Isospin nonconserving interaction in the $T = 1$ analogue states of the mass-70 region

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Mirror energy differences (MED) and triplet energy differences (TED) in the $T = 1$ analogue states are important probes of isospin-symmetry breaking. Inspired by the recent spectroscopic data of $^{66}$Se, we investigate these quantities for $A = 66 - 78$ nuclei with large-scale shell-model calculations. For the first time, we find clear evidences suggesting that the isospin nonconserving (INC) nuclear force has a significant effect for the upper $fp$ shell region. Detailed analysis shows that in addition to the INC force, the electromagnetic spin-orbit interaction plays an important role for the large, negative MED in all the $T = 1$ triplet nuclei. The INC force and its strength needed to reproduce the experimental data are compared with those from the G-matrix calculation using the modern charge-dependent nucleon-nucleon forces.

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The impact of the Wigner’s elegant concept, the isospin symmetry $I^+$, is maximal near the $N = Z$ line where nuclei have equal numbers of neutrons and protons. Breaking of this symmetry is generally attributed to the Coulomb and isospin-nonconserving (INC) nuclear forces. To study the isospin-symmetry breaking, information for nuclei with $N < Z$ is of particular interest but these nuclei are not easy to access experimentally. By comparison of nuclear masses $B$ and detailed spectroscopic information $\delta$ for nuclei having same isospin, $T$, one can study the isospin-related phenomena to explore the origin of the symmetry breaking.

Measurable quantities have been suggested to probe the isospin-symmetry breaking. Mirror energy differences (MED), which are the differences between excitation energies of the $T = 1$ isobaric analogue states (IAS), are regarded as measures of the charge-symmetry breaking. On the other hand, triplet energy differences (TED) among the triplet $T = 1$ nuclei are used to indicate the charge-independence breaking. MED were extensively studied for the $f_{7/2}$-shell nuclei up to high spins (see Ref. $^4$ for review). TED were discussed for the $A = 46$ $^5$, $A = 50$ $^7$, and $A = 54$ $^8$ $^9$ triplet nuclei. These studies have suggested that the INC nuclear interaction in the $f_{7/2}$ shell plays an important role in the explanation for the observed MED and TED $^4$. In the upper $sd$ shell, however, studies showed $^1$ that important contributions to the symmetry breaking come from the multipole Coulomb term and the electromagnetic spin-orbit interaction, but not from the INC nuclear interaction. Little has been explored for the upper $fp$-shell above the $N = Z = 28$ shell closure, and our knowledge on the isospin-symmetry breaking in the mass-70 region is presently very limited.

Recent advances in experiment have made it possible to collect very exotic spectroscopic data. In the past few years, experimental information on mirror nuclei of the upper $fp$-shell above the doubly-magic nucleus $^{56}$Ni became available. The MED in the $A \sim 60$ mass region were discussed $^4$. It was suggested that the large MED in the mirror pair $^{61}$Ga$^{61}$Zn are due to the Coulomb monopole interaction and the electromagnetic spin-orbit interaction. The positive-parity high-spin states for the mirror pair $^{67}$As$^{67}$Se were observed $^5$, and description of these states requires inclusion of the $g_{9/2}$ orbit into the $fp$ model space. In Ref. $^5$ we investigated $^{66}$Se MED and TED up to $J = 6$. As $^{66}$Se has been reported $^6$, $^{70}$Br$^{70}$Se can be explained by the electromagnetic spin-orbit interaction without the INC nuclear interactions. Thus this work $^6$ and Refs. $^4$-$^7$ seem to indicate that in contrast to what has been suggested for the $f_{7/2}$-shell nuclei, the important contribution to CED in the upper $fp$ shell comes from the multipole Coulomb term and the electromagnetic spin-orbit interaction, but not from the INC interaction.

However, we believe that the question whether the above conclusion is general or not should be further investigated. In particular, it is important to survey the entire mass region by using different probes such as MED and TED. Unfortunately, for mirror and triplet nuclei with $A > 66$, there are no experimental data on MED and TED available due to experimental difficulties with the $T = 1$, $T_z = -1$ nuclei. Very recently, new observation of low-lying levels in $^{66}$Se has been reported $^8$, which, with the data of $^{66}$As $^9$ and $^{66}$Ge $^{10}$, gives the experimental A $= 66$ MED and TED up to $J = 6$. This is by now the heaviest triplet nuclei having the TED data. It was shown $^{10}$ that the Coulomb interaction alone can not...
account for the observed $A=66$ TED.

The purpose of the present Rapid Communication is to investigate MED and TED for the even-even nuclei with $A=66-78$ to extract information on the isospin-symmetry breaking through detailed analysis of the shell-model results. We show that, in addition to the electromagnetic spin-orbit interaction, it is necessary to involve the INC interaction to explain the new $A=66$ MED and TED data. We discuss the type and strength of the INC force that is phenomenologically added into the usual effective interaction. We further show that the realistic nuclear interactions that contain the isospin-breaking terms do not provide similar strengths for the isoscalar component that are needed to reproduce the $A=66$ MED and TED data.

The MED in mirror-pair nuclei, defined by

$$\text{MED}(J) = E_z(J, T = 1, T_z = -1) - E_z(J, T = 1, T_z = 1),$$

are regarded as measures of the charge-symmetry breaking in effective nuclear interactions, which include the Coulomb force. In Eq. (1), $E_z(J, T, T_z)$ are the excitation energies of IAS with spin $J$ and isospin $T$, distinguished by different $T_z$. For $T = 1$, the experimental MED for $A=22-66$ are shown in Fig. 1(a). It is worth noting the behavior of the $J^p = 2^+, 4^+$, and $6^+$ states in $A = 42$ and 54. For each of these spin states, the two nuclei indicate nearly the same magnitude in MED but opposite signs. This is called the cross-conjugate symmetry in MED for the two extremes in the $f_{7/2}$ shell [8].

The TED of $T = 1$ states in triplet nuclei are defined by

$$\text{TED}(J) = E_z(J, T = 1, T_z = -1) + E_z(J, T = 1, T_z = 1) - 2E_z(J, T = 1, T_z = 0),$$

which measures the charge-independence breaking. The experimental TED for $A=22-66$ are shown in Fig. 1(b).

FIG. 1: (Color online) Experimentally-known MED and TED for masses of $A=22-66$. Data are taken from Refs. [17-29].

We first carry out a calculation with the same parameters taken from our previous works [15, 16], without considering the INC interaction in the $p f_{5/2} g_{9/2}$ valence space. In the numerical calculations, the recently-proposed SS method [30] is employed, which goes beyond the usual Lanczos method and makes diagonalizations for the current problem possible. We employ the modern JUN45 interaction [31], and add the multipole term $V_{CM}$ and monopole term $E_{ff}$ in the Coulomb interaction. In addition, the single-particle energy shift $\Delta E_s$ due to the electromagnetic spin-orbit interaction [32] is also included.

We now add the INC interaction with the $J=0$ pairing terms $V_{pp} = \beta_{pp} V_{pp}^{J=0}$, $V_{nn} = \beta_{nn} V_{nn}^{J=0}$, and $V_{pn} = \beta_{pn} V_{pn}^{J=0}$ for all the orbits in our model space, with $V_{pp}^{J=0}$, $V_{nn}^{J=0}$, and $V_{pn}^{J=0}$ being, respectively, the $pp$, $nn$, and $pn$ pairing interactions for the matrix elements having a unit value (see Ref. [33]). The strengths, $\beta_{pp}^{J=0} = \beta_{nn}^{J=0} = 100$ keV for the isoscalar and $\beta_{pn}^{J=0} = 300$ keV for the isovector, are chosen so as to reproduce the experimental CED, MED, and TED data for $A=66$ [20]. The isoscalar strength of 100 keV for $J=0$ is the same as that of the empirical TED of the characteristic feature is that all the TED have negative values and exhibit similar spin-dependence. For example, the behavior of the $A=46$ TED is almost identical to that of $A=50$ for the entire spin range.

We perform large-scale shell-model calculations in the $p f_{5/2} g_{9/2}$ valence space. In the numerical calculations, the recently-proposed SS method [30] is employed, which goes beyond the usual Lanczos method and makes diagonalizations for the current problem possible. We employ the modern JUN45 interaction [31], and add the multipole term $V_{CM}$ and monopole term $E_{ff}$ in the Coulomb interaction. In addition, the single-particle energy shift $\Delta E_s$ due to the electromagnetic spin-orbit interaction [32] is also included.
A = 42 triplet [14, 20] in the f_{7/2} shell.

Large differences have been found between the results with and without the INC interaction. As one can see from Fig. 2(a), the calculated MED with inclusion of INC can well reproduce the experimental data [21] for J = 2 and J = 4, while for J = 6 the agreement is improved as compared to the calculation without INC. The calculation shown in Fig. 2(b) reproduces the TED data [19, 21] remarkably well. We thus conclude that the INC interaction enhances the MED and TED significantly, and is responsible for the isospin symmetry breaking in the upper p shell. To reproduce the experimental MED for the 6+ state, the J = 2 INC pairing interaction alone may be used, as discussed in Ref. [9, 34]. As seen in Fig. 2, however, the J = 2 INC pairing calculation with \( J^{(2)} = J^{(+2)} = -200 \text{ keV} \) fails to describe the MED for J = 2 and TED for J = 4, although it reproduces the MED data for J = 6. From Fig. 2(b), it is clear that the experimental TED patterns are quite nicely reproduced by the J = 0 INC pairing interaction [10] alone.

We have carefully checked the proposed INC interaction to see whether the present parameter choice of INC also reproduces CED (the Coulomb energy difference between the T = 1 states in the odd-odd N = Z nuclei and the analogue states in their even-even partners). As seen in Fig. 3 inclusion of the same INC interaction gives essentially a similar description for CED of A = 66, 70, 74, and 78, although the agreement with data is slightly better for the results without INC [16]. We may thus conclude that the present two-parameter INC interaction can correctly describe all the existing data (MED, TED, and CED) for the mass A = 66.

With inclusion of the J = 0 INC interaction, Fig. 4 shows the calculated MED for the upper f-p-shell nuclei with A = 66, 70, 74, and 78. Large variations in MED are seen in these nuclei, in both the spin-dependent trend and the magnitude. We can analyze the shell-model results by studying the components of the Hamiltonian. In Fig. 4 the separated multipole, spin-orbit, and monopole parts are denoted by \( V_{CM}, \varepsilon_{ls}, \) and \( \varepsilon_{ll} \), respectively. For the A = 66 mirror pair \( ^{66}\text{Se}^{66}\text{Ge} \), \( \varepsilon_{ls} \) and \( V_{CM} \) have negative values for the \( J^2 = 0^+, 2^+ \) and \( 4^+ \) states, while \( \varepsilon_{ll} \) is positive. The net MED from summation of the three terms are small and negative, which reproduces the experimental MED for the \( 2^+ \) state [13, 21]. The MED components for the A = 70 mirror pair \( ^{70}\text{Kr}^{70}\text{Se} \) are large and negative for \( \varepsilon_{ls} \), but positive for \( V_{CM} \) and nearly zero for \( \varepsilon_{ll} \). Since the magnitudes of \( \varepsilon_{ls} \) are larger, the total MED indicate negative values with large magnitudes. This suggests that the spin-orbit contribution is responsible for the negative MED in \( ^{70}\text{Kr}^{70}\text{Se} \). For the A = 74 mirror pair \( ^{74}\text{Sr}^{74}\text{Kr} \), the components indicate a similar overall behavior as those in the A = 66 pair. However, \( \varepsilon_{ll} \) is found significantly larger in the A = 74 pair, and is dominant in the summation. Therefore, the A = 74 MED are positive. Comparison of the corresponding components of A = 66 and 74 suggests that the cross-conjugate feature of these two pairs, when only the Coulomb part in the interaction is considered, originates from the different contributions of the monopole term \( \varepsilon_{ll} \) in the Coulomb interaction. The INC interaction tends to break the cross-conjugate symmetry. For \( ^{78}\text{Zr}^{78}\text{Sr} \), all components are small and positive, and the total MED are therefore small and positive.

Next, we discuss TED in the T = 1 triplet nuclei. Figure 5 shows the calculated TED for A = 66, 70, 74, and 78. One sees that, in consistent with the known experimental TED for A = 22 – 66 shown in Fig. 1(b), all the total TED (denoted by \( V_{CM+ls+ll+INC} \)) have negative values. We can easily see the origin for the negative TED from its definition in Eq. [2]. This quantity is given by twice of the difference between the average excitation energy of two even-even analogue states, while \( \varepsilon_{ll} \) and \( \varepsilon_{ls} \) have negative values for the \( J^2 = 0^+, 2^+ \) and \( 4^+ \) states, while \( \varepsilon_{ll} \) is positive. The net MED from summation of the three terms are small and positive, which reproduces the experimental MED for the \( 2^+ \) state [13, 21]. The MED components for the A = 70 mirror pair \( ^{70}\text{Kr}^{70}\text{Se} \) are large and negative for \( \varepsilon_{ls} \), but positive for \( V_{CM} \) and nearly zero for \( \varepsilon_{ll} \). Since the magnitudes of \( \varepsilon_{ls} \) are larger, the total MED indicate negative values with large magnitudes. This suggests that the spin-orbit contribution is responsible for the negative MED in \( ^{70}\text{Kr}^{70}\text{Se} \). For the A = 74 mirror pair \( ^{74}\text{Sr}^{74}\text{Kr} \), the components indicate a similar overall behavior as those in the A = 66 pair. However, \( \varepsilon_{ll} \) is found significantly larger in the A = 74 pair, and is dominant in the summation. Therefore, the A = 74 MED are positive. Comparison of the corresponding components of A = 66 and 74 suggests that the cross-conjugate feature of these two pairs, when only the Coulomb part in the interaction is considered, originates from the different contributions of the monopole term \( \varepsilon_{ll} \) in the Coulomb interaction. The INC interaction tends to break the cross-conjugate symmetry. For \( ^{78}\text{Zr}^{78}\text{Sr} \), all components are small and positive, and the total MED are therefore small and positive.

Next, we discuss TED in the T = 1 triplet nuclei. Figure 5 shows the calculated TED for A = 66, 70, 74, and 78. One sees that, in consistent with the known experimental TED for A = 22 – 66 shown in Fig. 1(b), all the total TED (denoted by \( V_{CM+ls+ll+INC} \)) have negative values. We can easily see the origin for the negative TED from its definition in Eq. [2]. This quantity is given by twice of the difference between the average excitation energy of two even-even analogue states, while \( \varepsilon_{ll} \) and \( \varepsilon_{ls} \) have negative values for the \( J^2 = 0^+, 2^+ \) and \( 4^+ \) states, while \( \varepsilon_{ll} \) is positive. The net MED from summation of the three terms are small and positive, which reproduces the experimental MED for the \( 2^+ \) state [13, 21]. The MED components for the A = 70 mirror pair \( ^{70}\text{Kr}^{70}\text{Se} \) are large and negative for \( \varepsilon_{ls} \), but positive for \( V_{CM} \) and nearly zero for \( \varepsilon_{ll} \). Since the magnitudes of \( \varepsilon_{ls} \) are larger, the total MED indicate negative values with large magnitudes. This suggests that the spin-orbit contribution is responsible for the negative MED in \( ^{70}\text{Kr}^{70}\text{Se} \). For the A = 74 mirror pair \( ^{74}\text{Sr}^{74}\text{Kr} \), the components indicate a similar overall behavior as those in the A = 66 pair. However, \( \varepsilon_{ll} \) is found significantly larger in the A = 74 pair, and is dominant in the summation. Therefore, the A = 74 MED are positive. Comparison of the corresponding components of A = 66 and 74 suggests that the cross-conjugate feature of these two pairs, when only the Coulomb part in the interaction is considered, originates from the different contributions of the monopole term \( \varepsilon_{ll} \) in the Coulomb interaction. The INC interaction tends to break the cross-conjugate symmetry. For \( ^{78}\text{Zr}^{78}\text{Sr} \), all components are small and positive, and the total MED are therefore small and positive.
Experimental data indicate that the excitation energy of the odd-odd $T = 1, T_z = 0$ state must be larger than either of the even-even $T = 1, T_z = \pm 1$ analogue states, and therefore the TED are negative. This was explained in terms of the $T = 1$ proton-neutron pairing. With increasing spin, the $pp$ and $nn$ pairs re-couple in the two even-even nuclei, while the $pn$ pairs align in the odd-odd nuclei. The recoupling lowers the energy of the proton-rich nuclei with $T_z = -1$ due to the Coulomb effect. We have found that, although the Coulomb effect qualitatively accounts for the negative TED, the components in Fig. 5 show the significant contribution from the INC interaction. It is clear that without it, the calculated negative TED are less than half of the experimental ones. This is consistent with the conclusion of Ruotsalainen et al. (see Fig. 3(c) of Ref. [20]) that the Coulomb (mutipole) interaction alone does not account for the observed TED. As seen from Fig. 5(a), the INC force enhances the TED magnitudes, which explains well the experimental data for $A = 66$. We thus conclude that both the multipole component of the Coulomb force and the INC force are responsible for the negative TED.

We have found that the observed TED in $A = 66$ cannot be reproduced by using different single-particle energies for protons and neutrons alone. In other words, we do not see, at least for the $A = 66$ case, that the suggested INC effect can be effectively replaced by just shifting single-particle energies between protons and neutrons. This conclusion has been checked by using the single-particle energies proposed by Taché et al. in Ref. [26] as an example. The calculation tells us that there is essentially no difference between the results using our single-particle energies and those in Ref. [26]. However, the INC interaction is necessary to reproduce the observed TED in $A = 66$ no matter which set of single-particle energies is used.

In Ref. [15], some of the present authors performed MED calculations for the odd-mass $A = 67$ mirror pair nuclei. Now that problem is recalculated with inclusion of the same INC forces used in the present paper. It is found that the MED results presented in Ref. [15] are further improved. The new MED for the $3/2^-$ and $7/2^-$ states are $-45.2$ keV and $-30.8$ keV, respectively, which are compared to the experimental ones $-43$ keV and $-50$ keV. There is a clear improvement from our previous results shown in Ref. [15] ($-15.4$ keV and $-72.2$ keV) for which no INC forces were included. Furthermore, we confirm that the MED of the positive-parity band built on the $9/2^+$ state are also reproduced well by the new calculation. This is an additional support to the current treatment of the INC forces in the upper $fp$ shell region.

$^{70}$Kr lies in the transitional region where the shape-coexistence phenomenon has been discussed. It is interesting to examine the INC effects on the shape structure. The calculated results predict an oblate shape for the yrast states and a weakly prolate-deformation for the side band. By comparing the calculations with and without the INC interaction, we find only little difference in the results for both bands. We thus conclude that the INC force does not affect the bulk property such as deformation, which is consistent with the conclusion in Ref. [16] [18].

Realistic interactions based on the modern charge-dependent nucleon-nucleon (NN) forces, such as $N^3$LO, CD-Bonn, and AV18, can well reproduce the $NN$ scattering data. The isotensor strengths for the $NN$ forces have been calculated in the $G$ matrix formalism, which, based on low-momentum interactions $V_{\text{LOW}}$, sums the particle-particle ladders. The calculated strengths for $\beta_{f=0}^c$ are 225, 330, and 621 (all in keV) for $N^3$LO, CD-Bonn, and AV18, respectively. These values are two to six times larger than the strength adopted in the present work ($\beta_{f=0}^c = 100$ keV). Thus it is unlikely that the charge-dependent $NN$ forces will provide the same description for MED and TED in the upper $fp$-shell nuclei as the phenomenological treatment does. In the $f_{7/2}$ shell region, the observed $A = 54$ TED were investigated using the AV18 force. It was concluded that this force fails to reproduce the experimental data.

To summarize, the recent experimental results motivated us to carry out a detailed shell-model analysis for MED and TED in the upper $fp$ shell region, aiming at a better understanding of isospin-symmetry breaking in nuclear effective interactions. We have systematically investigated MED and TED for the $T = 1, T_z = 0, \pm 1$ nuclei with $A = 66 - 78$ by performing large-scale shell-model calculations. Our results for the upper $fp$-shell region have clearly shown that the observed MED and TED for $A = 66$ can only be explained by inclusion of the INC nuclear interaction, in addition to the Coulomb force. We have further predicted large, negative MED for $A = 70$, which is attributed to the INC interaction together with the same mechanism leading to the anomalous CED between the isospin $T = 1$ states in the odd-odd $N = Z$ nucleus $^{70}$Br and the analogue states in its even-even partner $^{70}$Se. It is also demonstrated that both the INC interac-
tion and the multipole Coulomb force determine the negative TED systematically for $A = 66, 70, 74,$ and $78$. We have found that the isotensor strengths derived from the modern charge-dependent forces ($N^3LO$, CD-Bonn, and AV18) deviate strongly from the required values that reproduce the experimental data. Presently it remains as an important open question why the above-mentioned modern charge-dependent forces can not account for the phenomenological strengths of the INC force. It would be interesting to see if the three-nucleon forces based on the chiral effective field theory [45] can provide a solution. Finally, experimental data for heavier nuclei are much desired to test our predictions and to understand the role of the INC force in nuclear spectroscopy.

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