, N \pm 1) \approx B(Z, N) + \Delta \pm \lambda$ based on standard BCS theory with pairing gap $\Delta$, the indicator $\Delta^{(3)}_{n}$ is often interpreted as a measure of the empirical pairing gap. However, it is well known that values of $\Delta^{(3)}_{n}(Z = \text{even}, N)$ are large for even-$N$ and small for odd-$N$. It was discussed that $\Delta^{(3)}_{n}(Z = \text{even}, N = \text{odd})$ is an excellent measure of $T = 1$ pairing correlations, and the differences of $\Delta^{(3)}_{n}$ at adjacent even- and odd-$N$ nuclei reflect the mean-field contributions. From a view point of the semi-empirical mass formula, the above indicator is well known to be affected by the symmetry energy term in the liquid-drop model. In the macroscopic-microscopic shell model, however, the curvature contribution cancels out the symmetry energy contribution as pointed out by Satultra et al. [3]. What does the magnitude of the pairing gap in the $N = Z$ nuclei mean? We suggest that $\Delta^{(3)}_{n}(Z, Z + 1)$ of odd-mass nucleus should be regarded as pure pairing gap in $N = Z$ adjacent even-even and odd-odd nuclei. For the $N = Z$ nuclei, the four and
five point indicators cannot be adopted because they include large contributions from mean filed and pn correlations \cite{2 3}. Figure 1 shows experimental values of $\Delta_n^{(3)}$ in odd-mass nuclei, where we plot $\Delta_n^{(3)}(Z, Z + 1)$ for $16 < A < 60$. When there is no data of $\Delta_n^{(3)}(Z, Z + 1)$ for $60 < A < 110$, we adopt $\Delta_n^{(3)}$ for nearest nuclei with $N = Z + 1$. The expected quenching of neutron pairing at magic (or semi-magic) particle number $N$ or $Z = 14, 28, 40,$ and $50$ is clearly seen in the figure. The standard curve $12A^{-1/2}$ is also shown as a guide eye in Fig. 1. We can see that the average pairing gap is smaller than the values of the curve $12A^{-1/2}$. The global trend can be fitted by the curve $5.18A^{-1/3}$ MeV, as discussed in recent analyses \cite{11 13}, where $T = 1$ pairing gap $\Delta_{T=1}$ obtained from some binding energy difference is fitted by the mass-dependence $A^{-1/3}$ different from the standard one $12A^{-1/2}$. The difference between the two curves is quite large for light nuclei, while it is small for heavy nuclei. The average gap was recently analyzed \cite{14} by $\Delta = \alpha + \beta A^{-1/3}$ which has theoretical foundation. This analysis also supports the weaker mass-dependence. We now consider the following pairing Hamiltonian to describe the $T = 1$ pairing correlations:

$$H = H_0 + H_P = \sum_\alpha \varepsilon_\alpha c_\alpha^\dagger c_\alpha - \frac{1}{2} G \sum_\kappa P_\kappa^\dagger P_\kappa,$$  \hspace{1cm} (2)

where $\varepsilon_\alpha$ is the single-particle energy and $P_\kappa$ is the $J = 0$ pair operator with isospin $T = 1, T_z = \kappa$. Implying isospin invariance to the above Hamiltonian, the pairing part $H_P$ includes the isovector pn interactions. The standard BCS calculations with the pairing Hamiltonian \cite{2} were performed in $sd$ and $fp$g shells. We adopted single-particle energies from a spherical Woods-Saxon potential in the BCS calculations. The pairing force strength $G = 24.5/A$ was chosen so as to fit the experimental odd-even mass difference $\Delta_n^{(3)}(Z = \text{even}, Z + 1)$ in odd-mass nuclei. The BCS results for $A > 40$ almost agree with the experimental odd-even mass differences, and moreover reproduce the shell effects. The BCS calculations reproduce well the behavior of the observed odd-even mass difference over a wide range of $N = Z$ nuclei. Thus the $T = 1$ pairing correlations can be estimated from the odd-even mass difference $\Delta_n^{(3)}(Z = \text{even}, Z + 1)$ in odd-mass nuclei.

To describe the $pn$ pairing correlations in odd-odd $N = Z$ nuclei, let us estimate the following double difference of binding energies \cite{2 13 16}:

$$\Delta_{pn}^T(Z, N) = \frac{1}{2} [B(Z, N)^T - B(Z, N - 1) - B(Z - 1, N) + B(Z - 1, N - 1)], \hspace{1cm} (3)$$

where $B(Z, N)^T$ is the binding energy of lowest state with isospin $T$ in odd-odd $N = Z$ nuclei. Figure 2 shows the double difference of binding energies calculated from the experimental binding energies. The odd-even mass differences for odd-mass nuclei are also displayed. Then we can see that the $\Delta_n^{(3)}(Z, Z + 1)$ agrees with the $\Delta_{pn}^{T=1}(Z + 1, Z + 1)$. This means that $T = 1$ pn pairing
for odd-odd $N = Z$ nuclei have the same correlation energy as the like-nucleon $nn$ pairing, $\Delta_n = \Delta_{pn}^{T=1}$, when assuming isospin symmetry. Thus, the indicator $\Delta_{pn}^{T=1}$ gives the $T = 1$ $pn$ pairing gap in $N = Z$ nuclei. The $\Delta_{pn}^{T=0}$ can be regarded as the $T = 0$ $pn$ pairing gap as well. Figure 2 with these estimations indicates that the $T = 0$ $pn$ correlations are superior to the $T = 1$ $pn$ correlations in the ground states of $sd$ shell nuclei, and the inversion occurs in the $pf$ shell nuclei. The $T = 0$ $pn$ pairing gap $\Delta_{p0}^{T=0}$ cannot be explained by the $T = 1$ pairing Hamiltonian.\(^2\)

In a previous paper \(^2\), it has been shown that the $T = 0$ matrix elements of the monopole field $V_{mn}^{T=0}(a,b)$ are significantly larger than the $T = 1$ ones, and are very important in determining the double differences of binding energies, where $a,b$ are the single particle orbitals. We can see that the matrix elements are quite large for isoscalar components but small for isovector components. In the USD interaction, the monopole matrix elements with $T = 0$ have values around -3 MeV and are strongly attractive. If we assume that the $T = 0$ monopole matrix elements are equal and independent of angular momentum $J$ and the single particle orbitals, $V_{mn}^{T=0}$ is reduced to the $J$-independent isoscalar $p-n$ pairing interaction. Neglecting $T = 1$ monopole components, let us add the $J$-independent $T = 0$ $pn$ pairing interaction \(^2,17\) to the pairing Hamiltonian \(^2\)

$$H = H_0 + H_P + H_{T=0}^{T=0}$$

$$= H_0 + H_P - k^0 \sum_{a \neq b} A_{J,M,00}^{\dagger}(ab)A_{J,M,00}(ab)$$

where $A_{J,M,00}^{\dagger}(ab)$ is the pair operator with spin $J$ and isospin $T = 0$. The $T = 1$ pairing interaction does not contribute to the double difference of binding energies $\Delta_{T=0}^{T=0}$, and $\Delta_{T=0}^{T=0} \approx k^0/2$. Then, the $T = 0$ pairing force strength $k^0 = 244.5(1 - 1.67A^{-1/3})/A$ is chosen so as to fit the $T = 0$ $pn$ pairing gap as seen in Fig. 2. The isovector monopole components in USD are small, except for $V_{mn}^{T=1}(s_{1/2},s_{1/2})$. The deviations from the curve $k^0/2$ for $^{30}$P and $^{34}$Cl in Fig. 2 would be attributed to the large value of isovector component $V_{mn}^{T=1}(s_{1/2},s_{1/2})$. We recently introduced \(^17\) monopole corrections to improve the energy levels of $^{48}$Ca, etc. In this paper, we ignore these correction terms.

If we assume degenerate single-particle energies $\varepsilon_n = 0.0$, the above Hamiltonian has SO(5) symmetry \(^18\) and the eigenenergy is assigned by the valence nucleon number $n$ and isospin $T$ \(^2\),

$$\langle H_{P_{0}} + H_{T=0}^{T=0} \rangle_{SO(5)} = \frac{1}{2} G n \left( \frac{(n - 6)}{4} \right)$$

$$- \frac{k^0}{2} \frac{n(n + 2)}{2} + \frac{1}{2} (G + k^0) T(T + 1),$$

(5)

where $\Omega = \sum_{\alpha_n}$ is the degeneracy of shell orbits. Note that the above equation includes the so-called symmetry energy term with coefficient $a(A)/A = (G + k^0)/2$. The parameters $G$ and $k^0$ used above give just the empirical symmetry energy formula $a(A) = 134.4(1 - 1.52A^{-1/3})$ determined by Door and Zuker \(^13\).

We next consider energy difference between the lowest $T = 0$ and $T = 1$ states in odd-odd $N = Z$ nuclei. Odd-odd $N = Z$ nuclei with $A < 40$ have the ground states with $T = 0, J > 0$ except for $^{34}$Cl, while the ground states of odd-odd $N = Z$ nuclei with $40 < A < 74$ are $T = 1$ and $J = 0$ except for $^{58}$Cu. Several authors discussed that this degeneracy is attributed to the delicate balance between the symmetry energy and pairing correlations, and that the energy difference between $T = 1$ and $T = 0$ states is well reproduced by $E_{T=1} - E_{T=0} = 2a(A)/A - 2\Delta_{T=1}$ using the value $\sim 75$ for $a(A)$ and the pairing gap $\Delta_{T=1} = 12A^{-1/2}$. However, if we substitute the odd-even mass difference $\Delta_{n}^{(3)}(Z = \text{even}, Z + 1)$ for $\Delta_{T=1}$, the energy difference $E_{T=1} - E_{T=0}$ becomes larger than the experimental value. The energy difference can be regarded as a measure of competition between the $T = 0$ and $T = 1$ pairing correlations as seen from the following identity,

$$E_{T=1} - E_{T=0} = 2(\Delta_{pn}^{T=0} - \Delta_{pn}^{T=1}).$$

(6)

The relationships $\Delta_{pn}^{T=0} \approx k^0/2$ and $\Delta_{pn}^{T=1} \approx \Delta_{n}^{(3)}$ offer an alternative relation $E_{T=1} - E_{T=0} \approx k^0 - 2\Delta_{n}^{(3)}$ for the energy difference except for $^{30}$P and $^{34}$Cl. If we adopt the parameter $k^0 = 244.5(1 - 1.67A^{-1/3})/A$ and the average value of pairing gap $5.18A^{-1/3}$ for $\Delta_{n}^{(3)}$, we get the dashed curve in Fig.3, which displays well the trend of the experimental values of energy difference $E_{T=1} - E_{T=0}$. Adopting the experimental odd-even mass

\[ \begin{array}{c|c|c}
\text{Symbols} & \text{Values} \\
\hline
G & 134.4 \\
\hline
k^0 & 244.5 \\
\hline
\end{array} \]

\[ \begin{array}{c|c|c}
\text{Parameters} & \text{Units} \\
\hline
a(A) & \text{MeV} \\
\Delta_{T=1} & \text{MeV} \\
\Delta_{n}^{(3)} & \text{MeV} \\
\hline
\end{array} \]
the ground state with $N$ though there are no experimental data of the energy differences for odd-odd $N = Z$ nuclei. The solid diamonds are the same as Fig. 3. The open circles denote the energy differences obtained by the BCS calculations. The dashed curve is $2a(A)/A$.

The energy differences for $\Delta_n^{(3)}$ and $k^0 = 244.5(1 - 1.67A^{-1/3})/A$, we obtain the energy difference $E_{T=1} - E_{T=0}$ denoted by the open squares. These values nicely reproduce the experimental values except for $^{30}\text{P}$ and $^{34}\text{Cl}$ as shown in Fig. 3. The disagreements in $^{30}\text{P}$ and $^{34}\text{Cl}$ are attributed to the large deviations of $T = 0$ pairing gap from the curve $k^0/2$ due to the neglect of the shell effects in Fig. 2.

Moreover, we calculated the $T = 0$ and $T = 1$ energy differences for odd-odd $N = Z$ nuclei with $A \geq 78$, although there are no experimental data of the energy difference. The calculation predicts that $^{82}\text{Nb}$ has possibly the ground state with $T = 0$, while the other odd-odd $N = Z$ nuclei have the $T = 1$ ground state. We call this isospin inversion hereafter. It is well known that a similar isospin inversion occurs at $^{58}\text{Cu}$. The isospin inversion is due to characteristic situation, where the Fermi energy lies between large spin and small spin orbits with large energy gap i.e., $1f_{7/2}$ and $2p_{3/2}$ for $^{58}\text{Cu}$, and $1g_{9/2}$ and $2p_{1/2}$ for $^{82}\text{Nb}$. In these cases, the $T = 1$ pairing gap is quite small as seen in Fig. 1, and energy difference becomes large from the simple relation $E_{T=1} - E_{T=0} \approx k^0 - 2\Delta_n^{(3)}(Z = \text{even}, Z + 1)$.

Figure 4 shows the calculated energy differences $E_{T=1} - E_{T=0}$ in odd-odd and even-even $N = Z$ nuclei. The energy differences in the BCS approximations are calculated by $2a(A)/A + \Delta_{BCS}$ for even-even $N = Z$ nuclei and by $k^0 - 2\Delta_{BCS}$ for odd-odd $N = Z$ nuclei where $a(A)$ is the empirical symmetry energy coefficient and $\Delta_{BCS}$ is the BCS pairing gap. The BCS calculations well reproduce the experimental values of energy differences, except for odd-odd $N = Z$ nuclei with $A < 40$.

The BCS calculations show that the $T = 0$ and $T = 1$ states in $^{82}\text{Nb}$ are almost degenerate, while the ground states of adjacent odd-odd $N = Z$ nuclei have isospin $T = 1$.

In conclusion, we investigated the $T = 0$ and $T = 1$ pairing correlations in $N = Z$ nuclei. The $T = 1$ pairing correlations in $N = Z$ nuclei are extracted from the odd-even mass differences of the neighboring odd-mass nuclei, which can be fitted by the curve $5.18A^{-1/3}$. The $pn$ pairing correlations are estimated from the double difference of binding energies. The $T = 1$ $pn$ pairing gap is the same as the $nn$ pairing gap. The indicator $\Delta_{pn}^{T=0}$ presents the magnitude of $T = 0$ $pn$ pairing correlations. The energy differences between the $T = 0$ and $T = 1$ states are well described by the $T = 1$ and $T = 0$ pairing model. In odd-odd $N = Z$ nuclei, the $T = 1$ pairing correlations compete with the $T = 0$ pairing correlations, and the degeneracy of the $T = 0$ and $T = 1$ states occurs. The empirical values and BCS results reproduced the energy difference. In particular, our results predict that odd-odd $N = Z$ nucleus $^{82}\text{Nb}$ has the $T = 0$ ground state or the $T = 0$ and $T = 1$ states are almost degenerate. The odd-even mass differences for even-even $N = Z$ nuclei are extremely larger than those of the neighboring even-even $N \neq Z$ nuclei. It would be affected by strong $pn$ correlations. Further studies in this direction are in progress.

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