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Isospin symmetry breaking in the mirror pair ^{73}Sr-^{73}Br

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The recent experimental observation of isospin symmetry breaking (ISB) in the ground states of the $T = 3/2$ mirror pair ^{73}Sr-^{73}Br is theoretically studied using large-scale shell-model calculations. The large valence space and the successful PFSDG-U effective interaction used for the nuclear part of the problem capture possible structural changes and provide a robust basis to treat the ISB effects of both electromagnetic and nonelectromagnetic origin. The calculated shifts and mirror-energy differences are consistent with the inversion of the $I^\pi = 1/2^-, 5/2^-$ states between ^{73}Sr and ^{73}Br and suggest that the role played by the Coulomb interaction is dominant. An isospin breaking contribution of nuclear origin is estimated to be $\approx$25 keV.

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I. Introduction. In a recent article entitled *"Mirror-symmetry violation in bound nuclear ground states"* [1], Hoff and collaborators reported the results of an experiment carried out at the National Superconducting Cyclotron Laboratory in which the decay of the proton-rich $T = 3/2$, $T_z = -3/2$ isotope ^{73}Sr was studied. Following a detailed and convincing analysis of the experimental data, they conclude that its ground state has $I^\pi = 5/2^-$. This observation is at odds with its mirror $T = 3/2$, $T_z = 3/2$ partner ^{73}Br which has a $I^\pi = 1/2^-$ ground state, and, thus, the topic of their paper. The theoretical interpretation, which accompanies the paper, cannot reproduce the inversion, and the authors conclude with two main points, one related to the well-known Thomas-Ehrman shift [2,3]: (sic) *Such a mechanism is not immediately apparent in the case of* ^{73}Sr / ^{73}Br, *and it may be that charge-symmetry-breaking forces need to be incorporated into the nuclear Hamiltonian to fully describe the presented results*, and the other one related to possible structural effects: (sic) *(the) inversion could be due to small changes in the two competing shapes, particularly, their degree of triaxiality, and the coupling to the proton continuum in the isobaric analog state of* ^{73}Rb.

Besides the fact that the $I^\pi = 1/2^-$ in ^{73}Sr is an excited state, there is no information available about its location. On the contrary, the level scheme of ^{73}Br is better known with an $I^\pi = 5/2^-$ state at 27 keV, an $I^\pi = 3/2^-$ at 178 keV and another $I^\pi = (3/2^-, 5/2^-)$ state at 241 keV. Given the above, it seems opportune to comment already that the mirror energy difference (MED) of the $1/2^-$ arising from the mirror symmetry violation can be as low as $\sim$30 keV. Note that MEDs as large as 300 keV have been measured for the 2^+ states of the ^{36}Ca-^{36}S mirror pair, which can be understood without invoking threshold effects [4]. Even further, in the same mirror pair, a prediction of a huge MED of 700 keV for the first excited 0^+ states has been made in Ref. [5], again without the need of threshold effects. There is abundant experimental and theoretical work on the subject of the MEDs which we believe provides a natural framework to interpret the new data. Actually, Ref. [6] places the new result within the context of the extensive body of available data, and the authors concluded that, being entirely consistent with normal behavior, the inversion does not provide further insight into isospin symmetry breaking (ISB).

Here, in line with the findings of Refs. [7,8], we propose an explanation based on the configuration-interaction shell model (SM-CI) to treat the nuclear (isospin conserving) part of the problem, plus a detailed analysis of both Coulomb and other ISB effects. The large valence space and the well-established effective interaction we use allow us to describe deformed nuclei in the laboratory frame without the restriction to axially symmetric shapes as considered in Ref. [1].

II. The shell-model framework. A. The nuclear input. We describe the $A = 73$, $T = 3/2$ system with the isospin conserving effective interaction PFSDG-U [9] which has been successful for a large region of nuclei from the pf shell to the $N = 40$ and $N = 50$ islands of inversion. Recently applied to the structure of ^{78}Ni [10], it can be considered as an extension of the Lenzi-Nowacki-Poves-Sieja interaction [11] which encompasses nuclei at and beyond $N = 50$.

The PFSDG-U interaction, defined for the full $pf + sdg$ shells, is, here, used in the valence space given by the orbits: $0f_{7/2}$, $1p_{3/2}$, $0f_{5/2}$, $1p_{1/2}$, $0g_{9/2}$, and $1d_{5/2}$ with the single-particle energies (SPEs) taken directly from the experimental spectra of ^{41}Ca as summarized in Table I. In the present calculation, an inert core of ^{56}Ni is adopted, and the number of excitations across $N = Z = 40$ are limited to four to achieve convergence for the states of interest which have dimension $\approx 10^9$. The isospin conserving (nuclear only) calculation produces a ground state $I^\pi = 5/2^-$ and the first excited state, $I^\pi = 1/2^-$ at 21 keV as shown schematically in Fig. 1 and in

TABLE I. Valence space and single-particle energies used in the present SM-CI calculations.

Orbit	$0f_{7/2}$	$1p_{3/2}$	$0f_{5/2}$	$1p_{1/2}$	$0g_{9/2}$	$1d_{5/2}$
SPE (MeV)	−8.363	−5.93	−1.525	−4.184	−0.013	0.937

agreement with the new measurement for ^{73}Sr. A $I^\pi = 3/2^-$ is found at 288 keV. With this as our starting point, we will next turn our attention to the role of the different ISB effects, responsible for the inversion of states in ^{73}Br.

B. Isospin symmetry-breaking analysis. In the following, we consider two methods to account for the ISB effects.

Method 1. The Coulomb interaction V_C is anticipated to be the most important mechanism contributing to the isospin breaking. In this first approach, it is simply added to the nuclear one in the SM-CI calculation,

$$H = H_N + V_C. \quad (1)$$

We have verified that nonperturbative and perturbative treatments give almost identical results. In the former, the Hamiltonian in Eq. (1) is directly diagonalized for each of the two mirror nuclei,

$$H|^{73}\text{Sr}, I^\pi\rangle = E_{I^\pi}(^{73}\text{Sr})|^{73}\text{Sr}, I^\pi\rangle,$$
$$H|^{73}\text{Br}, I^\pi\rangle = E_{I^\pi}(^{73}\text{Br})|^{73}\text{Br}, I^\pi\rangle.$$

In the latter, the eigenstates of H_N, $|A, T, I^\pi\rangle$ are used to compute the expectation value of the Coulomb interaction for each nucleus,

$$\delta E_{\text{pert}}(^{73}\text{Sr}, I^\pi) = \langle 73, 3/2, I^\pi|V_C(^{73}\text{Sr})|73, 3/2, I^\pi\rangle$$
$$\delta E_{\text{pert}}(^{73}\text{Br}, I^\pi) = \langle 73, 3/2, I^\pi|V_C(^{73}\text{Br})|73, 3/2, I^\pi\rangle.$$

V_C can be divided into three terms: core, one-body, and two-body. With the indices m, n representing the protons in

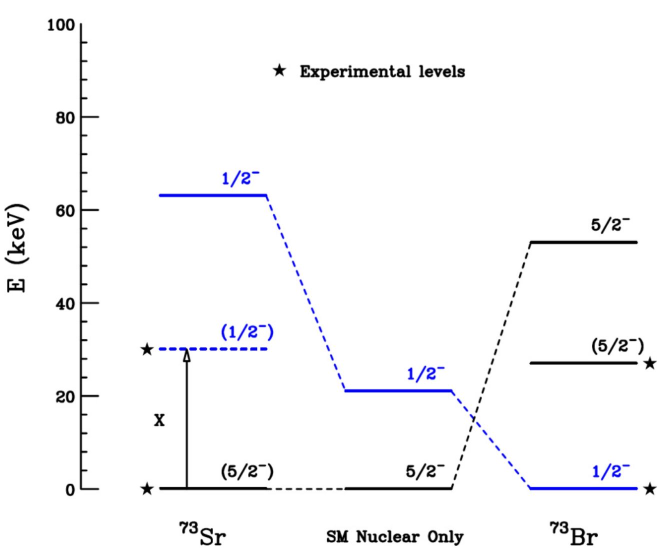

FIG. 1. Shell-model results compared to the experimental levels indicated by a star. The SM isospin conserving result with only the nuclear interaction is shown in the middle of the panel.

TABLE II. Method 1. Isospin symmetry-breaking contributions to the excitation energies of the lower states in ^{73}Sr and ^{73}Br, C1 (1B) and C2 (2B) (in keV). They are added to the nuclear only values to produce the total and MED columns, the ones to be eventually compared with experiment.

I^π	Nuclear	^{73}Sr			^{73}Br			MED
		$C1$	$C2$	Total	$C1$	$C2$	Total	
$5/2^-$	0	0	0	0	53	0	53	0
$1/2^-$	21	25	17	63	−27	6	0	116
$3/2^-$	288	3	−79	212	55	18	361	−96

the core and i, j the valence protons, we have

$$V_{C,\text{Core}} = \sum_{n,m} e^2/r_{n,m},$$

$$V_{C,1\text{B}} = \sum_j n_j \left(\sum_n e^2/r_{n,j}\right),$$

$$V_{C,2\text{B}} = \sum_{i,j} e^2/r_{i,j}.$$

The first term is the same for both nuclei and is not considered further. The one-body term affects only the single-particle energies of the proton orbits. We adopt the experimental spectrum of ^{41}Sc, where a lowering of 225 keV of the energies of the p orbits relative to the f orbits is observed. The two-body Coulomb matrix elements are calculated with harmonic-oscillator (HO) wave functions using $\hbar\omega = 45A^{-1/3}$–$25A^{-2/3}$ MeV. Their expectation values are denoted by $C1$ and $C2$, respectively. The results for the two mirror isotopes, including the individual contributions, are given in Table II and illustrated in Fig. 1.

It is clearly seen that: (i) This approach produces the desired inversion in ^{73}Br, and (ii) it is the one-body part of the Coulomb interaction, i.e., the shift in the proton single-particle energies of the p orbits relative to the f orbits, which is responsible for this phenomenon. If we shift the proton SPEs of the g and d orbits by the same quantity than the p orbits, we obtain qualitatively the same results and do not change appreciably even if we double the SPE correction. It is important to note that the difference of the SPE between protons and neutrons, taken from the experimental data, may not be only of electromagnetic origin. In addition, a reduction of the single-particle energy shift of the proton orbits of about 100 keV will line up the excitation energy of the $5/2^-$ state in ^{73}Br with the experimental value and halve the predicted excitation energy of the $1/2^-$ state in ^{73}Sr.

The MEDs are defined as the difference between the excitation energy of analog states, thus, putting the MED for the ground states to zero [7], which have, in general, the same spin and parity. As this is not the case here, we calculate the MED with respect to the $5/2^-$ state, that is the lowest state for the pure nuclear field. We report in the last column of Table II the MED obtained as

$$\text{MED}_{I^\pi} = E^*_{I^\pi}(^{73}\text{Sr}) - E^*_{I^\pi}(^{73}\text{Br}),$$

where $E^*_{I^\pi} = E_{I^\pi} - E_{5/2^-}$.

TABLE III. Method 2. Corrections to the SPEs of neutrons and protons (in keV), introduced by the electromagnetic $C_{\ell s}$ and $C_{\ell\ell}$ terms.

	$0f_{7/2}$	$1p_{3/2}$	$0f_{5/2}$	$1p_{1/2}$	$0g_{9/2}$	$1d_{5/2}$
Neutrons (ℓs)	52.5	17.5	−70	−35	70	35
Protons ($\ell s + \ell\ell$)	−100	65	47	128	−144	38

Method 2. Here, we follow the approach discussed in the review article [8] that considers several contributions to the MED:

Multipole Coulomb C_M. It is constructed as the Coulomb 2 in Method 1, the only difference is that only the multipole part of the two-body Coulomb matrix elements is considered. It is sensitive to microscopic features, such as the change in single-particle spin recoupling and alignment.

Single-particle energy corrections $C_{\ell s}$ and $C_{\ell\ell}$. Starting from identical single-particle orbits for protons and neutrons, given in Table I, relative shifts due to the electromagnetic spin-orbit interaction $C_{\ell s}$ [12] and the orbit-orbit term $C_{\ell\ell}$ [13] are introduced.

The electromagnetic spin-orbit interaction is as follows:

$$V_{\ell s} = (g_s - g_\ell)\frac{1}{2m_N^2c^2}\left(-\frac{1}{r}\frac{dV_C}{dr}\right)\vec{\ell}\cdot\vec{s},$$

where g_l and g_s are the g factors and m_N is the nucleon mass. The correction is given by

$$C_{\ell s} \simeq 14.7(g_s - g_\ell)\left(\frac{Z}{A}\right)[\ell(\ell+1) + s(s+1) - j(j+1)]\ \text{keV},$$

which, although ≈50 times smaller than the nuclear spin-orbit interaction, its effect on the excitation energies can be of several tens to hundreds of keV.

It is clear that this interaction contributes differently on protons and neutrons.

The $C_{\ell\ell}$ energy correction has been deduced in Ref. [13] and is given by

$$C_{\ell\ell} = \frac{-4.5Z_{cs}^{13/12}[2\ell(\ell+1) - N(N+3)]}{A^{1/3}(N+3/2)}\ \text{keV},$$

with Z_{cs} the atomic number of the closed shell. For $A = 73$, $Z_{cs} = 20$ and the corresponding HO principal quantum numbers $N = 3$ and $N = 4$, the energy shifts to be added to the bare energies in Table I are reported in Table III.

The corrections of electromagnetic origin introduced so far have no free parameters and affect the excitation energy of the analog states in each of the mirror nuclei. When added to the nuclear only result of Sec. II A, that places the $1/2^-$ state at 21-keV excitation energy, the multipole Coulomb interaction increases the energy of this state by 26 keV in ^{73}Sr and by 3 keV in ^{73}Br. The single-particle corrections $C_{\ell s}$ and $C_{\ell\ell}$ increase further the energy of the $1/2^-$ state in ^{73}Sr by 17 keV and by 6 keV in ^{73}Br. Although the effect is much larger in ^{73}Sr ($E_{1/2^-} = 64$ keV) than in its mirror ^{73}Br ($E_{1/2^-} = 30$ keV), these corrections do not reproduce the experimental inversion of the $1/2^-$ and $5/2^-$ states in ^{73}Br.

There are two additional corrections in Method 2 that have still to be considered. They are of pure isovector character, and we can calculate their contributions to the MEDs, but not the effects on the excitation energies in each mirror partner separately. However, as we will show, taking into account the data in ^{73}Br, the calculated MEDs are compatible with the inversion of the two states between ^{73}Sr and ^{73}Br. We describe in the following paragraphs these two empirical and schematic isovector contributions to the MEDs.

Radial term C_r. Of Coulomb origin, it takes into account changes of the nuclear radius for each excited state. These changes are due to differences in the nuclear configuration that depend on the occupation number of the orbits. Low-ℓ orbits have larger radii than the high-ℓ orbits in a main shell. This has a sizable effect in the MED: Protons in larger orbits suffer less repulsion than those in smaller orbits, which reflects in the binding energy of the nuclear states. Originally introduced in Ref. [14], the halo character of low-ℓ orbits has been recently discussed in detail in Ref. [15]. The isovector polarization effect in mirror nuclei tends to equalize proton and neutron radii. Thus, the contribution of the radial term to the MED at spin I^π can be parametrized as a function of the average of proton and neutron radii, considering the change in the occupation of low-ℓ orbits between the ground state (gs) and the state of angular momentum I^π [8],

$$C_r(I^\pi) = 2|T_z|\alpha_r\left(\frac{n_\pi(\text{gs}) + n_\nu(\text{gs})}{2} - \frac{n_\pi(I^\pi) + n_\nu(I^\pi)}{2}\right).$$

The value of $\alpha_r = 200$ keV has been used in extensive studies of MEDs in the pf shell [8]. In the present case, since we are also filling the shell $g_{9/2}$ and $d_{5/2}$ orbits, we have to include them as they have larger radii than the f orbits as well. We adopt the same value $\alpha_r = 200$ keV for the $p_{1/2}$ orbit, $\alpha_r = 100$ keV for the $p_{3/2}$ orbit that is almost full [16], and a larger value of $\alpha_r = 300$ keV for the $N = 4$ $g_{9/2}$ and $d_{5/2}$ orbits. The estimated radial contribution is $C_r(1/2^-) = -16$ keV.

Isospin-symmetry-breaking interaction V_B. This is an isovector correction deduced from the $A = 42$, $T = 1$ mirrors in Ref. [7] and more recently modified and generalized in Ref. [17]. It consists of a difference of −100 keV between the $I = 0$, $T = 1$ proton-proton and neutron-neutron matrix elements. Originally introduced for the $f_{7/2}$ shell, here, we apply it to all orbitals in the model space.

Taking into account all the corrections above, we compute the MEDs for the ^{73}Sr and ^{73}Br mirror pair in first-order perturbation theory as

$$\begin{aligned}\text{MED}_{I^\pi} &= E^*_{I^\pi}(^{73}\text{Sr}) - E^*_{I^\pi}(^{73}\text{Br}) \\ &= \Delta[\langle C_M\rangle(I^\pi) + \langle C_{\ell s+\ell\ell}\rangle(I^\pi)] \\ &\quad + C_r(I^\pi) + V_B(I^\pi), \end{aligned} \tag{2}$$

where the first two terms are obtained as the difference (Δ) of the expectation values of C_M, $C_{\ell s}$, and $C_{\ell\ell}$ between the two mirrors. We take the expectation values using the eigenstates that result from the diagonalization of the pure isoscalar nuclear Hamiltonian described in Sec. II A. The third and fourth terms correspond to the radial and ISB terms, respectively.

TABLE IV. Method 2. MEDs between ^{73}Sr and ^{73}Br and the contribution of each term in Eq. (2) (in keV).

I^{π}	C_M	$C_{\ell s+\ell\ell}$	C_r	V_B	MED
$5/2^-$	0	0	0	0	0
$1/2^-$	11	23	−16	25	43
$3/2^-$	−97	−130	6	−29	−250

The individual corrections and the total MEDs are given in Table IV.

Since the excitation energy of the $1/2^-$ state in ^{73}Sr is not yet known, we just have a lower limit for the MED of this state, which has to be greater than 27 keV. The MED value reported in Table IV is compatible with this limit, but there is room for further explorations using different values of α_r for the $p_{3/2}$, $p_{1/2}$, $g_{9/2}$, and $d_{5/2}$ orbits. A V_B contribution $\gtrsim$10 keV in Eq. (2) is needed to account for the MED experimental lower limit.

III. Conclusion. We have studied the inversion of the $I^{\pi} = 1/2^-, 5/2^-$ states between the mirror pair ^{73}Sr-^{73}Br within the framework of large-scale shell model calculations using the PFSDG-U effective interaction for the nuclear part of the problem. The Coulomb force and other isospin-symmetry-breaking effects were analyzed using two well-established methods which, not surprisingly, point to the prominent role played by Coulomb effects to explain the observed inversion. In Method 1, the Coulomb interaction is added to the nuclear Hamiltonian and treated both perturbatively and nonperturbatively with the calculated shifts in agreement with experiment. In this approach, possible nuclear ISB contributions might be included in the difference between neutron and proton SPEs which are empirically derived from the spectra of ^{41}Ca and ^{41}Sc. In Method 2, electromagnetic and non-Coulombic effects on the MEDs are evaluated. Although, as it follows from Eq. (2), MEDs do not give an absolute prediction, the relative changes between the mirror partners are robust. Thus, when referencing to the experimental level scheme of ^{73}Br and within the anticipated contributions of electromagnetic origin, our second approach suggests the need for an isospin breaking nuclear contribution to explain the inversion, in line with our estimate of $V_B \approx 25$ keV.

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