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Mechanisms of mirror energy difference for states exhibiting Thomas-Ehrman shift: Gamow shell model case studies of ^{18}Ne/^{18}O and ^{19}Na/^{19}O

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Abstract

The mirror energy difference (MED) of the mirror state, especially for states bearing the Thomas-Ehrman shift, serves as a sensitive probe of mirror symmetry breaking. We employ the Gamow shell model, which includes the inter-nucleon correlation and continuum coupling, to investigate the MED for *sd*-shell nuclei by taking the ^{18}Ne/^{18}O and ^{19}Na/^{19}O as examples. Our GSM provides good descriptions for the excitation energies and MEDs for the ^{18}Ne/^{18}O and ^{19}Na/^{19}O. Moreover, our calculations also reveal that the large MED of the mirror states is caused by the significant occupation of the weakly bound or unbound $s_{1/2}$ waves, giving the radial density distribution of the state in the proton-rich nucleus more extended than that of mirror states in deeply-bound neutron-rich nuclei. Moreover, our GSM calculation shows that the contribution of Coulomb is different for the low-lying states in proton-rich nuclei, which significantly contributes to MEDs of mirror states, which is well-recognized. Furthermore, our GSM calculation points out that the contributions of the nucleon-nucleon interaction are different for the mirror state, especially for the state of proton-rich nuclei bearing the Thomas-Ehrman shift, which also contributes to the significant mirror symmetry breaking with large MED.

Full Text

Preamble

Mechanisms of mirror energy difference for states exhibiting Thomas-Ehrman shift: Gamow shell model case studies of 18Ne/18O and 19Na/19O

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The mirror energy difference (MED) of mirror states, particularly for states bearing the Thomas-Ehrman shift, serves as a sensitive probe of mirror symmetry breaking. We employ the Gamow shell model, which includes inter-nucleon correlation and continuum coupling, to investigate the MED for sd-shell nuclei using 18Ne/18O and 19Na/19O as examples. Our GSM provides good descriptions for the excitation energies and MEDs of 18Ne/18O and 19Na/19O. Moreover, our calculations reveal that the large MED of mirror states is caused by the significant occupation of weakly bound or unbound s1/2 waves, giving the radial density distribution of the state in the proton-rich nucleus a more extended character than that of mirror states in deeply bound neutron-rich nuclei. Our GSM calculation also shows that the contribution of the Coulomb interaction differs for low-lying states in proton-rich nuclei, which significantly contributes to MEDs of mirror states, as is well recognized. Furthermore, our GSM calculation points out that the contributions of the nucleon-nucleon interaction are different for mirror states, particularly for states in proton-rich nuclei bearing the Thomas-Ehrman shift, which also contributes to significant mirror symmetry breaking with large MED.

Keywords: mirror symmetry breaking, Thomas-Ehrman shift, mirror energy difference, continuum coupling, Gamow shell model

INTRODUCTION

Exotic nuclear structures in drip-line nuclei have become a subject of great interest in recent years, as they are characterized by unique properties that exhibit significant differences compared to those of stable nuclei [**?**]. One of the most significant phenomena observed in these systems is the Thomas-Ehrman shift (TES) [**?**, **?**]. This effect is most pronounced in nuclei close to the proton drip lines, where the balance between the strong force and the Coulomb force is most delicate. States exhibiting TES effects are often weakly bound or unbound, characteristic of open quantum systems, while their neutron-rich mirror counterparts remain deeply bound, resulting in a large mirror energy difference

(MED) in their isobaric states [?]. These large MEDs are attributed to their proximity to near-threshold effects, in which continuum effects need to be properly treated. Consequently, a thorough comprehension of the Thomas-Ehrman shift is pivotal for elucidating the dynamics of weakly bound and unbound nuclear systems and understanding the mechanisms underlying mirror symmetry breaking in mirror nuclei.

Two possible reasons exist for states with large MED, of either external or internal character. If extended single-particle wave functions of weakly bound or unbound s- or p-waves are significantly occupied in the considered states, the large MED is of external nature, as in the TES states [?, ?, ?]. The second possibility, related to configuration mixing (see Refs. [?, ?]), is of internal nature. In this case, the extended wave function arises via strong configuration mixing in which a few nodal states of s or p waves are included in the calculations. These two external and internal effects are different but can be intertwined in a complex manner. For instance, the inversion of ground states in the 16F and 16N mirror nuclei is primarily due to the unbound proton 1s1/2 orbital, which can also be well described in GSM calculations within the configuration mixing framework [?, ?].

The sd-shell nuclei, situated at the boundary between light and heavy nuclei, exhibit a wide range of nuclear structure phenomena that remain somewhat mysterious [?]. In recent years, these nuclei have been extensively studied using a variety of experimental techniques [?]. A wealth of information on the Thomas-Ehrman shift has been gleaned from sd-shell proton drip-line nuclei, where numerous states exhibiting significant TES effects have been identified [?, ?]. For instance, the mirror pairs 18Ne/18O [?, ?] and 19Na/19O [?] serve as notable examples. For sd-shell nuclei, TES is mainly driven by s-waves. Indeed, the proton 1s1/2 orbital is weakly bound or unbound in proton drip-line nuclei, whereas the neutron 1s1/2 is well-bound in their mirror neutron-rich nuclei.

Several theoretical models have been developed to probe mirror asymmetry for mirror nuclei, such as the standard shell model (SM) [?], mean-field calculations [?, ?], and ab initio approaches [?, ?]. Within standard SM calculations, weakly bound and unbound wave functions on eigenenergies are indirectly considered via phenomenologically adjusting the matrix element related to the 1s1/2 orbit [?, ?]. Mean-field calculations, such as Skyrme-Hartree-Fock, have also been extensively employed in MED studies [?, ?]. However, these models involve parameters that are constrained by data [?, ?, ?]. In recent years, ab initio approaches such as the ab initio valence-space in-medium similarity renormalization group have also been applied to study MEDs of sd-shell nuclei [?, ?, ?, ?, ?], in which the extended many-body wavefunctions are partially described by using a large number of HO spaces.

Moreover, current theoretical calculations have pointed out that TES is caused by the repulsive Coulomb interaction and the occupations of weakly bound or unbound s- or p-waves for valence protons. However, detailed studies on the mechanism of TES are also lacking. In recent shell model calculations [?], TES has been investigated using calculated spectroscopic factors. Moreover, in our previous work [?], we compared MED results calculated using the shell model with spectroscopic factors and the ab initio valence-space in-medium similarity renormalization group approach, finding that the two models give similar results.

One of the major challenges in studying drip-line nuclei is accounting for the interplay between configuration mixing and continuum effects. The Gamow shell model (GSM) [?, ?, ?, ?, ?] has emerged as a powerful tool in this regard, as it provides a unified framework to describe the structure of nuclei close to the particle emission threshold and allows for an accurate understanding of exotic properties in drip-line nuclei. Based on this situation, we employ GSM to investigate significant mirror symmetry breaking with large MED values and the underlying mechanism for sd-shell nuclei, taking the 18Ne/18O and 19Na/19O mirror partners as examples.

II. METHOD

GSM is a multiconfiguration shell model framework that works in the picture of a core plus valence nucleons [?, ?, ?]. At the heart of GSM lies the utilization of the one-body Berggren basis [?], which possesses bound, resonance, and scattering states generated by a finite-range potential, typically of Woods-Saxon (WS) type (see details in Refs. [?, ?, ?]). The GSM Hamiltonian matrix is characterized as complex symmetric [?, ?]. The overlap method along with the Jacobi-Davidson method extended to complex-symmetric matrices is adopted to diagonalize and identify many-body resonance eigenstates [?, ?, ?]. Consequently, GSM calculations include both inter-nucleon correlations and continuum coupling [?, ?, ?].

The many-body Schrödinger equation of the GSM Hamiltonian can be solved within the so-called cluster orbital shell model (COSM) formalism [?] (see Refs. [?, ?, ?]). The GSM Hamiltonian in COSM coordinates reads [?, ?, ?]:

Aval(cid:88) ˆHGSM = (cid:18) p2 + ˆU (c) (cid:19) Aval(cid:88) (cid:18) ˆVij + (cid:19) pi · pj

where Aval is the number of valence nucleons, µi is the effective mass of the nucleon, ˆU(c) is represented by a one-body WS potential mimicking the inert core, ˆVij is the residual inter-nucleon interaction, which is modeled by a pionless effective field theory (EFT) interaction [?, ?], in which only two-body contact terms up to next-to-next-leading order are considered. The regularization approach adopted in Refs. [?, ?] is used. The last term embodies the recoil effects induced by the finite mass of the core Mc. The EFT interaction is optimized to reproduce the low-lying states of selected nuclei.

In the present work, the 18Ne/18O and 19Na/19O mirror partners are taken as examples. The doubly magic nucleus 16O is chosen as the inert core, and the s1/2, p1/2,3/2 and d3/2,5/2 partial waves are represented by the Berggren basis, in which 40 discretization points are used in total for continuum states in each partial wave, and the f5/2,7/2 partial waves are treated using the HO basis, in which 6 HO states are adopted for each partial wave. To estimate the effects of higher orbitals, we compare the results after adding the g7/2,9/2 partial waves under the HO basis; the difference in binding and excitation energy in the states studied in the present work is less than 5 keV. As such, higher partial waves are neglected. Only the Coulomb force is considered for the isospin non-conserving part of the GSM Hamiltonian. The contribution of the isospin-dependent part of nuclear interaction to TES is small and is neglected in the present GSM calculations. The Hamiltonian used in Ref. [?] is adopted in the present work. The calculated excitation energies of 18Ne/18O and 19Na/19O mirror partners are presented in Tables 1 and 2, which show good agreement with experimental data [?]. In the following section, the mechanics of the mirror energy difference for the 18Ne/18O and 19Na/19O mirror partners are investigated in detail.

III. RESULTS

Our GSM calculations accurately describe the excitation energies of low-lying states for the mirror partners 18Ne/18O and 19Na/19O. To delve deeper into the significant mirror symmetry breaking observed in these mirror nuclei, we define the MED for a given state Jπ as MED(Jπ) = Ex(T<z, Jπ) - Ex(T>z, Jπ), where Tz denote the negative and positive isospin projection Tz = (N - Z)/2, respectively, for a mirror pair. We have calculated MED values for mirror states in 18Ne/18O and 19Na/19O, as presented in Tables 1 and 2, along with experimental data. It is observed that in most states, the GSM-calculated MED values for low-lying states in the mirror partners 18Ne/18O and 19Na/19O align with experimental data. Although the numerical differences in excitation energies between calculated and experimental values for some states are relatively large, they still exhibit the expected qualitative trend of MED. Meanwhile, SM results perform poorly, which demonstrates that coupling to continuum states plays an essential role in the study of mirror states bearing significant mirror symmetry breaking. However, an exception is noted for the 0+2 state in the 18Ne/18O mirror nuclei, where our GSM calculations yield larger values than experimental data. Both our GSM calculations and experimental data highlight significant mirror symmetry breaking in the 3+1 state of the 18Ne/18O mirror nuclei and the 1/2+1 state of the 19Na/19O mirror nuclei, evidenced by their large MED values.

Table 1 . The calculated excitation energies of 18Ne/18O with GSM and SM calculations in harmonic oscillator single sd-shell model space without including higher orbitals, along with experimental data [?]. The unit of excitation energy is given in MeV, and the units of particle decay width and MED are given in keV.

Fig. 1 [Figure 1: see original paper]. The average occupation numbers for the s1/2 and d5/2 partial waves in the low-lying states of the 18Ne/18O mirror pair, calculated using the GSM above the 16O core.

Table 2 . Similar to Table 1, but for 19Na/19O.

Fig. 2 [Figure 2: see original paper]. Similar to Fig. 1, but for low-lying states in 19Na/19O.

To investigate the significant mirror symmetry breaking and the associated large MEDs, we begin by calculating the average occupations of low-lying states through GSM. The focus is particularly on the s1/2 and d5/2 partial waves above the 16O core for the 18Ne/18O and 19Na/19O mirror nuclei, as illustrated in Figs. 1 and 2. Notably, other partial waves like d3/2, f5/2,7/2 exhibit negligible occupations and are therefore excluded from these figures. The calculated average occupations reveal almost identical patterns for mirror states within the 18Ne/18O and 19Na/19O pairs. Our GSM calculations further indicate that states exhibiting significant mirror symmetry breaking with large MED values also show significant occupancy in the s1/2 partial waves—markedly higher than in their respective ground states. For instance, the occupations of the s1/2 partial wave for the 3+1 and 1/2+1 states in the 18Ne/18O and 19Na/19O mirror pairs, respectively, are substantially greater than those of the ground states. Additionally, our calculations show that the 0+2 states of 18Ne/18O demonstrate notable s1/2 partial wave occupations compared to the ground states, resulting in a large MED. Contrastingly, experimental data give a smaller MED value, hinting at a complex structure of the 0+2 states in 18Ne/18O that might not be fully captured by the 16O plus valence particles picture.

Aligned with results from other theoretical frameworks, such as the standard shell model and the ab initio VS-IMSRG approach, our results indicate that the significant mirror symmetry breaking with large MEDs observed in mirror states stems primarily from the extensive occupation of the s1/2 partial waves, which are weakly bound or unbound in the proton-rich nucleus but deeply bound in its mirror neutron-rich nucleus—this is the TES. However, a deeper understanding of mirror states bearing significant mirror symmetry breaking with large MED values is lacking. GSM is a very suitable model that properly treats both inter-nucleon correlations and continuum coupling to describe the properties of dripline nuclei, including a precise description of the many-body wave function in the asymptotic regions [**?**, **?**, **?**, **?**].

To elucidate the underlying mechanism of large MEDs, we conduct a detailed analysis of the radial density distributions of mirror states in 18Ne/18O and 19Na/19O pairs using GSM. The results allow us to systematically compare the radial distributions of valence protons in proton-rich nuclei and valence neutrons in their neutron-rich mirror counterparts, as presented in Figs. 3 and 4 for 18Ne/18O and 19Na/19O mirror partners, respectively. Our GSM results reveal that states characterized by minor mirror symmetry breaking with small MEDs exhibit almost identical radial density distributions, which decline sharply in the asymptotic regions, such as the ground states of both 18Ne/18O and 19Na/19O. This phenomenon is largely attributed to the dominance of d5/2 partial waves, which are constrained within the nuclear region by high centrifugal and Coulomb barriers, despite the state being unbound. Conversely, GSM calculations depict the radial density distributions of the 3+1 state of 18Ne and the 1/2+1 state of 19Na as more extended in the asymptotic region than their neutron-rich counterparts, 18O and 19O, respectively. This disparity stems from the non-existent centrifugal barrier for the s1/2 partial wave, leading to a more pronounced distribution in the proton-rich nucleus due to the weakly bound or unbound nature of the s1/2 partial wave.

A similar mechanism underlies the formation of halo nuclei, where valence nucleons occupy weakly bound s- or p-partial waves, resulting in an extended density distribution due to the minimal or absent centrifugal barrier [?, ?, ?]. In previous works, these exotic phenomena resulting from the mechanism for the extension of the s-partial wave have been widely recognized. However, in reality, most theoretical models cannot directly provide the properties of this extension and its impact on physical phenomena when performing calculations. For example, the results of our SM calculations within a single sd-shell model space in Table 1 show that the MEDs of all states for 18Ne/18O are quite small.

However, mirror symmetry breaking can be calculated using traditional SM by introducing further approximations and modifications. For example, traditional SM calculations using the USDC interaction give the MED of the mirror 1/2+1 state of 19Na/19O as -225 keV, which is significantly smaller than the experimental value of -727 keV. Moreover, the MED of the mirror 1/2+1 state of 19Na/19O is mainly caused by the difference in optimized single-particle energy for valence protons and neutrons in the USDC interaction [?]. Nevertheless, since the calculated MED is significantly smaller than experimental data, they simulated the TES arising from continuum coupling through TEStotal C2Ss1/2 TESsp, where C2Ss1/2 is the spectroscopic factor of the proton s1/2 orbital and TESsp is the single-particle TES [?]. This approximate treatment of TES gives MED values of mirror states close to experimental data. Based on this, the relationship between TES and the extended s1/2 partial wave in the mirror partner was indirectly determined; however, SM calculations cannot provide a direct description of TES. Moreover, phenomenological adjustments to the matrix elements related to the proton s1/2 orbital have also been employed in SM to describe the indirect effects of weakly bound and unbound wave functions on eigenenergies. For A 20 nuclei, the strength of effective SM interactions involving the loosely bound proton s1/2 orbit is significantly reduced in comparison with their mirror nuclei to calculate significant mirror symmetry [?], where reduction factors of the two-body matrix elements related to the proton s1/2 orbital are evaluated using the Woods-Saxon potential. The large MEDs in 18Ne/18O and 19Na/19O are well reproduced.

Unlike SM calculations with the aforementioned corrections, our GSM calculations provide a more self-consistent direct calculation of the radial density distribution, yielding the expected MEDs without relying on other corrections and modifications. Moreover, our calculations directly unveil that mirror states demonstrating significant mirror symmetry breaking with large MEDs possess many-body wave functions in proton-rich nuclei that are more extended than those in their neutron-rich mirror states, which further helps us understand the role of mirror symmetry breaking in shaping their properties.

Fig. 3 [Figure 3: see original paper]. The calculated radial density distribution of valence protons and valence neutrons for low-lying mirror states in 18Ne/18O, respectively, above the 16O inner core, using GSM.

Fig. 4 [Figure 4: see original paper]. Similar to Fig. 3, but for low-lying states in 19Na/19O.

The GSM Hamiltonian, as shown in Eq. (1), can be divided into nuclear interaction (encompassing core-nucleons and nucleon-nucleon interaction) and Coulomb interaction (including one-body Coulomb (1BC) interaction between the inner core and valence protons, and two-body Coulomb (2BC) interaction between valence protons). We delve into further calculations to dissect the contributions from different parts of the Hamiltonian, aiming to shed light on the underlying mechanisms in mirror states exhibiting significant mirror symmetry breaking with large MED.

The computed energies for the low-lying mirror states in the pairs 18Ne/18O and 19Na/19O, along with experimental data [?], are showcased in Figs. 5 and 6, respectively. To gain deeper insights, we also present the energy minus 2BC contribution (GSM-2BC) and energy minus 1BC and 2BC contribution (GSM-1BC-2BC) in proton-rich nuclei 18Ne and 19Na. Indeed, GSM-1BC-2BC corresponds to the contribution of nuclear interaction. Within the isospin symmetry picture, the difference in mirror state energies should solely stem from Coulomb interactions, implying that the GSM-1BC-2BC values for a state in a proton-rich nucleus would be the same as its mirror state in the neutron-rich nucleus.

Our GSM calculation gives that the GSM-1BC-2BC values for the ground states of 18Ne and 19Na closely align with the computed ground-state energies of their neutron-rich counterparts, 18O and 19O, respectively, indicating the preservation of mirror symmetry for these ground states. Conversely, for the excited 3+1 state in 18Ne/18O and the 1/2+1 state in 19Na/19O, our GSM calculations showcase a deviation from this symmetry. To quantitatively examine this discrepancy, we introduce ΔE as the differential metric for significant mirror symmetry breaking. ΔE encapsulates the disparity between the GSM-1BC-2BC values in the state of the proton-rich nucleus and the energy calculated for the corresponding state in the neutron-rich mirror nucleus, which reads as $\Delta E = \Psi\text{proton}|HNN|\Psi\text{proton} - \Psi\text{neutron}|HNN|\Psi\text{neutron}$, where Ψproton and Ψneutron correspond to the many-body wave functions of proton-rich and neutron-rich nuclei, respectively. The ΔE corresponds to the difference in the contribution of nuclear interactions in the mirror state.

Our GSM calculations show that both ΔE and Coulomb interactions, including 1BC and 2BC, significantly influence the energy discrepancies observed in mirror states. Predominantly, the Coulomb interaction emerges as the dominant factor contributing to these differences. Illustrated in the lower panels of Figs.

5 and 6, we detail the ΔE, 1BC, and 2BC contributions to the energy differences in the low-lying mirror states of 18Ne/18O and 19Na/19O mirror pairs. Our GSM results indicate that the energy differences in the ground states of 18Ne/18O primarily stem from Coulomb interactions, with ΔE making a minimal contribution. Furthermore, for 19Na/19O, the ΔE contribution is noted to be around 100 keV. Interestingly, we find varying contributions of ΔE, 1BC, and 2BC across different mirror states within each nucleus. For instance, the 3+1 states in 18Ne/18O exhibit a higher ΔE contribution and lower Coulomb interactions relative to their ground states. The heightened ΔE values underscore the distinct nuclear interaction contributions to mirror symmetry breaking in these systems, showcasing the complex interplay of forces that shape the energy landscapes of mirror nuclei.

In evaluating the MED, the ground state energy of mirror nuclei serves as the baseline, with MED being determined by the discrepancy in excitation energies of corresponding mirror states. Adopting the energy difference of the ground states of mirror nuclei as a reference—illustrated by red dashed lines in Figs. 5 and 6—the difference between the values of ground and excited mirror states corresponds to the MED, highlighted by the red arrows in these figures. The results reveal that both the ΔE values and the Coulomb interaction exhibit significant variations across different mirror states, both contributing to the MED.

Furthermore, to validate our conclusion, we performed Gamow shell model calculations using an optimized Hamiltonian fitted to reproduce a series of selected experimental data for sd-shell nuclei. This optimized Hamiltonian has been employed to investigate the low-lying states in 21Al [**?**] and 22Si [**?**], as well as isospin symmetry breaking in those nuclei. While the calculated excitation energies exhibit slight differences, the MED results align with both the current GSM calculations and the established conclusions regarding the MED mechanism.

Fig. 5 [Figure 5: see original paper]. Upper panel: calculated energies (GSM), energies minus the two-body Coulomb contribution (GSM-2BC), and energies minus one- and two-body Coulomb total contributions (GSM-1BC-2BC) of low-lying states of 18Ne using GSM, along with the energies of mirror states in 18O, with respect to the 16O inner core. The GSM results are also compared with experimental data. Lower panel: the contribution for the calculated energy difference between the mirror states.

Fig. 6 [Figure 6: see original paper]. Similar to Fig. 5, but for low-lying states in 19Na/19O.

IV. SUMMARY

Based on GSM calculations, in which both inter-nucleon correlation and continuum coupling are properly treated, we deduce that significant mirror symmetry breaking in mirror states, leading to large MED values, arises from the occupation of weakly bound or unbound s1/2 partial waves in the proton-rich nucleus, while its counterpart in the neutron-rich nucleus remains deeply bound. This dichotomy culminates in a more expansive radial density distribution for states within the proton-rich nucleus, as opposed to their mirror counterparts. Additionally, the difference in radial density distributions between mirror states implies disparate contributions from nuclear interactions, underscored by significant ΔE values, which further highlight the presence of mirror symmetry breaking. Moreover, states with an extended radial density distribution tend to yield smaller Coulomb contributions compared to ground states characterized by more localized distributions. This factor chiefly accounts for the reduced excitation energies in states influenced by the Thomas-Ehrman shift effect, thereby engendering substantial negative MED values in mirror states. Our GSM calculations corroborate that both nuclear and Coulomb interactions play crucial roles in manifesting the significant mirror symmetry breaking associated with large MED values.

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