Isospin symmetry breaking at high spins in the mirror pair ^{67}Se and ^{67}As

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Recent experimental data have revealed large mirror energy differences (MED) between high-spin states in the mirror nuclei ^{67}Se and ^{67}As, the heaviest pair where MED have been determined so far. The MED are generally attributed to the isospin symmetry breaking caused by the Coulomb force and by the isospin nonconserving part of the nucleon-nucleon residual interaction. The different contributions of the various terms have been extensively studied in the fp shell. By employing large-scale shell model calculations, we show that the inclusion of the $g_{9/2}$ orbit causes interference between the electromagnetic spin-orbit and the Coulomb monopole radial terms at high spin. The large MED are attributed to the aligned proton pair excitations from the $p_{3/2}$ and $f_{5/2}$ orbits to the $g_{9/2}$ orbit. The relation of the MED to deformation is discussed.

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One of the current topics in nuclear structure physics is the isospin symmetry breaking due to the Coulomb force and the strong nucleon-nucleon (NN) interaction. Assuming isospin symmetry, mirror pair nuclei, i.e. a pair of nuclei with exchanged proton and neutron numbers, have identical level schemes. However, the Coulomb effects and the isospin nonconserving NN interaction break this symmetry, leading to observable differences between energy levels of analogue states. The so-called mirror energy differences (MED) are defined by

$$\mathrm{MED}_J \;=\; E_x(J,T,T_z=-T)-E_x(J,T,T_z=T), \qquad (1)$$

where $E_x(J,T,T_z)$ are the excitation energies of analogue states with spin J and isospin T, T_z. The MED are thus regarded as a measure of isospin symmetry breaking in an effective interaction which includes the Coulomb force. The MED have been extensively studied for mirror pair nuclei in the upper *sd* and the lower fp shell regions (see Ref. [1] for review). In both cases, a remarkable agreement between experimental data and shell model calculations has been achieved, allowing a clear identification of the origin of the MED based on the isospin nonconserving Coulomb and strong NN forces [2–18].

For mirror nuclei in the upper part of the fp shell the situation is different. The experimental information on MED is relatively scarce and only recent large-scale shell model calculations including the $g_{9/2}$ orbit have become available [19, 20]. Moreover due to the deformation driving effect of the $g_{9/2}$ orbit, variations in the MED are expected to be strongly related to the change in the nuclear deformation. Recently new data on the A=67 mirror nuclei ^{67}Se and ^{67}As have become available [21]. Investigations [22] for ^{66}Ge suggested that the spin alignment of the $g_{9/2}$ neutrons occurs at $J^\pi = 8^+$. As the positive-parity band built on the $9/2^+$ state in ^{67}As can be interpreted as a $g_{9/2}$ proton weakly coupled to the ^{66}Ge core, the neutron spin alignment is expected to occur at spin $25/2^+(=8^+ + 9/2^+)$ in ^{67}As [22, 23]. On the other hand, the proton spin alignment takes place at the same spin in its mirror partner ^{67}Se. As the response to the Coulomb field is different for the corresponding high-spin states in such mirror nuclei, one expects the Coulomb based MED contribution in ^{67}Se and ^{67}As to give large negative value suddenly at $25/2^+$ where the proton/neutron spin alignment occurs. In the lower fp-shell region, due to the active role played by the $f_{7/2}$ shell, in the MED the isospin nonconserving NN interaction has been suggested to be at least as important as the Coulomb part [24]. In the upper fp-shell region the situation is different and one does not expect a major contribution because the $f_{7/2}$ shell is almost not active.

For the $A = 67$ mirror pair nuclei, excited states have been known for ^{67}As [23, 25], and have been recently determined for the mirror partner ^{67}Se [26]. This is the heaviest mirror pair where the excited energy levels have been identified with detailed experimental information. In both cases, the low-lying $9/2^+$ state has been found to be isomeric, allowing the determination of the degree of isospin symmetry breaking through the measurement of the mirror $9/2^+ \to 7/2^-$ $E1$ strengths [21]. In our previous paper [19], the structure of this isomeric state has been investigated using large-scale shell model calculations. The isomerism of the $9/2^+$ state was understood as due to proton and neutron configuration mixing based on the $g_{9/2}$ intruder orbit as well as on the fp-shell structures.

In this Rapid Communication, we investigate the MED in the mirror pair ^{67}Se and ^{67}As discussing the origin of isospin symmetry breaking in the upper fp-shell region. Theoretical calculations are performed using the spherical shell model in the $pf_{5/2}g_{9/2}$ model space. We employ the recently proposed JUN45 interaction [20], a realistic effective interaction based on the Bonn-C potential and ajusted to the experimental data of nuclei in the $A = 63 \sim 96$ mass region. To describe the MED, the first attempt was carried out by adding the

Coulomb term to the KB3 interaction matrix elements [27]. However, those calculations did not succeed to describe the experimental MED for the mirror pairs of mass $A = 47$ and $A = 49$. A better agreement with the data has been obtained using the formalism introduced by Zuker *et al.* [24]. In this description the Coulomb matrix elements in the valence space represent only the multipole part of the Coulomb interaction whereas the contribution of the other nucleons is described by the Coulomb monopole effect. The Coulomb interaction is therefore separated into a monopole term V_{Cm} and a multipole term V_{CM}. While V_{Cm} accounts for single-particle and bulk effects, V_{CM} contains all the rest. The monopole term V_{Cm} is further divided into the single particle correction ε_{ll}, the radial term V_{Cr} and the spin orbit term ε_{ls}. The contribution of ε_{ll} to the monopole term is given by [6]

$$\varepsilon_{ll} \;=\; \frac{-4.5 Z_{cs}^{13/12}[2l(l+1)-p(p+3)]}{A^{1/3}(p+3/2)}, \qquad (2)$$

where Z_{cs} is the proton number corresponding to a closed shell, p the principal quantum number, and l the orbital momentum. Due to such single particle correction, in ^{67}Se the proton $g_{9/2}$ and $f_{5/2}$ orbits are lowered roughly by 95 keV and 58 keV, respectively, while the energy of the $p_{3/2}$ orbit is raised by about 135 keV. The relative energy gap between the proton $g_{9/2}$ and $f_{5/2}$ orbits is reduced of only 37 keV, and therefore there is basically no effect on single-particle levels due to the ε_{ll} term.

The radial term V_{Cr} reflects the change in radii along the rotational band, and in the fp shell is proportional to the change in occupancy of the $p_{3/2}$ orbit as a function of spin J. It can be expressed as $\Delta_{MED}(V_{Cr}) = a_m(\langle m_{p3/2}\rangle_{9/2}/2 - \langle m_{p3/2}\rangle_J/2)$, where $\langle m_{p3/2}\rangle_J$ with $m_{p3/2} = z_{p3/2} + n_{p3/2}$ is the expectation value of the proton and neutron number in the $p_{3/2}$ orbit at spin J and a_m is the strength parameter fitted to the experimental data. When the occupation of the $p_{3/2}$ protons decreases, valence protons in orbits with smaller radii are nearer to the charged core, which results in a gain of Coulomb energy [1]. In the $pf_{5/2}g_{9/2}$ shell, the $p_{3/2}$ orbit has larger radius than the $f_{5/2}$ and $g_{9/2}$ orbits and therefore the Coulomb repulsion increases as the number of protons increases. Here the role of the $p_{1/2}$ orbit is less important simply because the $p_{1/2}$ occupancy is small, and furthermore it does not change very much as a function of the angular momentum J.

The single-particle shift ε_{ls} takes into account the relativistic spin-orbit interaction [28]. This interaction comes from the Larmor precession of the nucleons in the electric field due to their magnetic moments, which, as well known, affects the single-particle energy spectrum. ε_{ls} can be written as [28]

$$\varepsilon_{ls} \;=\; (g_s - g_l)\frac{1}{2m_N^2c^2}\left(\frac{1}{r}\frac{dV_c}{dr}\right)\langle \hat{l}\cdot\hat{s}\rangle, \qquad (3)$$

where m_N is the nucleon mass, and the free values of the gyromagnetic factors, g_s^{π}=5.586, g_l^{π}=1 for protons and g_s^{ν}=-3.828, g_l^{ν}=0 for neutrons, are used. In the present work, by assuming a uniformly charged sphere, ε_{ls} is calculated using the harmonic oscillator single-particle wave function. Depending on proton or neutron orbit, the shift can have opposite signs. It depends also on the spin-orbit coupling, as for instance $\langle \hat{l}\cdot\hat{s}\rangle = l/2$ when $j = l+s$ and $\langle \hat{l}\cdot\hat{s}\rangle = -(l+1)/2$ when $j = l-s$. As this term influences differently on neutrons and protons, its effect becomes very important for some particular states. In ^{67}Se, the proton $g_{9/2}$ orbit is lowered by about 66 keV, while the $f_{5/2}$ orbit is raised by about 66 keV, the effect being opposite for ^{67}As. Also the relative energy gap between the proton $g_{9/2}$ and $f_{5/2}$ orbits decreases roughly by 132 keV, providing a large contribution to the MED. Since the spin-orbit contribution leads to a reduction of the energy gap between the proton $g_{9/2}$ and $f_{5/2}$ orbits, excitations from those orbits into the $g_{9/2}$ orbit are enhanced. The opposite effect is predicted to happen in ^{67}As for the neutron orbits.

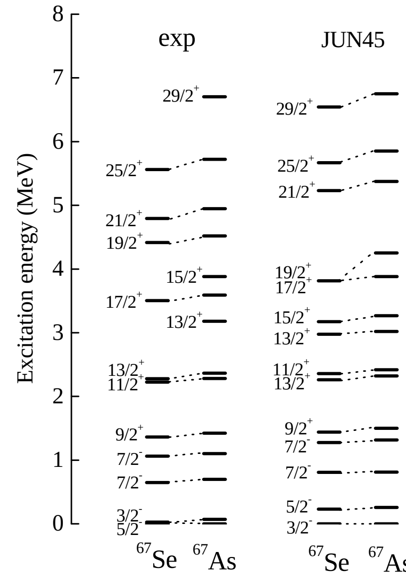

FIG. 1: Comparison of calculated energy levels (JUN45) with experimental data (exp) for ^{67}Se and ^{67}As.

With inclusion of V_{CM}, ε_{ll} and ε_{ls}, shell-model calculations are carried out in the $pf_{5/2}g_{9/2}$ shell for the $A = 67$ mirror nuclei. The isospin nonconserving term is neglected in the upper half of fp shell region because the $f_{7/2}$ orbit is almost not active. The calculation uses the code MSHELL [29] and the effective interaction JUN45. After solving the eigenvalue problem, contribution of the Coulomb monopole radial term V_{Cr} is included into the energy E_J obtained in the shell model calculation, where the strength parameter a_m was fix to 280 keV so as to fit the MED of the postive-parity high-spin states, and taken as 0.0 keV for the negative-parity states.

In Fig. 1, the calculated energy levels are shown, and compared with the experimental data for ^{67}Se and ^{67}As. As one can see, the calculation with the JUN45 interaction reproduces well the experimental data. The energy differences of the analogue states are in a reasonable agreement with experiment. The structure of the negative-parity states at low-excitation energies are mainly dominated by the fp shell configurations.

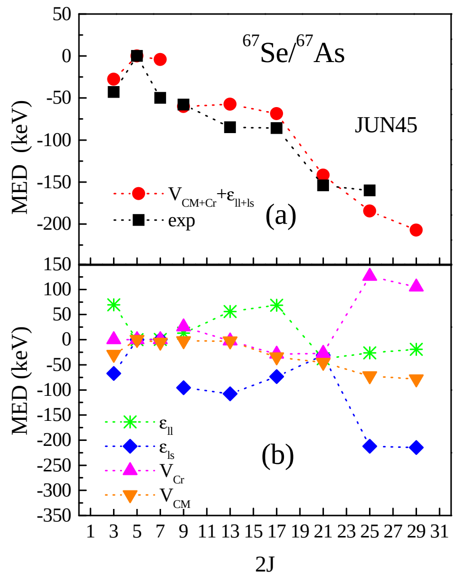

FIG. 2: (Color online) The MED for states shown in Fig. 1. Upper graph: Comparison of calculated MED with available data. Lower graph: Decomposition of theoretical MED into four terms (see text for explanation).

The positive-parity states built at higher spin strongly involve the $g_{9/2}$ orbit. The structural difference of such configurations strongly reduces the transition strengths explaining the isomeric character of the $9/2^+$ levels [19]. We note however that the calculated level energy for the $19/2^+$ state lies lower than the experimental value.

In the past few years, experimental data on mirror nuclei above the doubly magic ^{56}Ni have become available. Ekman *et al.* [13] discussed the MED of the $A \sim 60$ mass region based on the results of the shell model calculations. It was reported that for the MED the contribution of the electromagnetic spin-orbit term ε_{ls} is significant, but the monopole Coulomb ε_{ll} term is not. Energy shifts due to ε_{ls} increase the gap between the $p_{3/2}$, $f_{5/2}$ and the $g_{9/2}$ orbits for neutrons but reduce it for protons. As a consequence excitations involving those orbits have important contribution to MED.

In Fig. 2 (a), the experimental MED along the positive-parity excited band with $\Delta J = 2$ built on the $9/2^+$ state and the low-lying negative-parity states $(3/2^-, 5/2^-, 7/2^-)$ are compared with the results of our JUN45 calculations as a function of spin $2J$. The agreement is excellent. In particular, the calculation reproduces correctly the large negative value in the MED at the high-spin $21/2^+$ and $25/2^+$ states. It is now interesting to examine which terms contribute to such drastic changes in the MED. In order to see this, the four different contributions to MED have been plotted separately in Fig. 2 (b). The Coulomb multipole term V_{CM} reflects the alignment effects at high spin and follows the negative trend of the MED. It is in fact well known that spin alignments affect the MED, which is a behavior first suggested by Sheikh *et al.* [30] based on results from the deformed cranked shell model. In the mirror pair ^{49}Mn and ^{49}Cr the alignment process has been examined based on the shell-model calculations by counting the number of proton pairs in the shell j coupled to the maximum spin $J = 2j - 1$ [5]. It was shown that this number is closely correlated with the MED. For the present case of ^{67}Se, two protons and one neutron jump up from the fp-shell to $g_{9/2}$ at spin of $25/2^+$ and $29/2^+$. The spin alignment of the two protons in the $g_{9/2}$ orbit increases the spatial separation between them, leading to a smaller Coulomb energy. Thus, the alignment effect for protons reduces the excitation energy in ^{67}Se while the same does not happen in the analogue states in ^{67}As. However, as can be seen in Fig. 2 (b), the V_{CM} term alone underestimates the MED by a factor of three. As already noticed the contribution of the ε_{ll} term is only marginal. V_{Cr} gives the largest positive contribution in particular for the $25/2^+$ and $29/2^+$ states due to the increased occupation of the $g_{9/2}$ orbit. On the other hand, the ε_{ls} contribution to the MED is strongly negative for the $25/2^+$ and $29/2^+$ spin values. When the V_{Cr}, V_{CM}, ε_{ls} and ε_{ll} terms are all included, the theoretical MED reproduce well the experimental data. We note, however, that the strength of V_{Cr} was fitted to data and not determined in an independent way. The ε_{ls} and V_{Cr} terms contribute to the MED from the opposite directions, causing a large cancelation at the highest spins. For the $21/2^+$ state, all terms give almost the same contribution of about 40 keV, providing in total large MED. Below $21/2$, the ε_{ls} term competes with the ε_{ll} term, while the V_{Cr} and V_{CM} values are small. In our conclusion therefore the observed MED behaviour in the ^{67}Se and ^{67}As pair is characterized by a strong competition among the different terms, dominated at high spin by the interference of the spin orbit and radial contributions.

A question that we now address concerns the importance of the isospin nonconserving term of the NN interaction. The good results shown in Fig. 2 have been obtained through the inclusion of the V_{Cr} term whose strength is however fitted to the experimental data. As seen in Fig. 2, calculations without V_{Cr} cannot reproduce the data in the high-spin region. In the $f_{7/2}$ shell nuclei the isospin nonconserving NN term is important mainly at the low spin region [1]. If one speculates that a similar behavior occurs also in the $g_{9/2}$ shell, this would imply a limited contribution of the isospin nonconserving term to the high spin region in the current discussion. The calculation presented in this work indeed shows that we can obtain a good agreement with the experimental data for the MED without including an explicit isospin breaking NN term. All these seem to suggest that the isospin nonconserving NN term is not important. However, since we have normalised a part of the interaction by fitting to the experimental data, we cannot make a strong conclusion about the role of the isospin nonconserving part that in principle contributes to the MED.

To support the above picture, Fig. 3 shows the calculated occupancies of the excited band with $\Delta J = 2$ built on the $9/2^+$ state in ^{67}Se. The upper and lower graphs are for protons and neutrons, respectively. From the upper graph, one can see that for the $9/2^+$ state, protons occupy mainly the fp-shell and partially the $g_{9/2}$ orbit. The occupations change gradually such that the fp occupancies increase but the $g_{9/2}$ one

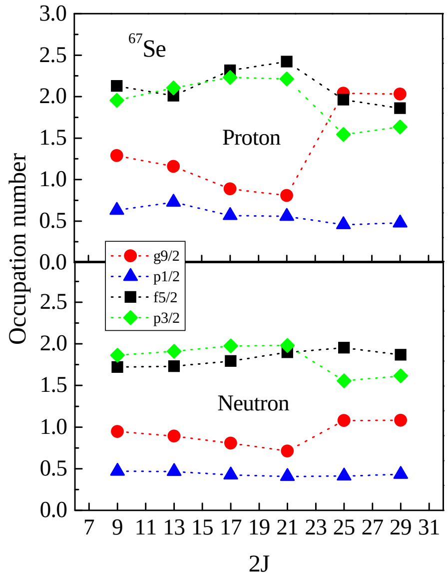

FIG. 3: (Color online) Calculated occupation numbers for proton orbits (upper graph) and neutron orbits (lower graph) in ^{67}Se.

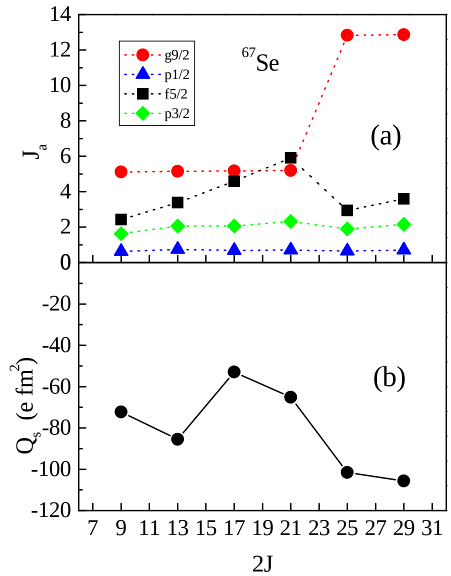

FIG. 4: (Color online) Calculated spin distribution in each orbit (upper graph) and spectroscopic quadrupole moment (lower graph) in ^{67}Se. The spin distribution is the spin value J_a on a single-particle orbit a for the excited states (see text for explanation).

decreases as a function of $2J$. However, it is notable that the proton $g_{9/2}$ occupation increase suddenly at spin $25/2$, and the proton $p_{3/2}$ and $f_{5/2}$ occupations decrease at the same spin. This means that two protons and one neutron jump up from the fp-shell to the $g_{9/2}$ orbit at spin $25/2$. This drastic change of occupations is in clear contrast to that of the $f_{7/2}$-shell nuclei, where the occupations of $p_{3/2}$ and $f_{7/2}$ orbits change gradually with increasing spin [1]. The lower graph indicates a similar pattern for neutrons, but the variation is not so large. As already mentioned above, the change in occupancy of the $p_{3/2}$ orbit affects strongly the MED through the Coulomb monopole radial term V_{Cr}. Since the $p_{3/2}$ orbit has larger radius than the $g_{9/2}$ orbit, when at high spin nucleons are filling the $g_{9/2}$ shell the Coulomb monopole contribution is larger than that at low spins.

We finally show the calculated spin alignment and spectroscopic quadrupole moment in ^{67}Se. In Fig. 4 (a), the spin distribution of the expectation value $J_a = \sqrt{\langle \vec{j}_a \rangle^2}$ is plotted as a function of spin $2J$, where $\vec{j}_a$ is angular momentum operator for each orbit a. As the neutron orbits are blocked for this odd-neutron nucleus, the first alignment will be that of a pair of $g_{9/2}$ protons which brings additional 8 units of angular momentum. It is clearly visible that the proton pair and one neutron alignment in ^{67}Se occur at spin $25/2$. The $29/2^+$ state also shows a large aligned spin value. This alignment is interpreted as five-quasiparticle configuration involving two protons and three neutrons. Figure 4 (b) shows the calculated spectroscopic quadrupole moment Q_s (in $e$fm^2) for the excited states built on the $9/2^+$ level in ^{67}Se. The Q_s absolute value has sudden increase at spin $25/2$ corresponding to the sudden increase in spin alignment (see the upper graph). This suggests that the quadrupole moment is closely related to the spin alignment of the $g_{9/2}$ proton pair, which correlates with the multipole term V_{CM} of the MED. Therefore, change in deformation seems to affect the MED, but its influence is not large. It should be noted that the present V_{Cr} calculation and the discussion on occupation of the single-particle orbits are carried out in a spherical basis, and therefore, the deformation effects (such as changes of single-particle levels by the shape-driving effect) are not explicitly seen. To study the deformation effects in the MED, a shell model based on deformed single-particle states [31, 32] would have to be employed.

In conclusion, we investigated the MED between high-spin states in the mirror pair ^{67}Se and ^{67}As using large-scale shell model calculations. The calculations reproduce well the experimental level schemes, and confirm the suitableness of the JUN45 effective interaction for this mass region. The need for inclusion of the $g_{9/2}$ orbit in the description for the MED in the upper fp shell nuclei was demonstrated. In this mass region, the electromagnetic spin-orbit interaction and the Coulomb monopole radial term are responsible for producing the large MED at high-spin states, while the contribution from the Coulomb multipole term is small. The occupations of the relevant orbits and the spin alignment in the $g_{9/2}$ orbit affect the variation of the MED along the band built on the $9/2^+$ state. We obtained a good agreement with the experimental data for the MED without involving the isospin nonconserving part. However, it cannot be concluded that the isospin nonconserving NN term is not important. This remains an open question.

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