Shell gaps and $pn$ pairing interaction in $N = Z$ nuclei

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**A B S T R A C T**

We analyze the observed shell gaps in $N = Z$ nuclei determined from the binding energy differences. It is found that the shell gaps can be described by the combined contributions from the single-particle level spacing, the like-nucleon pairing, and the proton–neutron pairing interaction. This conclusion is consistent with that of Chasman in [R.R. Chasman, Phys. Rev. Lett. 99 (2007) 082501]. For the double-closed shell $N = Z$ nuclei, the single-particle level spacings calculated with Woods–Saxon potential are very close to those obtained by subtracting the $nn$ pairing interaction from the observed shell gap. For the sub-closed or non-closed shell $N = Z$ nuclei, the $pn$ pairing interaction is shown to be important for the observed shell gaps.

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A long-standing problem in nuclear structure is that for the double-closed and sub-closed shell nuclei the single-particle energy-level orderings and spacings obtained from mean-field calculations underestimate the observed shell gaps. The observed shell gaps are defined by taking differences of ground-state masses, which are usually given as twice the odd–even mass difference extracted from the binding energy. However, this method assumes that there are no many-body effects involved in the mass differences at the closed shell. Chasman [1] has recently investigated this problem, and pointed out that the correlation energy due to pairings can resolve this discrepancy. As addressed in Ref. [1], there are changes in binding energy due to many-body effects even for double-closed shell nuclei. In this Letter, two main interactions have been considered to affect the observed shell gaps: One is the pairing interaction in like nucleons (neutron–neutron ($nn$) and proton–proton ($pp$)), and the other is the proton–neutron ($pn$) pairing interaction. Previously, one of us (K.K.) studied [2–4] these empirical interactions in $N \approx Z$ nuclei using the odd–even mass difference and the double difference of binding energies [5,6], which is different from the other one [7].

A typical indicator for $T = 1$ $nn$ pairing interactions is well known, which is given by the following three-point odd–even mass difference:

$$
\Delta_n^{(3)}(Z, N) = (-1)^N \left[ B(Z, N + 1) \\
- 2B(Z, N) + B(Z, N - 1) \right],
$$

(1)

where $B(Z, N)$ is the negative binding energy of a nucleus. According to the standard BCS theory for the $nn$ pairing gap $\Delta_n$, $B(Z, N + 1) \approx B(Z, N) + \Delta_n \pm \lambda_n$. Therefore, $\Delta_n^{(3)}(Z, N)$ is roughly $\Delta_n$. Thus, $\Delta_n^{(3)}$ is often interpreted as a measure of the empirical $mn$ pairing gap. However, because of the odd–even staggering effect, values of $\Delta_n^{(3)}(Z = \text{even}, N)$ are large for even-$N$ and small for odd-$N$ nuclei. It has been suggested [8,9] 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 interactions in neighboring even–even nucleus, although it is still controversial [10]. Thus, the differences of $\Delta_n^{(3)}$ in adjacent even- and odd-$N$ nuclei reflect the mean-field contributions. To extract the mean-field shell gap, we can apply this idea to the even–even $N = Z$ nuclei.

Fig. 1 shows experimental values of $\Delta_n^{(3)}$ obtained by using Eq. (1). We plot $\Delta_n^{(3)}(Z, Z)$ and $\Delta_n^{(3)}(Z, Z + 1)$ for the even–even $N = Z$ and the adjacent odd-mass $N = Z + 1$ nuclei ranging from...
A = 12 to A = 61. It can be seen that the large $\Delta_{n}^{(3)}(Z,Z)$ in $N = Z$ nuclei decreases steadily with increasing particle number. The expected quenching in the $nn$ pairing interaction at the magic or semi-magic number $N$ or $Z = 14$ and 28 is clearly seen. As also observed from the figure, the differences between $\Delta_{n}^{(3)}(Z,Z)$ and $\Delta_{n}^{(3)}(Z,Z+1)$ are remarkable. The $N = Z$ nuclei have additional binding energy due to the so-called Wigner effect. The differences in $\Delta_{n}^{(3)}$ between neighboring even- and odd-$N$ nuclei reflect the single-particle (mean-field) contributions and the correlation energies.

To investigate the physical source of the differences between $\Delta_{n}^{(3)}(Z,Z)$ and $\Delta_{n}^{(3)}(Z,Z+1)$, we first adopt a spherical single-particle model without considering the two-body interactions. In this case, the binding energy is simply expressed as

$$B_{sp}(N) = \sum_{j} N_{j} \epsilon_{j},$$

with $N_{j}$ and $\epsilon_{j}$ being the occupation number and single-particle energy, respectively, and the particle number $N = \sum_{j} N_{j}$. In a double-closed and sub-closed shell nucleus with $N = Z$, energy levels are fully occupied up to the level $j_{0}$, while in the neighboring odd-$N = Z+1$ system, the last neutron occupies the next level $j_{1}$. This implies

$$\Delta_{sp}^{(3)}(N = Z + 1) = 0,$$

$$\Delta_{sp}^{(3)}(N = Z) = \frac{1}{2}(\epsilon_{1} - \epsilon_{0}),$$

where $\epsilon_{0}$ and $\epsilon_{1}$ are the level energies for $j_{0}$ and $j_{1}$, respectively. Thus, for the double-closed and sub-closed shell nuclei with $N = Z$, the indicator (1) vanishes for $N = Z + 1$, but gives half of the single-particle level spacings for $N = Z$. On the other hand, for non-closed shell nuclei with $N = Z$ particles partially occupy the last level $j_{0}$. The odd-even mass difference is then expressed as

$$\Delta_{sp}^{(3)}(N = Z + 1) = 0,$$

$$\Delta_{sp}^{(3)}(N = Z) = 0.$$  

This means that the single-particle energies do not contribute to the odd-even mass difference or the observed shell gap for non-closed shell nuclei with $N = Z$. It is important to note that polarization effects for odd-$A$ nuclei may affect the filters (3) and (4). For this reason, the formulae (3) and (4) are considered as approximations.

The many-body contributions beyond the single-particle model are characterized by the amount that deviates from Eq. (3). By subtracting the many-body contributions from the indicator (1) at $N = Z$ and $N = Z + 1$, we may obtain information about the single-particle level spacing. Since for non-double-closed or non-sub-closed shell nuclei both values in (3) vanish in a single-particle model, the many-body contributions are dominated by the odd-even mass difference in these nuclei.

We consider the observed shell gap defined as twice the odd-even mass difference $\Delta_{n}^{(3)}(Z,Z)$. By subtracting the $nn$ pairing gap $\Delta_{sp}^{(3)}(Z,Z+1)$ from $\Delta_{n}^{(3)}(Z,Z)$, we can define the extracted gap as

$$\delta \Delta_{n}^{(3)}(Z,Z) = \Delta_{n}^{(3)}(Z,Z) - \Delta_{n}^{(3)}(Z,Z+1).$$

In Fig. 2, we plot twice the observed shell gap $2\Delta_{sp}^{(3)}(Z,Z)$, twice the extracted gap $\delta \Delta_{n}^{(3)}(Z,Z)$, and the single-particle spacing $\delta \epsilon_{WS}$, for the double-closed and sub-closed shell nuclei ranging from $A = 12$ to $A = 56$. Comparing the extracted gaps with the single-particle spacings $\delta \epsilon_{WS}$ obtained from a Woods-Saxon (WS) potential, we can see that the agreement between these two quantities is fairly good for the double-closed shell nuclei $^{16}O$, $^{40}Ca$, and $^{56}Ni$. This is expected because the $nn$ pairing interaction is dominated in these nuclei and any other interactions would be small due to the large shell gaps. Thus, for the double-closed shell nuclei, the $nn$ pairing interaction is considered to be the extracted gaps $\delta \Delta_{n}^{(3)}(Z,Z)$. For sub-closed shell nuclei such as $^{14}C$ and $^{28}Si$, however, the difference between the extracted gaps and the Woods-Saxon calculations, defined as

$$\delta \Delta_{n}(Z,Z) = \delta \Delta_{n}^{(3)}(Z,Z) - \frac{1}{2} \delta \epsilon_{WS},$$

is quite large. This suggests that the many-body interactions beyond the $nn$ pairing interaction would be significant. It should be mentioned here that the WS potential model is by no means a consistent microscopic mean-field model. A recent paper [11] has demonstrated that the single-particle energies can be improved systematically by refitting the spin-orbit and tensor part of the energy density functional method. Inclusion of the tensor effect may modify the shell gaps in sub-closed-shell nuclei.

Next, we study the many-body effects in the shell gaps for the sub-closed and non-closed shell $N = Z$ nuclei. The odd-even mass differences in even-even $N = Z$ nuclei are larger than those in the neighboring even-even $N = Z + 2$ nuclei, which reflects the gain in pairing energy due to stronger $nn$ interactions in $N = Z$ systems [2] and is referred as the Wigner energy [12]. The previous work [2] studied the indicator (1) for the Cr isotopes by performing
experimental binding energies. The open triangles denote the T shell nuclei, the gap. Fig. 3 further suggests that for the ground states of odd–even mass differences in odd–mass nuclei with N = Z + 1 are shown by the open squares.

shell model calculations, and suggested that the pn pairing interactions play an important rule for the odd–even mass difference as well as the nn pairing at N = Z. To describe the pn pairing interactions in odd–odd N = Z nuclei, we estimate the following double difference of binding energies [2–6]:

$$\Delta_{pn}^{(4T)}(Z, N) = \frac{(-1)^N}{2} \left[ B(Z, N)^T - B(Z, N - 1) - B(Z - 1, N) + B(Z - 1, N - 1) \right],$$  

where $B(Z, N)^T$ is the binding energy of the lowest state of isospin T in odd–odd N = Z nuclei. Fig. 3 shows such double differences calculated from the experimental binding energies. The odd–even mass differences for odd-mass nuclei are also displayed. One sees that $\Delta_n^{(3)}(Z = even, Z + 1)$ agrees with $\Delta_{pn}^{(4T)=1}(Z + 1, Z + 1)$, which means that the T = 1 pn pairing interaction for odd–odd N = Z nuclei have the same interaction energy as the nn pairing interaction, namely $\Delta_{nn} = \Delta_{pn}^{(4T)=1}$, if isospin symmetry is assumed. Thus, the indicator $\Delta_{pn}^{(4T)=1}$ provides the T = 1 pn pairing gap in N = Z nuclei. Similarly, $\Delta_{pn}^{(4T)=0}$ can be regarded as the T = 0 pn pairing gap. Fig. 3 further suggests that for the ground states of sd shell nuclei, the T = 0 pn interactions are stronger than the T = 1 pn interactions, whereas an opposite situation occurs in the pf shell nuclei where the T = 1 pn interactions are stronger. Thus, the T = 0 pn pairing gap $\Delta_{pn}^{(4T)=0}$ cannot be explained by the T = 1 pairing Hamiltonian.

In Fig. 4, we compare the extracted gap obtained from Eq. (5) with the pn pairing gap $\Delta_{pn}^{(4T)}(Z + 1, Z + 1)$ after subtracting the WS single-particle spacing from $\delta\Delta_n^{(3)}(Z, Z)$. One can see that overall, the extracted gaps correlate fairly well with the pn pairing interaction, with only two exceptions $^{20}\text{Ne}$ and $^{24}\text{Mg}$ (see discussions below). Thus, we may conclude that $\Delta_n^{(3)}(Z, Z)$ generally contains contributions from the single-particle spacing $\delta\epsilon$, the nn pairing gap $\Delta_n$, and the pn pairing gap $\Delta_{pn}$:

$$\Delta_n^{(3)}(Z, Z) = \frac{1}{2} \delta\epsilon + \Delta_n + \Delta_{pn}. \quad (8)$$

It is important to note that $\Delta_{pn} \approx 0$ for the double-closed shell nuclei and $\delta\epsilon \approx 0$ for the non-closed shell nuclei.

Using shell model calculations with the USD interaction in the sd shell, we now explain why the extracted gaps of $^{20}\text{Ne}$ and $^{24}\text{Mg}$ in Fig. 4 are larger than the pn pairing interaction. To understand this, we first extract the J = 0 pairing and monopole interaction from the USD interaction [13]

$$H_{pn} = H_0 + H_p + H_m. \quad (9)$$

In Eq. (9), $H_0$ is the single-particle Hamiltonian and the pairing term $H_p$ has the J = 0 components of the two-body matrix elements $\langle a, b, J, T | V[a, b, J, T] \rangle$ in the USD interaction. Hence the matrix elements of the monopole interaction $H_m$ take the form

$$V_m^{(T)}(a, b) = \frac{\sum_j (2J + 1) \langle a, b, J, T | V[a, b, J, T] \rangle}{\sum_j (2J + 1)}, \quad (10)$$

where a, b are single particle orbitals and the J = 0 components are neglected from the summation. The residual interaction is then defined by $H_{res} = H - H_{pn}$. It is well known that this interaction is dominated by the multipole interactions such as the quadrupole, octupole, and hexadecapole interactions [14]. In this sense, the residual interaction $H_{res}$ provides the collective correlations [15,16]. On the other hand, the monopole interaction does not lead to the collective correlations but it is important for the binding energy. It has been shown [2–4] that the T = 0 matrix elements of the monopole field $V_m^{(T)}(a, b)$ are significantly larger than those with T = 1, and are very important in determining the double differences of binding energies [6–8]. We can see that the matrix elements are quite large for the isoscalar components but small for the isovector components [3]. In the USD interaction, the monopole matrix elements (10) with T = 0 have values about −3 MeV and are strongly attractive, while the T = 1 monopole components are quite small.

The experimental and theoretical odd–even mass differences $\Delta_n^{(3)}(Z, Z)$ for N = Z nuclei in the sd-shell region are compared in Fig. 5. The calculated results with the USD interaction reproduce very well the odd–even mass difference for the N = Z nuclei. The shell model calculations with the J = 0 pairing and monopole interactions are in good agreement with the experimental values for $^{25}\text{Si}$, $^{32}\text{S}$, and $^{38}\text{Ar}$, but not for $^{20}\text{Ne}$ and $^{24}\text{Mg}$. It is obvious that the differences for $^{20}\text{Ne}$ and $^{24}\text{Mg}$ are attributed to the residual interaction $H_{res}$, and are consistent with the previous finding that the extracted gaps are larger than the pn pairing interactions in Fig. 4.

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**Fig. 3.** (Color online.) The pn pairing gaps estimated from the double differences of experimental binding energies. The open triangles denote the T = 0 pn pairing gap, while the solid circles the T = 1 pn pairing gap. The odd–even mass differences in odd–mass nuclei with N = Z + 1 are shown by the open squares.

**Fig. 4.** (Color online.) Comparison of the extracted gap with the pn pairing interaction. The solid squares and solid circles are for non-closed and sub-closed shell nuclei, respectively. For the extracted gap of sub-closed shell nuclei, we subtracted the WS part from the extracted gap $\delta\Delta_n^{(3)}(Z, Z)$, using Eq. (6).
Fig. 5. (Color online.) Comparison of the odd–even mass difference $\Delta_n^{(3)}(Z,Z)$ for $N=Z$ nuclei in the sd-shell. For each nuclide, the ordering is the experimental values, the calculated values in the USD interaction, and the calculated values in the $H_{pm}$ interaction.

To summarize, we have studied in detail the observed shell gaps determined from the binding energy differences for $N=Z$ nuclei. We have shown that the observed shell gaps can be described by the single-particle level spacing, the $nn$ pairing interaction, and the $pn$ pairing. This conclusion is consistent with that of Chasman [1]. In particular, the $pn$ pairing interactions are important for the non-closed and sub-closed shell nuclei, while they can be neglected for double-closed shell nuclei. For $^{20}\text{Ne}$ and $^{24}\text{Mg}$, it has been found that the residual interactions after removing the $J=0$ pairing and monopole interactions contribute to the shell gaps as well. Although we have considered in this Letter the neutron shell gap only, similar conclusions for the proton shell gap can also be obtained.

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