Breakdown of the Isobaric Multiplet Mass Equation as An Effect of the Isospin-Symmetry Breaking

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The breakdown of the quadratic form of isobaric multiplet mass equation (IMME), presents a long-standing challenge to the existing theoretical models. In particular, recent high-precision nuclear mass measurements have indicated a dramatic failure of the IMME for several isobaric multiplets. We propose a new mechanism that the isospin-projection \( T_z \) dependence of the 1st-order symmetry energy coefficient (SEC) drives a significant breakdown of the IMME, where the 1st-order SEC is primarily induced by the isospin-symmetry breaking (ISB) of strong nuclear force. Completely different from the existing knowledge, the deviation from the IMME cannot be measured simply by the high-order terms such as cubic term \( dT_z^3 \).

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Introduction. Isospin, as a fundamental concept in nuclear and particle physics, was introduced by Heisenberg more than eighty years ago after the discovery of neutron to describe the different charge state of a nucleon \([1]\). Proton (\( p \)) and neutron (\( n \)) with nearly identical mass belong to an isospin \( T = 1/2 \) doublet distinguished by different projections \( T_z(p) = -1/2 \) and \( T_z(n) = +1/2 \). Isobaric nuclei with the same \( T \) as well as spin-parity \( J^\pi \) and similar properties but different \( T_z \), form an isobaric multiplet, where an excited state of a nucleus is called as an isobaric analog state (IAS). The strong nuclear force is exactly isospin symmetric under the assumption of its charge-independence and charge-symmetry. However, the isospin symmetry is weakly broken by the \( u-d \) quark mass difference and the electromagnetic interactions between quarks \([2]\). The nucleon-nucleon scattering data have already suggested a distinguishable difference between \( nn \), \( np \) and \( pp \) interactions \([3–5]\). Understanding this isospin-symmetry breaking (ISB) is of particular importance as it is connected to a deeper cognition of the nuclear force. One intriguing approach to explore the ISB is implemented via the deviation of the isobaric multiplet mass equation (IMME) \([6, 7]\).

The IMME predicts in the first-order perturbation theory that the mass excesses \( ME(A, T, T_z) \) of the isospin multiplet members follow the parabolic expression \([8, 9]\)

\[
ME(A, T, T_z) = a + bT_z + cT_z^2,
\]

where \( A \), \( T \) and \( T_z = (N - Z)/2 \) are the mass number, total isospin and the isospin projection of the multiplet. \( a \), \( b \) and \( c \) are the coefficients depending on the mass number and total isospin. The quadratic form of the IMME was found to work well for most cases, and hence it has been used as a powerful tool to perform the widespread mass predictions for the cases where some members of a multiplet are known, in particular for the neutron-deficient nuclei with unknown or insufficiently precise masses that are involved in the astrophysical \( rp \)-process path. Nevertheless, a large discrepancy from the quadratic form of the IMME was reported for some isobaric multiplets, and an extra cubic term \( dT_z^3 \) or even a quartic term \( eT_z^4 \) is generally included to measure any deviation from the IMME. With the improvement of radioactive beam facilities, a wealth of nuclear masses has been being measured with increasingly high precision and allows one to test the breakdown of the quadratic form of the IMME with an enhanced accuracy. Although several theoretical explanations have been suggested to explain the \( dT_z^3 \) term, including the isospin mixing, high-order Coulomb effects and charge-dependent nucleon-nucleon interaction \([10–13]\), the breakdown mechanism of
the quadratic form of the IMME remains a great continual challenge to the existing nuclear theories. In this Letter, we explore this bewildering issue in a distinctive approach.

The 1st-order symmetry energy caused by the ISB. Without the inclusion of the \( n-p \) mass difference, an isobaric multiplet would be completely energetically degenerate in the absence of Coulomb interaction if the strong nuclear force were isospin symmetric. Yet, the ISB leads to the breaking of this degeneracy slightly, which serves exactly our starting point to explore the breakdown mechanism of the IMME. We measure this breaking by the density-dependent 1st-order symmetry energy coefficient (SEC) of nuclei. To derive the 1st-order SEC of nuclei, we should firstly fall back on the 1st-order SEC of infinite nuclear matter.

The 1st-order SEC of nuclear matter with density \( \rho \) and isospin asymmetry \( \beta \) is given as

\[
S_1(\rho) = \frac{\partial E(\rho, \beta)}{\partial \beta} |_{\beta=0}.
\]  

(2)

The origin of \( S_1(\rho) \) is twofold: the ISB of nucleon-nucleon interaction and the \( n-p \) mass difference (npMD). The npMD is also an ISB effect. Accordingly, \( S_1(\rho) \) is written as \( S_1(\rho) = S_1^{(\text{ISB})}(\rho) + S_1^{(\text{npMD})}(\rho) \). \( S_1^{(\text{ISB})} \) is determined by the Brueckner Hartree-Fock theory [14] with the AV18 interaction, where the AV18 is a high-quality nucleon-nucleon potential with explicit charge dependence and charge asymmetry [15]. To achieve a reliable accuracy, it is determined with the following formula

\[
\frac{E(\rho, \beta) - E(\rho, -\beta)}{2\beta} = S_1^{(\text{ISB})}(\rho) + S_1^{(\text{ISB})}(\rho)\beta^2 + ..., 
\]

(3)
to cancel out the systematical uncertainty available. The 3rd-order SEC \( S_3(\rho) \) is found to be much less than the 1st-order one and thus is completely insignificant. The mass excess is defined as \( \text{ME} = (m - Au)^2 = [m_0 - B(Z,A) - Au]c^2 \), where \( m_0 = Zm_p + (A - Z)m_n \) is the total rest mass of the nucleons and \( B(Z,A) \) is the binding energy. The \( n-p \) mass difference in \( m_0 \) (labeled \( \Delta m_{n-p}^{(0)} \)) contributes in a manner of \( T_z(m_n - m_p) \) to the IMME and does not break the IMME. Nevertheless, the mass difference in \( B(Z,A) \) (labeled \( \Delta m_{n-p}^{(B)} \)) leads to a part of the 1st-order symmetry energy. The model-independent 1st-order SEC caused by the \( n-p \) mass difference can be expressed as

\[
S_1^{(\text{npMD})}(\rho) = -\frac{\hbar^2}{2m^*} \left( \frac{3\pi^2}{2} \right)^{2/3} \left( \frac{m_n - m_p}{m_n + m_p} \right)^2 \rho^2 ,
\]

(4)

where \( m^* \) is the reduced mass \( m^* = 2m_pm_p/(m_n + m_p) \). The nucleonic masses \( m_n = 939.56533 \) and \( m_p = 938.27199 \) are used [16] in the calculations. The density-dependent 1st-order SEC \( S_1(\rho) \) is illustrated in Fig. 1 which is found to be mainly from the ISB of nucleon-nucleon interaction, and indeed dramatically less than the 2nd-order one and often reasonably neglected.

The calculated \( S_1(\rho) \) is used to estimate the 1st-order symmetry energy \( E_{\text{sym},1}(A) = a_{\text{sym},1}(A)(N - Z) \) of the spherical nuclei with mass number \( A \), where \( a_{\text{sym},1}(A) \) is the corresponding 1st-order SEC. Adopting the local density approximation, \( E_{\text{sym},1}(A) \) is calculated within the framework of the nuclear energy-density functional approach by directly integrating the following density functional

\[
E_{\text{sym},1}(A) = \int_0^{\infty} 4\pi r^2 \rho(r)S_1(\rho)\beta(r)dr .
\]

(5)
after subtracting the Coulomb polarization effect. \( \beta(r) = (\rho_n(r) - \rho_p(r))/\rho(r) \) is the local isospin asymmetry in which \( \rho_p(r) \) and \( \rho_n(r) \) are the proton and neutron density distributions inside a nucleus. The 1st-order symmetry energy effect here is treated as a small perturbation that cannot affect the density distributions distinctly, and hence the \( E_{\text{sym},1}(A) \) can be reliably extracted since it is isolated, and additionally we have \( a_{\text{sym},1}(A, T_z) = a_{\text{sym},1}(A, -T_z) \) in isobaric multiplets.

To estimate the \( E_{\text{sym},1}(A) \) of an IAS, its nucleonic density distributions \( \rho_n \) and \( \rho_p \) should be determined firstly. Excluding the Coulomb interaction and considering the ISB of nuclear force is just a small perturbation to its ground state, the wave function
FIG. 1: Density-dependent 1st-order symmetry energy coefficient \( S_1(\rho) \) of infinite nuclear matter, where the \( S_1^{(\text{ISB})} \) is determined by the Brueckner Hartree-Fock theory with the AV18 interaction and \( S_1^{(\text{npMD})} \) is calculated with Eq. (4).

The IAS with \( N - 1 \) neutrons and \( Z + 1 \) protons (\( N > Z \)) is obtained with \( |\text{IAS} > = |T, T_z = T - 1 > = \frac{1}{\sqrt{2T}} T_0 > \),

\[ (6) \]

where \( T_- \) is the isospin lowering operator with \( T_- = \sum L_-(j), j \in \text{excess neutron orbits in } |0 > \). \( |0 > \) is the ground state of the parent nucleus with \( N \) neutrons and \( Z \) protons, as a member of a multiplet with \( T = T_z \). As a result, \( (\rho_n + \rho_p)_{\text{IAS}} = (\rho_n + \rho_p)_{\text{parent}} \) and \( (\rho_n - \rho_p)_{\text{IAS}} = (\rho_n - \rho_p)_{\text{parent}} - \frac{1}{\sqrt{2}} \rho_{n,\text{exc.}} \) can be obtained without introducing isospin mixing, where \( \rho_{n,\text{exc.}} \) is the density of the \( (N - Z) \) excess neutrons in the parent nucleus.

**TABLE I:** Calculated 1st-order symmetry energies \( E_{\text{sym},1}(A) \) of finite nuclei (in units of MeV) with Eq. (5).

| Nuclide | SLy4  | SLy5  | KDE   |
|---------|-------|-------|-------|
| \( ^{53}\text{Mn} \) | -0.303 | -0.300 | -0.311 |
| \( ^{20}\text{O} \)  | -0.289 | -0.286 | -0.302 |
| \( ^{208}\text{Pb} \) | -5.021 | -5.024 | -5.226 |

We give a brief discussion on the calculated 1st-order symmetry energy \( E_{\text{sym},1}(A) \) of finite nuclei. In our previous work \[20\], we constrained the neutron skin thickness in \( ^{208}\text{Pb} \) and density-dependent behavior of the SEC. The derived SEC, reference density and neutron skin thickness of \( ^{208}\text{Pb} \), along with the SEC of nuclear matter at its saturation density, serve as important calibrations for the effective interactions in nuclear energy density functionals. The three most excellent interactions that satisfy those constraints are selected among the interactions to calculate \( E_{\text{sym},1}(A) \) with Eq. (5). They are the SLy4 \[21\], SLy5 \[21\] and KDE \[22\] interactions and displayed also in the Fig. 1 in Ref. \[20\]. Table I lists the calculated \( E_{\text{sym},1}(A) \), taking \( ^{53}\text{Mn} \) (a member of \( A = 53 \) quartet), \( ^{20}\text{O} \) (a member of \( A = 20 \) quintet) and a heavy nucleus \( ^{208}\text{Pb} \) as examples. \( E_{\text{sym},1}(A) \) is found to be only weakly model-dependent because different interactions generate almost identical nucleonic density profiles. For \( ^{53}\text{Mn} \) and \( ^{20}\text{O} \), the values of \( E_{\text{sym},1}(A) \) are very small due to their low isospin asymmetries and the undersized \( S_1(\rho) \) indicates the validity of the perturbation treatment for the ISB of nuclear force. \( E_{\text{sym},1}(A) \) for \( ^{208}\text{Pb} \) is however as large as \(-5 \text{ MeV} \). At present, nuclear masses can be predicted accurately with deviations of several hundred keV by employing macroscopic-microscopic mass models \[23, 25\]. We thus conclude that the 1st-order symmetry energy \( E_{\text{sym},1}(A) \) is so sizable that it can not be neglected.
simply for the nuclei with a large isospin asymmetry since it can be comparable to the pairing or shell energy, as a byproduct of the present work. On the other hand, the ISB has been shown to play a significant role in some interesting subjects in nuclear structure [26]. It is also expected to exhibit perceptible effects in spin-isospin excitations, such as the charge-exchange reaction, Gamow-Teller transition and $\beta$-decay. It is thus necessary to consider the ISB effect in a reliable construction of new effective interactions in nuclear many-body models.

**Breakdown mechanism of the IMME.** Mass measurements of exotic nuclei are a topic of great interest driven by many important issues in nuclear physics and astrophysics, which provide critical information about nuclear force [27–29], nuclear structure [30–32] and astrophysical applications [32]. Recently, the accurate mass data coming mainly from the Penning trap and isochronous mass spectrometry facilities have enabled one to further test the validity of the quadratic form of the IMME given in Eq. (1) stringently and hence promote the exploration of its breakdown mechanism theoretically. Contrary to the common belief that the 1st-order SEC $a_{\text{sym},1}(A)$ induced by the ISB of nuclear force as well as $n-p$ mass difference $\Delta m_{np}^{(0)}$ also contributes to the nonzero value of $c$ in the IMME stems from the Coulomb energy [33, 34] and is also attributable to the Coulomb energy.

Breakdown of the IMME. In our framework, where $\delta \rho = \rho_{n}^{\text{core}} - \rho_{p}(r)$ is the difference between the neutron and proton densities in the core consisting of the $Z$ protons and $Z$ neutrons in the corresponding orbits for the nucleus with $T_z = T$. Therefore, the $d$ value is attributed to the difference of the 1st-order symmetry energy of the $N = Z$ core among the $2T + 1$ members of the multiplet.
FIG. 2: The calculated $d$ values compared with the experimental data. For the $T = 3/2$ quartets with $A = 53, 49, 45, 41$ [35], $A = 35$ [36] and $A = 21$ [37], the experimental $d$ values are derived via Eq. (8) combined with measured mass excesses, and the calculated $d$ values are obtained with Eq. (10). For the $T = 2$ quintet with $A = 20$ [37, 38], the calculated $d$ values are from Eq. (11).

Figure 2 summarizes the measured $d$ coefficients of the quartets and quintets with a strong breakdown of the IMME given in Eq. (1) from several different collaborations. Our calculated values of $d$ with Eqs. (10), (11) are also presented in Fig. 2 for comparison to test the validity of our theoretical approach. We would like to point out again that the coefficient $d$ is not the coefficient appearing in the cubic term as we do not introduce a $dT_z^3$ term.

The $T_z = 3/2$ quartets of the nuclides $A = 53, 49, 45, 41$ serve as the first test of the IMME in the $fp$-shell nuclei [35], indicating a dramatic failure of the quadratic form of the IMME. The theoretical values based on the two isospin nonconserving Hamiltonians, namely, the $f_{7/2}$ model space [39] and the full $pf$ model space with GPFX1A isospin conserving Hamiltonian [40–42] plus the Ormand-Brown (OB) isospin nonconserving Hamiltonian [43], cannot reproduce the experimental data in order of magnitude [35]. Our calculated $d$ values are in marginal agreement with the experimental ones for the $T_z = 3/2$ quartets of the nuclides $A = 49, 45, 41$, but substantially underestimate the $d$ value for the $A = 53$ quartet. The underlying physical reason should be further investigated. On the other hand, the improved experimental data with a much higher precision are desired, noting that the uncertainties for the experimental $d$ coefficients are very large. The large experimental $d$ value for the $A = 53$ quartet, if finally verified, will extend our knowledge about the nuclear force to new depths. The $A = 35$ [36] and $A = 21$ [37] quartets are measured with relatively smaller uncertainties, and the $d$ coefficients we obtained agree excellently with the experimental ones. As pointed out in Ref. [37], the $A = 20$ and 21 multiplets provide an excellent test of the IMME in the $sd$-shell nuclei as they are the lightest isospin multiplets where all members are stable against particle emission, and strong deviations from the quadratic form of the IMME were discovered. The universal $sd$ USDA and USDB isospin-conserving Hamiltonians [44] supplemented with an isospin nonconserving part [45] yield too small $d$ values, $d = -0.3$ keV (USDA) and $d = 0.3$ keV (USDB) for the $A = 21, J^\pi = 5/2^+$ quartet [37]. In addition, the valence-space calculations based on low-momentum two-nucleon and three-nucleon forces derived from chiral effective field theory [45] give $d = -38$ keV for the $A = 21$ quartet [37], disagreeing also with the experimental finding of 6.7(13) keV. Our approach yields $d = 6.8 \sim 8.0$ keV for the $A = 21$ quartet, being in good agreement with the experimental measurements. Two months ago, an unexpected breakdown of the IMME in the $A = 20, T = 2$ quintet compared with a large $d$ value in Ref. [37] was reported [38]. Our calculated value is in between them, as shown in Fig. 2 while the calculations in Ref. [37] deviate substantially from both of the two measurements.
Herfurth et al. [46] measured the mass of $^{33}\text{Ar}$ and combined with the known masses of the other members of the $T = 3/2$ quartet and achieved $d = -2.95 \pm 0.90 \text{ keV}$ for the $J^\pi = 1/2^+$ multiplet. Shortly thereafter, however, Pyle et al. [47] determined the mass of $^{33}\text{Cl}$ with a new result that disagrees with the previously accepted value, and they concluded that the validity of the IMME was restored. The predicted $d$ value for the $A = 33$ quartet with our method is $-2.5 \sim -1.5 \text{ keV}$, suggesting that the significant deviation of the IMME as that for the above $pf$-shell multiplets is not expected, in accordance with the measurements qualitatively. The test of the IMME for the $T = 2$ quintet at $A = 32$ has been carried out by several collaborations [48–52] for more than ten years. It appears that the derived $d$ value is not very large. Our estimated value of $d = -1.1 \sim -0.6 \text{ keV}$ is not sizable either. However, the masses of some members of the multiplet are still controversial [52]. Consequently, more direct mass measurements need to be done for a final verification of the breakdown of the IMME, as suggested in Ref. [52].

Although the determination of the 1st-order symmetry energy $E_{\text{sym},1}(A)$ is weakly model-dependent since different interactions yield the almost identical nucleonic density distribution, the calculated $d$ values are not so fortunate because the $d$ values tend to be very small. Due to the fundamental difficulty and complexity of nuclear many-body systems, to estimate the $d$ coefficient accurately is unavailable at present. Nevertheless, we proposed an alternative strategy towards exploring the breakdown of the IMME and achieved satisfactory results on the whole, which enhances our understanding of the isospin-symmetry breaking of nuclear force. Meanwhile, other effects, such as isospin mixing and high-order Coulomb effects should also be investigated in further depth to achieve a more comprehensive cognition of the breakdown of the IMME. For instance, a strongly isospin mixing has been revealed in the form of a splitted IAS in the daughter nucleus $^{55}\text{Ni}$ [53].

**Summary.** The breakdown mechanism of the quadratic form of the IMME, as a long-standing heavy challenge to the fundamental nuclear theory, has been explained with a completely distinctive strategy in this letter. Completely different from the conventional conception introducing higher-order terms in the IMME such as a cubic term $dT_z^3$ to measure the deviation from the IMME, we have showed that the $T_z$-dependence of the $b$ coefficient induced by the 1st-order symmetry energy coefficient $a_{\text{sym},1}(A)$ drives the breakdown of the IMME, where $a_{\text{sym},1}(A)$ primarily originates from the isospin-symmetry breaking of nuclear force. Accordingly, the IMME should be revised to include the contribution of $a_{\text{sym},1}(A)$, as described by Eq. (7). Our theoretical results for the first time are in satisfactory agreement with the recent high-precision experimental measurements, deepening our understanding of the isospin-symmetry breaking. In addition, as a byproduct of this work, it is found that for a neutron-rich nucleus, the 1st-order symmetry energy $E_{\text{sym},1}(A)$ that is generally dropped is rather sizable as it can be as important as the pairing or shell energy, so that it could trigger many relevant studies in future about its effects on nuclear structure, such as on accurate nuclear mass estimations and construction of nuclear energy density functionals.

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