Microscopic analysis of $T = 1$ and $T = 0$ proton-neutron correlations in $N = Z$ nuclei

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Abstract

The competition between the isovector ($T = 1$) and isoscalar ($T = 0$) proton-neutron ($p - n$) correlations in $N = Z$ nuclei is investigated by calculating their correlation energies with a realistic effective interaction which reproduces observed nuclear properties very well, in a strict shell model treatment. It is shown in the realistic shell model that the double-differences of binding energies ($B(A + pm : T) + B(A) - B(A + p) - B(A + n)$) ($B(A)$ being the binding energy) are good indicators of the $T = 1$ and $T = 0$ $p - n$ correlations. Each of them, however, originates in plural kinds of correlations with $T = 1$ or $T = 0$.

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1 Introduction

The competition between isovector ($T = 1$) and isoscalar ($T = 0$) pairing correlations has been a matter of renewed concern in nuclear structure studies of $N \approx Z$ nuclei [1,2,3]. The competition appears in the near degeneracy of the lowest $T = 1$ and $T = 0$ states in odd-odd $N = Z$ nuclei. The $T = 0$ proton-neutron ($p - n$) pairing correlations in $N \approx Z$ nuclei have been studied by the two approaches [2,3] with different treatments of the symmetry energy. The two conclusions about the importance of the $T = 0$ $p - n$ pairing correlations are in opposition to one another. The $T = 1$ and $T = 0$ pairing correlations, which are considered to be induced by $T = 1$ and $T = 0$ nuclear interactions, should be treated consistently on the same footing [3]. The structure of $N = Z$ nuclei has been well described by the shell model which does treat $T = 1$ and $T = 0$ pairing consistently. Large-scale shell model calculations were applied to the investigation of the isovector and isoscalar pairing correlations in Refs. [4,5,6], where the contributions of $T = 1$, $J = 0$ and $T = 0$, $J = 1$ interactions are compared [4] and the contributions of the quadrupole-quadrupole ($QQ$)
force are also considered [5]. The authors have recently shown that the competition between the $T = 1$ and $T = 0$ pairing correlations are approximately explained with the $T = 1$, $J = 0$ pairing force ($P_0$) and a $T = 0$ $p-n$ force ($V_{mp}^{T=0}$ below) [7]. In order to understand the competition in detail, it is important to evaluate the two types of correlations induced by realistic effective interactions.

In this paper, we investigate the competition between $T = 1$ and $T = 0$ $p-n$ correlations in the lowest states of $N = Z$ nuclei using a realistic effective interaction in a strict shell model treatment. The spherical shell model, which gives an excellent description of various properties of $N \approx Z$ nuclei (not only the binding energies but also other properties), has the advantage that the correlation energies of respective interactions are properly calculated. A shell model Hamiltonian is composed of the $T = 0$ and $T = 1$ interactions,

\[ H = H_{sp} + V_{T=0} + V_{T=1}, \]

\[ V_T = \sum_{a \leq b} \sum_{c \leq d} G_{JT}(ab : cd) A_{JMTK}^\dagger(ab) A_{JMTK}(cd) \quad (T = 0, 1), \]

where $H_{sp}$ stands for the single-particle energies, $A_{JMTK}^\dagger(ab)$ is the creation operator of a nucleon pair with the spin $JM$ and the isospin $TK$ in the single-particle orbits $(a,b)$, and $G_{JT}(ab : cd)$ denotes the interaction matrix elements. The so-called realistic effective interactions contain multipole ($J \geq 0$) pairing forces of $T = 0$ and $T = 1$ in the expression (2). In this sense, the shell model with a realistic effective interaction is to deal with all the multipole pairing correlations. We investigate the competition between the $T = 0$ and $T = 1$ correlations induced by the $T = 0$ and $T = 1$ interactions.

The realistic effective interactions have the property that the centroid of $T = 0$ diagonal interaction matrix elements \( G_{T=0}(ab) = \sum_J (2J + 1) G_{J0}(ab : ab) / \sum_J (2J + 1) \) has a roughly constant value, being independent on the orbits $(ab)$ [8]. By setting \(-k_0 = \sum_{ab} G_{T=0}(ab) / \sum_{ab} \), we obtain the average $T = 0$ $p-n$ force

\[ V_{mp}^{T=0} = -k_0 \sum_{a \leq b} A_{JM00}^\dagger(ab) A_{JM00}(ab). \]

Let us write residual $T = 0$ interactions as $V_{res}^{T=0} = V_{T=0} - V_{mp}^{T=0}$ and rewrite the Hamiltonian as

\[ H = H_{sp} + V_{mp}^{T=0} + V_{res}^{T=0} + V_{T=1}. \]

The separation of $V_{mp}^{T=0}$ in Eq. (4) follows the procedure of Dufour and Zuker in Ref. [9], where the Hamiltonian is divided into the monopole and multi-
pole parts as $H = H_m + H_M$. The monopole field $V_{mp}^{T=0}$ is exactly written as $-(k^0/2)\{\hat{n}_v/2(\hat{n}_v/2 + 1) - \hat{T}(\hat{T} + 1)\}$, where $\hat{n}_v$ stands for the number of valence nucleons and $\hat{T}$ stands for the total isospin. This equation shows that the force $V_{mp}^{T=0}$ which yields only energy gain depending on $n_v$ and $T$ is completely irrelevant to wave-functions, even to whether the nucleus is spherical or deformed, and configuration mixing is caused by $V_{res}^{T=0}$ and $V^{T=1}$. The force strength $k^0$ extracted from the realistic effective interaction USD [10] is, for instance, 2.8 MeV for $^{22}$Na. We know that $V_{mp}^{T=0}$ makes a large contribution to the binding energy and gives a bonus 2.8 MeV to the $T = 0$ states against the $T = 1$ states in $^{22}$Na. In this paper, we do not separate the $T = 1$ monopole field which is much smaller than the $T = 0$ one (we shall mention another reason for it later). We analyze roles of the three interactions $V_{mp}^{T=0}$, $V_{res}^{T=0}$ and $V^{T=1}$ in the competition between the $T = 0$ and $T = 1$ correlations.

2 Indicators of $T = 0$ and $T = 1$ $p-n$ correlations

It is well known that the even-even $N = Z$ nuclei are more deeply bound than the $T = 1$, 0$^+$ states of neighboring nuclei. The difference in mass between the nuclei with mass number $A = m\alpha$ and $A = m\alpha + 2$ (where the unit $\alpha$ consists of two protons ($2p$) and two neutrons ($2n$) and $m$ is an integer) is a good indicator of the $\alpha$-like $2p - 2n$ correlations according to Ref. [11]. If the difference is large, it shows the $\alpha$-like superfluidity of the $A = m\alpha$ system. In fact, we see such a signature in the whole region of $N \approx Z$ nuclei. We can regard the $T = 1$ (or $T = 0$) lowest state of the odd-odd $N = Z$ nuclei as a correlated state of the last $p-n$ pair coupled with the $\alpha$-like superfluid state of $A = m\alpha$. Based on this picture, we attempted to analyze the single-difference of binding energies $B(m\alpha + pn) - B(m\alpha)$, but we were unable to obtain simple information about the $T = 1$ or $T = 0$ correlations of the last $p-n$ pair.

The $p-n$ correlation energy in the odd-odd $N = Z$ nuclei with $A = m\alpha + pn$ can be evaluated by the double-difference of binding energies [12,13,14]

$$-\delta^2 V_{pn}(A + pn : T) = (B(A + pn : T) + B(A))$$
$$-(B(A + p) + B(A + n)) \quad (T = 0, 1),$$

(5)

where $B(A)$ stands for the binding energy. It is popular to calculate the odd-even mass difference for evaluation of the $T = 1$ pairing correlations. Using the odd-even mass difference $\Delta M_{oe}(A + n)$, the correlation energy of the $T = 1$ neutron pair in the $A + 2n$ (even) nuclei is evaluated by

$$-\delta^2 V_{nn}(A + 2n) = -2\Delta M_{oe}(A + n)$$
\[ = B(A + 2n) + B(A) - 2B(A + n). \] (6)

In the BCS approximation for the \( T = 1, J = 0 \) pairing correlations, the odd-\( A \) system is described as one neutron quasi-particle on the pairing superfluid vacuum as the average state of adjacent even-\( A \) systems, and the quasi-particle energy \( E_{qp} \) is approximately equal to the gap \( \Delta_n \), i.e., \( \Delta_{Me} \approx E_{qp} \approx \Delta_n \). Since the isospin is a good quantum number in \( N \approx Z \) nuclei, the \( m\alpha + 2p \), \( m\alpha + 2n \) and \( m\alpha + pn \) nuclei with \( T = 1 \) (or \( m\alpha + p \) and \( m\alpha + n \) nuclei) have approximately the same energy if the Coulomb energy is subtracted from the binding energy. We have the approximate relation

\[ -\delta^2 V_{pn}(m\alpha + pn : T = 1) \approx -\delta^2 V_{nn}(m\alpha + 2n). \]

We can suppose that the quantity \( -\delta^2 V_{pn}(m\alpha + pn : T = 1) \) represents the correlation energy of the last \( p - n \) pair as \( -\delta^2 V_{nn}(m\alpha + 2n) \) does that of the last neutron pair. Similarly, \( -\delta^2 V_{pn}(m\alpha + pn : T = 0) \) represents the correlation energy of the last \( p - n \) pair with \( T = 0 \) outside the \( A = m\alpha \) system.

Let us illustrate empirical values of \( -\delta^2 V_{pn}(T = 0) \) and \( -\delta^2 V_{pn}(T = 1) \) for the lowest \( T = 0 \) and \( T = 1 \) states of odd-odd \( N = Z \) nuclei, in Fig. 1. The difference \( \delta^2 V_{pn}(T = 0) - \delta^2 V_{pn}(T = 1) \) is equal to the energy difference between the lowest \( T = 0 \) and \( T = 1 \) states, from the definition (5). It is considered in phenomenology that the quantities \( -\delta^2 V_{pn}(T = 0) \) and \( -\delta^2 V_{pn}(T = 1) \) are indicators of the \( T = 0 \) and \( T = 1 \) pairing correlations. The odd-even mass difference expressed as \( 5.18A^{-1/3} \) in the mass formula [15] corresponds well with \( \delta^2 V_{pn}(T = 1)/2 \), as shown in Fig. 1. If we write the symmetry energy plus Wigner energy as \( a_T T(T + 1) \) in a mass formula, we have the relation \( \delta^2 V_{pn}(T = 0) \approx 3a_T/2 \) (note that if the Wigner energy proportional to \( T \) is neglected, \( \delta^2 V_{pn}(T = 0) \approx a_T/2 \)). The empirical value \( a_T \approx 134.4(1 - 1.52A^{-1/3}) \) in the mass formula [15] explains the \( A \)-dependent value of \( \delta^2 V_{pn}(T = 0) \) in Fig. 1. The empirical values of \( \delta^2 V_{pn}(T = 1) \) and \( \delta^2 V_{pn}(T = 0) \) show large

![Fig. 1. Empirical values of \(-\delta^2 V_{pn}\) for the lowest \( T = 0 \) and \( T = 1 \) states of odd-odd \( N = Z \) nuclei.](image-url)
fluctuations, which indicates shell effects. Basically, however, $\delta^2 V_{pn}(T = 0)$ is larger than $\delta^2 V_{pn}(T = 1)$ in the $sd$ shell nuclei, while the latter is larger than the former in the $pf$ shell nuclei. The empirical trend depending on the mass $A$ is well explained by using the parameters of the mass formula [15]. The trend of $\delta^2 V_{pn}(T = 0)$ is also reproduced by $3a_T/2$ with somewhat different parameters of other modern mass formulas which have the symmetry energy and Wigner energy in the form $a_T T (T + 1)$. This suggests an intimate relation between the $T = 0$ correlations and the symmetry energy. The model calculations using the $T = 1$ pairing force and a $T = 0$ $p - n$ force on a deformed base [3] and on a spherical base [7] gave a microscopic explanation of the competition between the $T = 1$ and $T = 0$ correlations, reproducing the energy difference $\delta^2 V_{pn}(T = 0) - \delta^2 V_{pn}(T = 1)$.

Our subject is to analyze in more detail the $p-n$ correlation energies $-\delta^2 V_{pn}(T = 0)$ and $-\delta^2 V_{pn}(T = 1)$ in the shell model calculations with realistic effective interactions. Let us illustrate the results obtained with the USD interaction [10] for the $sd$-shell nuclei, in Fig. 2, where contributions from $V_{mp} T = 0$, $V_{res} T = 0$ and $V_{T = 1}$ to $-\delta^2 V_{pn}$ are denoted by the dash, dot and solid lines respectively, and $-\delta^2 \langle H_{sp} \rangle$ denotes the contribution from $H_{sp}$. The double-difference of single-particle energies $-\delta^2 \langle H_{sp} \rangle$ is evaluated by substituting the expectation value $\langle H_{sp} \rangle$ for $B$ in Eq. (5). The quantity $-\delta^2 \langle H_{sp} \rangle$ gives the starting point of $-\delta^2 V_{pn}$ with no interactions in the shell model calculation. In Fig. 2, the calculated values of $-\delta^2 V_{pn}(T = 0)$ and $-\delta^2 V_{pn}(T = 1)$ finely reproduce their empirical values. We see mixed contributions from the $T = 0$ and $T = 1$ interactions to the final states with $T = 0$ or $T = 1$ and some deviations.
coming from the single-particle energy part $H_{sp}$. Still, Fig. 2 shows that the
double-differences of binding energies $-\delta^2 V_{pn}(T = 0)$ and $-\delta^2 V_{pn}(T = 1)$ are
good indicators of the $T = 0$ and $T = 1$ $p-n$ correlations. It is notable that
not only $V_{mp}^{T=0}$ but also $V_{res}^{T=0}$ contributes to $-\delta^2 V_{pn}(T = 0)$. We calculated
separately the contributions from the $T = 1$, $J = 0$ interactions and the other
$(T = 1, J > 0)$ interactions to the $T = 1$ $p-n$ correlation energy. The
calculated indicator $-\delta^2 V_{pn}(T = 1)$ includes the contributions from the $T = 1,$
$J > 0$ interactions as well as the $T = 1$, $J = 0$ interactions. The results show
that the $T = 1$, $J > 0$ interactions contribute greatly to the binding energy
but reduce the value of $-\delta^2 V_{pn}(T = 1)$ considerably. If we consider only the
$T = 1$, $J = 0$ pairing force $P_0$ and adjust the force strength so as to explain
the quantities $\delta^2 V_{pn}(T = 1)$ and $\delta^2 V_{nn}$ for the last nucleon pair, the binding
energy will not be reproduced, revealing a contradiction.

We can evaluate the $p-n$ correlation energy in even-even $N = Z$ nuclei using
the following double-difference of binding energies [8,14,16,17,18]:

\[- \delta^2 V_{2p2n}(A + 2p2n) = (B(A + 2p2n) + B(A))
\]

\[- (B(A + 2p) + B(A + 2n)). \] (7)

When we consider the $A = m\alpha$ systems, the quantity $\delta^2 V_{2p2n}$ is nothing but the
difference in mass caused by the $\alpha$-like correlations [11,19]. The large values
of $\delta^2 V_{2p2n}$ observed in the even-even $N = Z$ nuclei show the $\alpha$-like superfluid-
ity. The definition of $\delta^2 V_{2p2n}$ based on the picture of the $\alpha$-like superfluidity
corresponds well with that of $\delta^2 V_{nn}$ based on the pairing superfluidity. The
quantity $-\delta^2 V_{2p2n}$ represents the $p-n$ correlation energy between $2p$ and $2n$
A quarter of $-\delta^2 V_{2p2n} (-\delta^2 V_{2p2n}/4)$ is regarded as the $p-n$ correlation energy
per one $p-n$ bond.

In Fig. 2, we show the calculated and empirical values of $-\delta^2 V_{2p2n}/4$ for the sd-shell nuclei $^{24}$Mg and $^{28}$Si. This figure indicates that the quantity $-\delta^2 V_{2p2n}/4$
evaluates the $T = 0$ $p-n$ correlation energy as the quantity $-\delta^2 V_{pn}(T = 0)$.
The value of $\delta^2 V_{2p2n}/4$ is smaller than that of $\delta^2 V_{pn}(T = 0)$, which means that
the $p-n$ correlations of the last $p-n$ pair with $T = 0$ in the $A = m\alpha + pn$
nuclei are a little stronger than the $p-n$ correlations between $2p$ and $2n$.
By the way, $\delta^2 V_{2p2n}$ corresponds to the symmetry energy of the $A + 2p$ or
$A + 2n$ system with $T = 1$ in the framework of the mass formula [20]. Thus,
the indicators $\delta^2 V_{pn}(T = 0)$ and $\delta^2 V_{2p2n}$ represent the $T = 0$ $p-n$ correlation
energy in the shell model, while they are attributed to the symmetry energy
in the mass formulas. If one excludes the symmetry energy from the binding
energy as done in Ref. [2], one inevitably misses the contribution from the
$T = 0$ $p-n$ interactions to the total energy and hence is likely to miss the
signature of the $T = 0$ correlations.
3 Further discussions of $T = 0$ and $T = 1$ correlations

It is instructive for our study of the $T = 1$ and $T = 0$ correlations to see the expectation values of $V^{T=0}_{mp}$, $V^{T=0}_{res}$ and $V^{T=1}$ in addition to the double-differences of binding energies. We calculated their expectation values in the lowest states with $T = 0$ and $T = 1$. We call the expectation values “interaction energies” and write them such as $\langle V^{T=1} \rangle$. The interaction energies obtained by using the USD interaction for the $N = Z$ sd-shell nuclei from $^{20}$Ne to $^{32}$S are shown with three different lines in Fig. 3. This figure shows the indivisible cooperation of the $T = 1$ correlations and the $T = 0$ $p - n$ correlations, and indicates a significant role of the average $T = 0$ $p - n$ force $V_{mp}^{T=0}$ in the realistic effective interaction. The larger the valence-nucleon number is, the greater is the $V_{mp}^{T=0}$ contribution to the binding energy. Figure 3 shows that the $T = 0$ $p - n$ interactions including $V_{mp}^{T=0}$ make a larger contribution to the binding energy than the $T = 1$ interactions. However, if we neglect $V_{mp}^{T=0}$ which does not affect the structure, the $T = 1$ interactions are more important than the $T = 0$ residual interactions.

Dufour and Zuker [9] indicated that the realistic effective interactions are represented approximately by the monopole field $V_{mp}$, the $P_0$ force and the $QQ$ force. In fact, it was shown in Ref. [21] that the interaction $V_{mp} + P_0 + QQ$ with the $T = 1$, $J = 2$ pairing force ($P_2$) reproduces various properties of the $f_{7/2}$-subshell nuclei as comparably as the realistic effective interactions. The extended $P + QQ$ interaction describes well also the sd-shell nuclei in our calculations (unpublished). These results showed that the essential part of the monopole field is the $T = 0$ one ($V_{mp}^{T=0}$) and the $T = 1$ monopole field can be neglected, although some monopole corrections ($\Delta V_{mp}^{T=0}$ and $\Delta V_{mp}^{T=1}$)
depending on respective orbits remain. This is another reason why we do not extract the $T = 1$ monopole field in Eq. (4). The realistic effective interactions are well approximated by

$$V_{mp}^{T=0} + \Delta V_{mp}^{T=0} + \Delta V_{mp}^{T=1} + P_0 + P_2 + QQ.$$ (8)

We have a useful insight into the $T = 0$ and $T = 1$ correlations in this model. The $T = 0$ correlations are induced by $T = 0$ re-coupling terms of the QQ force and $\Delta V_{mp}^{T=0}$ except for $V_{mp}^{T=0}$, while the $T = 1$ correlations are induced by the monopole and quadrupole pairing forces ($P_0$ and $P_2$), and also by $T = 1$ re-coupling terms of the QQ force and $\Delta V_{mp}^{T=1}$.

As is well-known, the $T = 0$ states are the ground states in the odd-odd $N = Z$ nuclei except for $^{34}$Cl in the $sd$ shell. It is curious that the interaction energy gain of the $T = 1$, $0^+$ state is larger than that of the lowest $T = 0$ state for $^{26}$Al and $^{30}$P in Fig. 3. In the shell model, the $T = 0$ states of $^{26}$Al and $^{30}$P suffer less energy loss due to the single-particle energy part $\langle H_{sp} \rangle$ and hence become the ground states. This happens because the $T = 1$ correlations are stronger than the $T = 0$ residual $p - n$ ones, thus making more nucleons jump up to the $d_{3/2}$ orbit. If we lower the $d_{3/2}$ orbit, the $T = 1$ state becomes lowest in $^{26}$Al. The shell structure thus affects the competition between the $T = 0$ and $T = 1$ states for the ground-state position in the odd-odd $N = Z$ nuclei.

4 Conclusion

In conclusion, we have investigated the competition of the $T = 0$ and $T = 1$ $p - n$ correlations in an exact treatment of the shell model with a realistic effective interaction. By dividing the $T = 0$ $p - n$ interactions into the average monopole field and the residual interactions, we evaluated interaction energies of them and the $T = 1$ interactions. The calculations show that the cooperation of the average $T = 0$ $p - n$ force, $T = 0$ residual $p - n$ interactions and $T = 1$ interactions produce the large binding energies of the $N = Z$ nuclei. It is shown that the double-difference of binding energies $-\delta^2 V_{pn}(T = 0)$ or $-\delta^2 V_{pn}(T = 1)$ defined by Eq. (5) can be used to evaluate the correlation energy of the last $p - n$ pair with $T = 0$ or $T = 1$ in the odd-odd $N = Z$ nuclei. The realistic shell model calculations, however, show that the indicator $-\delta^2 V_{pn}(T = 0)$ or $-\delta^2 V_{pn}(T = 1)$ does not originate in a single kind of pairing correlations, but contains the contributions from plural kinds of correlations with $T = 0$ or $T = 1$.

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