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Broken mirror symmetry in ^{36}S and ^{36}Ca

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Shape coexistence is a ubiquitous phenomenon in the neutron-rich nuclei belonging to (or sitting at the shores of) the $N = 20$ island of inversion (IoI). Exact isospin symmetry predicts the same behavior for their mirrors and the existence of a proton-rich IoI around $Z = 20$, centered in the (surely unbound) nucleus ^{32}Ca. In this article we show that in ^{36}Ca and ^{36}S, Coulomb effects break dramatically the mirror symmetry in the excitation energies due to the different structures of the intruder and normal states. The mirror energy difference (MED) of their 2^+ states is known to be very large at -246 keV. We reproduce this value and predict the first excited state in ^{36}Ca to be a 0^+ at 2.7 MeV, 250 keV below the first 2^+. In its mirror ^{36}S the 0^+ lies at 55 keV above the 2^+ measured at 3.291 MeV. Our calculations predict a huge MED of -720 keV, that we dub the "colossal" mirror energy difference. A possible reaction mechanism to access the 0_2^+ in ^{36}Ca will be discussed. In addition, we theoretically address the MEDs of the $A = 34,\ T = 3$ and $A = 32,\ T = 4$ mirrors.

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The study of the effects of the isospin symmetry breaking (ISB) terms of the nucleon-nucleon interaction on nuclear properties, particularly the Coulomb repulsion among the protons, has a long-standing history, starting with the Nolen and Schiffer anomaly [1], which involves the mass difference of a pair of mirror nuclei, and following up with their effects in spectroscopic properties like the mirror energy differences (MEDs) and the triplet energy differences extracted from the comparison of the excitation spectra of the members of an isobaric multiplet [2,3]. These studies have shown that the MEDs reflect nicely some structural properties of the states in question, such as deformation, alignment, and occupancies of particular orbits. On another register, the study of neutron-rich nuclei near the neutron magic shell closures has lead to the discovery of the so-called islands of inversion (IoIs), groups of nuclei which, unexpectedly, have their ground states dominated by intruder configurations, most often of a deformed nature. The relevant IoI for our present purpose is at $N = 20$, centered about ^{31}Na [4–13]. At or around these IoIs it is very common to find states of different shapes coexisting in the same nucleus. Therefore, if isospin symmetry holds (and we know it does to a very large extent) each IoI at the neutron-rich side should have a mirror IoI at the proton-rich side. However, only for relatively light nuclei can one hope to reach or even approach such proton IoIs. For the $Z = 20$ isotopes, ^{32}Ca most likely is experimentally out of reach, perhaps we can reach ^{34}Ca, and there is already some information about ^{36}Ca in Refs. [14,15].

The structure and location of coexisting intruder 0^+ states at $N = 20$ evolve as we move away from $N = Z$. Indeed, the first excited state in ^{40}Ca at 3.353 MeV is the head of a deformed band of a 4-particle–4-hole (4p-4h) nature. The relevant experimental information about the $A = 38,\ T = 1$ mirrors is gathered in Table I. The second 0^+ and 2^+ states are again of intruder nature: neutron 2p-2h in ^{38}Ar and proton 2p-2h in ^{38}Ca. And this is clearly manifested in their MEDs which are very large, because the two protons promoted to the pf shell suffer less Coulomb repulsion than when occupying the sd shell, which is why the excitation energies of the intruders are reduced in ^{38}Ca. With this anchor we can proceed further into the proton-rich side $A = 36$ looking for an enhanced ISB effect associated with shape coexistence.

^{36}S is stable and extensively studied experimentally. We list the states of interest in Table II, the normal 0^+ and 2^+ states and the intruder 0^+. For ^{36}Ca the only spectroscopic information available is the excitation energy of the first 2^+ state [16] from Refs. [14,15]. Note the very large experimental MED for the spherical 2^+ state of $-246(3)$ keV, at variance with the situation in the $A = 38$ mirrors, where the MED is $+45$ keV. Indeed this large shift in the $A = 36$ mirrors cannot have the same origin as the ones found in the intruder states of $A = 38$.

We proceed now with the theoretical description of the $A = 36,\ T = 2$ mirrors in the framework of the shell model with configuration interaction [17]. We adopt the valence space and the effective interaction (sdpfu-mix) which has been successfully applied in the simultaneous description of the $N = 20$ and $N = 28$ IoIs in Ref. [18]. We add to the nuclear interaction the two-body matrix elements of the Coulomb potential computed in an oscillator basis with the appropriate oscillator parameter $\hbar\omega = 45A^{-1/3} - 25A^{-2/3}$. The proton sd-shell single-particle energies (SPEs) could be derived from the experimental spectra of ^{17}F and that of the proton pf-shell orbits from the spectrum of ^{41}Sc. The value of the Coulomb shift of the $1s_{1/2}$ proton single-particle energy relative to the corresponding neutron single-particle energy would then be 375 keV and that of the $1p_{3/2}$ and $1p_{1/2}$ proton orbits 200 keV. However, it is seen experimentally that the MEDs in the mirrors

TABLE I. Experimental excitation energies (in MeV) and MEDs (in keV) for the mirror nuclei $A = 38,\ T = 1$.

J^π	^{38}Ca (expt.)	^{38}Ar (expt.)	MED (expt.)	MED (theor.)
0_1^+	0.0	0.0		
2_1^+	2.213	2.168	+45	−25
0_2^+	3.084	3.378	−294	−340
2_2^+	3.684	3.936	−252	−340

^{39}Ca-^{39}K and ^{37}Ca-^{37}Cl are much smaller: 56 and 120 keV, respectively. Drawing from the findings of Ref. [19] which concludes that the $1s_{1/2}$ orbit has a very large radius when empty at the mean-field level, independent of any energy threshold effect, becoming smaller as it is filled. We take an interpolated value of 300 keV for the shift in $A = 36$. However, these SPEs have unwanted effects in some MEDs directly related to the $Z = 14$ gap. Hence, following the analysis of Ref. [14], we have resorted to a minimal modification of the proton SPEs. Our ansatz is the following: the $Z = 14$ proton gap remains unchanged whereas the $Z = 16$ gap is reduced by 300 keV. This choice of the proton SPEs results in a MED for the ^{29}S-^{29}Al mirror pair of –46 keV, in reasonable agreement with the experimental value –176(20) keV from Ref. [20]. The experimental $Z = 20$ and $N = 20$ shell gaps at ^{40}Ca are essentially equal, they differ by just 29 keV, and our calculations reproduce nicely this difference, a theoretical value of 27 keV is obtained. The MEDs of the $A = 38$ mirror pair are also well reproduced, as can be seen in Table I. Since the choice of proton SPEs is irrelevant for this case and the neutron and proton gaps are equal, the large MEDs of the intruder states have their origin only in the two-body Coulomb repulsion.

The results for the mirror pair ^{36}Ca-^{36}S are shown in Table II. The calculation reproduces the large MED of the 2^+, with the same mechanism discussed in Ref. [14]. The origin of this large MED is easily grasped if we compare the spectra of ^{36}S and ^{36}Ca, shown in Fig. 1, with the spectrum obtained in the calculation without the Coulomb interaction. Whereas the excitation energy of the 2^+ in ^{36}Ca barely moves with respect to the no-Coulomb reference, in ^{36}S it goes up by 280 keV. The reason lies in the fact that the proton $1s_{1/2}$ orbit is more tightly bound than the neutron $1s_{1/2}$, relative to the corresponding $0d_{3/2}$ orbits. As the configuration of the 2^+ is $1s^1_{1/2}\ 0d^1_{3/2}$ the result follows trivially.

TABLE II. Excitation energies (in MeV) and MEDs (in keV). In the column labeled "$A = 36,\ T = 2$" we list the results of a calculation without the Coulomb interaction.

J^π	$A = 36, T = 2$	^{36}Ca		^{36}S		MED (theor.)
		Expt.	Theor.	Expt.	Theor.	
0_1^+	0.0	0.0	0.0	0.0	0.0	
2_1^+	2.97	3.045	2.95	3.291	3.25	−300
0_2^+	2.97		2.70	3.346	3.42	−720

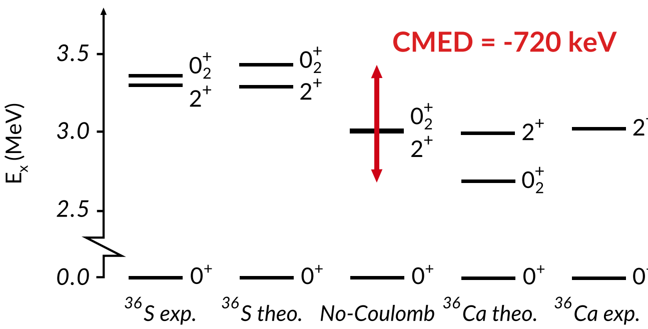

FIG. 1. Low-lying excited states in the mirror pair ^{36}Ca-^{36}S. The known experimental information is shown together with shell-model calculations using the sdpfu-mix interaction. At the center of the figure, the results without the Coulomb interaction are shown. The main configurations for ^{36}S are $0^+_{\mathrm{g.s.}}\ d^6_{5/2}s^2_{1/2}$ (protons) and $(sd)^{12}$ (neutrons); $2^+\ d^6_{5/2}s^1_{1/2}d^1_{3/2}$ (protons) and $(sd)^{12}$ (neutrons). For the intruder second 0^+ the main configuration is $d^6_{5/2}s^1_{1/2}d^1_{3/2}$ (protons), $d^6_{5/2}s^2_{1/2}d^2_{3/2}(pf)^2$ (neutrons). For ^{36}Ca it suffices to exchange the role of protons and neutrons.

But what happens for the intruder 0^+ state? Let's compare again the two mirrors with the no-Coulomb case. In ^{36}S the 0_2^+ excitation energy increases by the same amount as in the 2^+ case. And this may seem unexpected because one might naïvely think that its proton configuration is close to $1s^2_{1/2}$. Which is not the case indeed, because due to the deformed nature of the intruder band, the sd shell occupancies approach the pseudo-SU3 limit, being rather close to $1s^1_{1/2}\,0d^1_{3/2}$. Moving to ^{36}Ca, the proton configuration becomes $(sd)^{10}$-$(pf)^2$ which, as discussed for the $A = 38$ pair, has less Coulomb repulsion than the $(sd)^{12}$ configuration of the 0^+ ground state. These two shifts of quite different origin add constructively to produce a colossal mirror energy difference (CMED) of −720 keV, without advocating energy threshold effects. This is our main prediction. As a consequence, the intruder 0^+ becomes the first excited state of ^{36}Ca, decaying by an $E0$ transition to the ground state. We do not expect energy threshold effects due to the proximity of the excitation energy of the 0^+ intruder to the two-proton $(2p)$ separation energy, because of the Coulomb barrier which makes the (less bound) 2^+ a very narrow state [the one- and two-proton separation energies, S(p) and S($2p$) are about 2.6 MeV in ^{36}Ca]. Our prediction agrees nicely with what can be naïvely expected from the known experimental MED nearby. Indeed, the experimental MED of the excited 0^+ state of the $A = 38$ mirrors gives a hint of the extra contribution to the MED in the case of intruder states, whereas the experimental MED of the 2^+ state in the ^{36}Ca-^{36}S mirror pair does the same for the contribution to the MED of a configuration $1s^1_{1/2}\ 0d^1_{3/2}$. Knowing from theory that this is indeed the neutron (proton) configuration in the intruder 0^+ of ^{36}Ca (^{36}S), one can conclude that both contributions add constructively to produce a MED of about –600 keV. In this discussion we have not adopted any theoretical ansatz for the one- and two-body Coulomb effects, we have just made an educated guess drawing from the available experimental data.

There are a few other known cases of MEDs of similar size. However, all of them are dominated by energy threshold effects, i.e., they involve an excited state with an important $1s_{1/2}$ content which is well above the proton separation energy of the proton-rich mirror. For instance, the ^{19}Na-^{19}O pair has an MED of −750 keV because both the $5/2^+$ ground state and the $1/2^+$ excited state are proton unbound. The latter has a width of 110 keV, therefore the very large spatial extension of the $1s_{1/2}$ proton wave function should be solely responsible for the huge value of the MED. Similar arguments apply to the ^{14}O-^{14}C (MED = −669 keV) [21] and ^{12}O-^{12}Be (MED = −630 keV) [22] mirror pairs.

The calculated $B(E2;2^+ \rightarrow 0^+_{\mathrm{g.s.}})$ for ^{36}Ca is very small, 4.7 e^2 fm^4 (the Dufour-Zuker [23] effective charges $e_\pi = 1.31e$ and $e_\nu = 0.46e$ have been used). In fact this value is the smallest of all the calcium isotopes together with that of ^{50}Ca, 7.5 ± 0.2 e^2 fm^4 [24]. The 2^+ decay to the intruder 0^+ is suppressed by a factor 2×10^4 with respect to the decay to the ground state due to the phase-space factor. For completeness, our prediction for the $B(E2;2^+ \rightarrow 0^+_{\mathrm{g.s.}})$ in ^{36}S is 19.5 e^2 fm^4, which is in good agreement with the experimental value, $17.7^{+1.7}_{-1.0}$ e^2 fm^4 [25]. The calculated $\rho^2(E0)$ for the decay of the 0^+_2 state to the ground state in ^{36}Ca is 40×10^{-3}, which corresponds to a lifetime of $\tau(E0) = 8.3$ ns. An effective isoscalar $E0$ charge of $1.0e$ has been assumed. This effective $E0$ charge has been deduced from the known experimental value in ^{36}S, where the 0^+_2 has been observed to decay directly via an $E0$ transition to the 0^+ ground state and its half-life has been measured to be 8.8 ± 0.2 ns [26], no γ transition has been observed from the 0^+_2 state to the 2^+ state. Therefore, using Eq. (1) of Ref. [27], we can compute an upper limit for the $\rho^2(E0)$, considering an experimental sensitivity limit of 1% for the 0^+_2 to 2^+ decay branch $\rho^2(E0) = \frac{I(E0)}{I_\gamma(E2)} \times \frac{1}{\Omega(E0)} \times \frac{1}{\tau_\gamma} = 9 \times 10^{-3}$. The electronic $\Omega(E0) = 8.7 \times 10^9$ s^{-1} factor has been calculated with BRICC [28].

As discussed previously, the $T = 2$ mirrors ^{36}Ca and ^{36}S are known experimentally very unequally. While the ^{36}Ca isotope is the heaviest acknowledged $T_z = -2$ nucleus, just two neutrons away from the proton drip line, the ^{36}S is stable. The excitation energy of the 2^+ state, for the $N = 20$ ^{36}Ca isotope, was measured both at GSI [14] and GANIL [15] by using a knock-out reaction from a secondary ^{37}Ca beam. In these two experiments a unique γ was observed at an energy of 3015(16) keV at GSI and 3036(11) keV at GANIL. The momentum distribution measurement of the ^{36}Ca at GANIL with the SPEG spectrometer indicates an $\ell = 0$, $\ell = 2$ character of the excited 2^+ state, which agrees well with our calculations, where the 2^+ state has a dominant sd configuration. This is all the information that currently exists for the $T_z = -2$ ^{36}Ca; in contrast, the experimental information available for the stable ^{36}S is copious. Over the last decades many reactions have been used to study the semimagic nature of this ($N = 20$) isotope.

The intruder 0^+_2 state in the mirror ^{36}S, which has mainly a neutron $(sd)^{10}$-$(pf)^2$ nature, was selectively populated via a two-neutron transfer reaction ^{34}S$(t,p)^{36}$S [26], ^{34}S$(t,p\gamma)^{36}$S [29], as well as via a less selective reaction such as inelastic scattering with protons and α particles: ^{36}S$(p,p)^{36}$S and ^{36}S$(\alpha,\alpha)^{36}$S [30]. Considering the proton nature, $(sd)^{10}$-$(pf)^2$ predicted by our calculations, of the intruder 0^+_2 state in ^{36}Ca, one could experimentally access this state by using a two-proton transfer reaction with a radioactive ^{34}Ar beam, such as ^{34}Ar$(^3$He$,n)^{36}$Ca. The 0^+_2 would decay directly to the $0^+_{\mathrm{g.s.}}$ with a 2.63 MeV $E0$ transition with an expected lifetime of 8.3 ns. The internal pair formation, according to BRICC [28] calculations is more than 50 times larger than the internal conversion. For the $T = 4$, $T_z = +4$, ^{32}Mg which represents the pivotal nucleus in the $N = 20$ IoI, the second 0^+ state was also populated via a two-neutron transfer reaction since it presents a neutron nature [31]. While the second 0^+ state in the $T = 3$, $T_z = +3$, ^{34}Si was directly observed via β decay of a 1^+ isomer in ^{34}Al [32], so in this case no transfer reaction was needed to measure the properties of the intruder state. For the ^{36}Ca isotope, one cannot populate the intruder state via β decay since its progenitor ^{36}Sc is unbound.

TABLE III. Theoretical excitation energies (in MeV) and MEDs (in keV). In the column labeled "$A = 34$ $T = 3$" we list the results of a calculation without the Coulomb interaction.

J^π	$A = 34,\ T = 3$	^{34}Ca	^{34}Si	MED
0^+_1	0.0	0.0	0.0	
0^+_2	2.57	2.33	2.75	−420
2^+_1	3.45	3.20	3.62	−420
2^+_2	4.46	4.43	4.49	−60

As a purely academic exercise, because of their almost certain unbound nature, we examine now what happens when we go to the $A = 34$, $T = 3$ and $A = 32$, $T = 4$ mirrors, where the intruder configurations become more significant. The theoretical results for the $A = 34$, $T = 3$ mirrors ^{34}Ca and ^{34}Si are displayed in Table III. The ground state and the 2^+_2 are dominated by the "normal" sd configurations $0d^6_{5/2}$ and $0d^5_{5/2}1s^1_{1/2}$ respectively. This results in the small MED of the 2^+_2. The intruders 0^+_2 and 2^+_1 decrease by 400 keV in ^{34}Ca with respect to the no-Coulomb result, as they did in ^{36}Ca. However, different from what happened in ^{36}S, this does not add constructively with a large pure sd-shell effect in ^{34}Si and the resulting MEDs are very large but not huge.

Even farther beyond the proton drip line would eventually sit ^{32}Ca, the mirror of the prominent member of the $N = 20$ IoI ^{32}Mg. In Table IV we give the (rather exotic) structure of the

TABLE IV. Theoretical excitation energies (in MeV) and MEDs (in keV). In the column labeled "$A = 32,\ T = 4$" we list the results of a calculation without the Coulomb interaction. In the last three columns,, we give the amplitudes of the np-nh configurations (in percentage) for the calculation without the Coulomb contribution.

J^π	$A = 32,\ T = 4$	^{32}Ca	^{32}Mg	MED	0p-0h	2p-2h	4p-4h
0^+_1	0.0	0.0	0.0		9	54	35
2^+_1	0.85	0.77	0.85	−80	2	46	50
0^+_2	1.20	1.18	1.20	−20	33	12	54
0^+_3	1.91	2.09	1.91	180	48	37	15

low-lying states according to the no-Coulomb calculation. The only state dominated by the normal (closed $N = 20$ or closed $Z = 20$) configurations is the 0_3^+. Due to the presence of 4p-4h configurations in addition to the 2p-2h ones, the two lowest states have quite small MEDs. Only the 0_3^+ has a large MED due to its mainly spherical nature. In fact, when we include the Coulomb interaction in the calculation, the percentage of the 0p-0h configuration in the 0_3^+ of ^{32}Ca increases to 70%. For this state only, the Coulomb interaction induces important differences in the structure of the wave functions of the two mirrors, due to the quasidegeneracy of the different np-nh configurations before their mixing by the nuclear interaction. The evolution of the MEDs as a function of the isospin of the mirror pair T is shown in Fig. 2. All in all, it seems that the CMED is elusive and the opportunity to observe it might be confined to the $A = 36$, $T = 2$ mirrors.

In summary, we predict a first excited 0_2^+ state at 2.7 MeV in ^{36}Ca, 250 keV below the first 2^+, in the framework of the shell model with configuration interaction, using the effective interaction sdpfu-mix. This large decrease in the excitation energy of the intruder 0_2^+ state gives origin to the largest ever predicted MED between bound states: −720 keV, which we name the colossal MED (CMED). The calculated $B(E2; 2^+ \rightarrow 0^+_{\mathrm{g.s.}})$ transition probability of 4.7 e^2 fm^4 represents the smallest value in the calcium isotopic chain. The theoretical $\rho^2(E0) = 40 \times 10^{-3}$, leads to a lifetime $\tau(E0) = 8.3$ ns for the intruder 0^+ state. According to our calculations, disregarding energy threshold considerations, the CMED would not be present in the more exotic mirror pairs $A = 34$, $T = 3$ and $A = 32$, $T = 4$. A two-proton transfer reaction, such as ^{34}Ar(^{3}He, n)^{36}Ca, will give access to the 0_2^+ intruder state that is predicted to have a proton $(sd)^{10}$-$(pf)^2$ configuration.

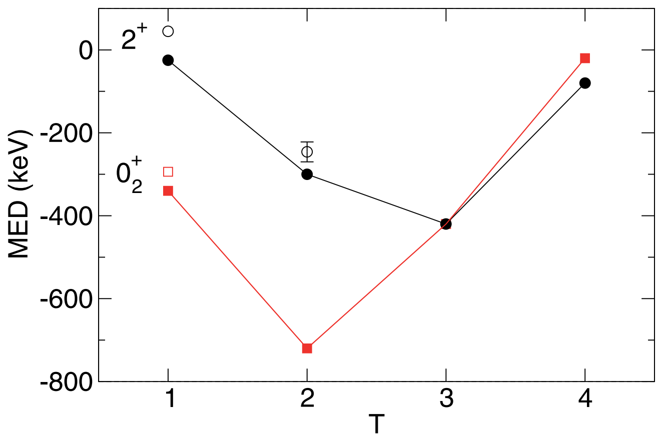

FIG. 2. MED (in keV) as a function of the isospin of the mirror pair for the proton-rich calcium isotopes. Open and full symbols indicate experimental data and theoretical predictions, respectively. For the $T = 1$ mirror pair the experimental errors are within the symbols.

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