Coulomb energy differences in mirror nuclei

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Abstract. By comparing the excitation energies of analogue states in mirror nuclei, several nuclear structure properties can be studied as a function of the angular momentum up to high spin states. They can be described in the shell model framework by including electromagnetic and nuclear isospin-non-conserving interactions. Calculations for the mirror energy differences in nuclei of the $f_{7/2}$ shell are described and compared with recent experimental data. These studies are extended to mirror nuclei in the upper $sd$ and $fp$ shells.

1. Introduction
One of the central topics in nuclear physics is the isospin symmetry. It shows experimentally in nearly identical spectra in pairs of mirror nuclei (obtained interchanging protons and neutrons) and, more generally, in isobaric multiplets. Even if the Coulomb force breaks this symmetry, the isospin can be considered a good quantum number that characterises the nuclear states. Studying mirror nuclei, signatures of the isospin symmetry breaking of the effective interaction can be deduced from the differences between the excitation energy of analogue states, called mirror energy differences (MED).

From the analysis of these differences, remarkable properties can be studied as a function of the angular momentum up to high spin states, and in many cases, along rotational bands. Nuclei of the $f_{7/2}$ shell have been extensively studied in the last years, both from the experimental and the theoretical sides. These energy differences amount to 50-100 keV, and it is because of their smallness that they become a very delicate probe of nuclear structure. In fact, it has been shown how the MED can account for nuclear features such as nucleon alignment at the backbending [1, 2] and changes of the nuclear radius with increasing spin [3, 4, 5, 6]. Recently, evidence of a nuclear isospin non-conserving (INC) term in the residual nuclear interaction has been suggested [6].

Interesting results concerning isospin multiplets have been obtained in the last years in the $sd$ shell thanks to important experimental developments [7, 8, 9, 10]. From the theoretical point of view, to obtain a description of the MED, high quality shell model calculations with modern techniques are needed. An important issue in describing nuclei of mass $A$~30-40 with the shell model is that the $sd$-shell space is not able to account for the high spin and negative parity states. Intruder configurations involving higher orbitals become relevant and therefore effective interactions that take into account two main shells ($sd$ and $fp$) are needed. Recently, mirror nuclei in the upper $fp$ shell have been investigated experimentally [11] and a new effective interaction, GXPF1 [12], has been proposed for the description of the entire $fp$ shell.

In this work, after a brief description of the theoretical method, recent applications to mirror energy differences in the $sd$ and $fp$ shells by means of shell model calculations are reported.
2. Theoretical survey

Different terms of the electromagnetic and nuclear effective interactions contribute to the MED. The calculation of the MED in the shell model framework, is performed here following the method described by Zuker et al. in Ref. [6]. The Coulomb interaction is separated into the multipole $V_{C M}$ and the monopole $V_{C m}$ components. An INC nuclear term $V_R$ is also considered. The experimental MED are defined as

$$MED_{exp}(J) = E^*(Z_>, J) - E^*(Z_<, J)$$ (1)

Assuming good isospin wave functions, the contributions to the MED can be obtained as differences of the expectation values at each state of spin $J$,

$$MED_{th}(J) = \Delta_M(V_{Cr}(J)) + \Delta_M(V_{CM}(J)) + \Delta_M(V_B^{(1)}(J))$$ (2)

where $\Delta_M$ means the difference between the mirror nuclei, as in Eq. (1). For the mirror nuclei in the $f^2_7$ shell we have obtained the good isospin wavefunctions using the KB3G [13] effective interaction, while for the mirror nuclei in the upper sd shell, the sdfp [14] interaction has been used. Finally, the GXPF1 [12] interaction has been applied to upper fp-shell mirror nuclei. Coulomb matrix elements are calculated in the harmonic oscillator representation. The nuclear isospin-non-conserving interaction for nuclei in the $f^2_{7/2}$ shell has been deduced from the spectra of the mirror $A = 42$ by A.P. Zuker in Ref [6]. Here we use the same schematic parametrisation which consists on a single matrix element for two protons in the $f^2_{7/2}$ mirror partner) from the $\text{sd}$ shell coupled to $J = 2$ with a strength of 100 keV.

Recently, it has been shown [7, 8, 9] that single-particle effects, induced by the electromagnetic spin-orbit (EMSO) interaction, $E_{ls}$, and the Coulomb orbital term $E_{C_{O}}$, deduced in Ref. [15], produce large effects in the MED for nuclei in the upper $sd$ and $fp$ shells. The shifts in the single-particle energies due to the electromagnetic spin-orbit interaction can be obtained as [16]:

$$E_{ls} = (g_s - g_l) \frac{1}{2m_N c^2} \frac{1}{r} \left( \frac{dV_e}{dr} \right) \langle \tilde{r} \cdot \tilde{s} \rangle \simeq (g_s - g_l) \frac{1}{2m_N c^2} \left( \frac{Ze^2}{R_C^3} \right) \langle \tilde{r} \cdot \tilde{s} \rangle$$ (3)

where $g_s$ and $g_l$ are the gyromagnetic factors, $m_N$ is the nucleon mass and $R_C$ is the charge radius. It is easy to see that the energy shift will have different sign for a proton orbit than for a neutron one. The sign will also depend on the spin-orbit coupling, as $\langle \tilde{l} \cdot \tilde{s} \rangle = -l$ when $j = l + s$ and $\langle \tilde{l} \cdot \tilde{s} \rangle = l + 1$ when $j = l - s$. For upper sd-shell nuclei, the effect of the EMSO is to reduce the energy gap between the $f_{7/2}$ and $d_{3/2}$ orbitals for protons by $\sim$120 keV and to increase it for neutrons by a similar amount. The MED will be influenced much by this effect whenever a pure single-particle excitation (a proton in one nucleus and a neutron in its mirror partner) from the $d_{3/2}$ to the $f_{7/2}$ will dominate the configuration of the negative-parity states.

In Ref. [15], Duflou and Zuker show that the contribution of the monopole Coulomb interaction to the energy differences induces single-particle corrections that account for shell effects. They affect the energy of the proton orbits proportionally to the square of the orbital momentum $l$ in the harmonic oscillator representation. The expression for the single-particle splittings for a proton in a main shell, with principal quantum number $N$, above closed shell $Z_{cs}$ results [15]

$$E_{ll} = \frac{-4.5 Z_{cs}^{13/12}}{A^{1/3}(N + \frac{3}{2})} [2l(l + 1) - N(N + 3)] \text{keV}. \quad (4)$$

Its effect on the single-particle energies is sizable. In $^{41}\text{Sc}$ ($Z_{cs} = 20$, $N = 3$), proton $f$ orbits are lowered by $\sim 45$ keV while the energy of $p$ orbits is raised by $\sim 105$ keV with respect to the
neutron levels. The relative energy between the proton $f_7^2$ and $p_7^2$ orbitals is therefore increased by $\sim 150$ keV with respect to the neutron energy difference.

In the nuclei of the $f_7/2$ shell - where well deformed nuclei have been studied up to the band termination - the multipole Coulomb term accounts for the nucleon alignment along the rotational yrast bands, as has been shown in different works [1, 17]. This is due to the fact that when a pair of nucleons are in time-reversed orbits the Coulomb interaction is maximum but when the pair breaks and couples to $J \neq 0$ angular momentum, the repulsive force decreases. Of course this has an effect on the nucleus where a proton pair aligns, while, in the mirror nucleus, a neutron aligns without any Coulomb effect, producing a jump in the MED.

The monopole Coulomb contribution to the MED corresponds to the difference of the Coulomb energy of the mirror partners (uniform charged spheres) as a function of the nuclear spin, referred to the ground state:

$$\Delta M < V_{Cr}(J) > = \frac{3}{5} n(2Z - n)e^2 \left( \frac{1}{R_C(J)} - \frac{1}{R_C(0)} \right)$$

where, $n = 2|T|$, $Z_\geq = Z_\leq + n$, and $Z = Z_\geq$. For nuclei in the $f_7/2$ shell, where the $f_7/2$ component in the wave functions is dominant, and the contribution of the $f_5/2$ and $p_1/2$ is almost constant with $J$, changes in radii are due to changes in the occupation numbers of the $p_3/2$ shell, as the nucleus passes from a well deformed shape at low spin to a non-collective high spin regime, aligning the nucleons in the $f_7/2$ shell. The contribution is therefore parametrised in terms of the average of the occupation number ($m$) of protons plus neutrons in the $p_3/2$ shell.

$$\Delta M < V_{Cr}(J) > = n \alpha_r \left( \frac{m_\pi(0)}{2} + \frac{m_\nu(0)}{2} - \frac{m_\pi(J)}{2} - \frac{m_\nu(J)}{2} \right)$$

where the constant $\alpha_r$ can be deduced from the single-particle relative energies in mass $A = 41$, after taking into account the contributions of $E_{ls}$ and $E_{CI}$.  

3. The results

The formalism described above has been applied with success to several $f_7/2$-shell mirror nuclei of mass $A = 47 - 51$ in Ref. [6], only the single-particle effects were not taken into account. Their role is, however, not very significant in this mass region. In the present work we calculate the MED for some $T = 1$ isobaric states in even-even and odd-odd mirror nuclei in the $f_7/2$ shell. The same parametrization has been used in all cases. The constant $\alpha_r$ in Eq. (6) has been fixed to 200 keV, the same strength as in Ref. [6] (100 keV) has been used for $V_B$, and single-particle energies have been obtained from Eqs. (3) and (4).

The results, obtained with the code ANTOINE [18], are reported in Fig. 1 in comparison with the experimental data. The different terms of Eq. (2) are shown in the figure. The values labelled “VCM” include the single-particle effects of Eqs. (3) and (4). It is interesting to see how the relative weight of the different terms changes in each case. For the odd-odd $A = 48$ mirror pair, data have been recently obtained by Bentley and collaborators [19]. The main contribution to the MED arises from the monopole Coulomb term, because, as discussed in Ref. [19], in this particular case, multipole effects are hindered due to self conjugation. In the middle panel, the $A = 50$ mirror pair is shown [5]. In this case, all components have similar weights in the construction of the MED. Finally, the bottom panel shows the recently measured [20] mirror
Figure 1. $T=1$ isobaric states in mirror nuclei of the $f_{7/2}$ shell compared with shell model calculations (see text for details).

Figure 2. $T=1/2$ isobaric states in mirror nuclei of the $sd$ and $fp$ shells compared with shell model calculations (see text for details).

pair $A = 54$. While for $A = 48$ and $A = 50$ calculations have been done in the full $fp$ shell, in this case, a truncation $t = 8$ has been applied, which means that a maximum of 8 nucleons are allowed to be excited from the $f_{7/2}$ shell to the upper $fp$ orbitals. As shown in the figure, monopole effects are hindered in the $A = 54$ case, as the closed shell is approached, and the dominant term is the multipole Coulomb which puts in evidence the gradual recoupling of the two holes in the $f_{7/2}$ shell. Note, however, that the contribution of the isospin-non-conserving “nuclear” interaction is crucial for the description of the $J = 2$ state. This effect, also known as the “$J = 2$ anomaly”, is important for all the $f_{7/2}$-shell nuclei studied so far [21, 22]. Its interpretation is an open question and constitutes a theoretical challenge.

It is important to note here that the theoretical curves in Fig. 1 do not intend to be a best fit of the data. Of course a better description for the single cases is possible. The important point is that with the same parametrisation it is possible to describe with very good accuracy the MED data up to high spin in the mirror nuclei known so far from $A = 47$ to $A = 54$ (see Ref. [21]), including the energy differences in isobaric triplets too. This means that the method works
and that the different terms that contribute to the MED are under control. Moreover, we can learn from the behaviour of the MED several nuclear structure properties. These investigations, undertaken in the $f_{7/2}$ shell, encouraged the extension of these studies to other mass regions such as the $sd$ shell or the upper $fp$ shell where recent measurements have produced interesting MED data.

In nuclei of the $sd$ shell large MED values, of the order of 300 keV, have been observed in a few non-natural-parity states in the $T_z = \pm 1/2$ mirror pairs of mass $A = 31, 35, 39$ [7, 9, 23, 24]. These states present particular configurations where a single nucleon (a proton or a neutron) is excited from the $sd$ to the $fp$ shell. In these cases, single-particle effects become very important in constructing the MED. More recently, sizable single-particle effects in the MED have been encountered in natural-parity states in the $A \sim 60$ mass region [11]. The nuclear wave functions in these latter cases involve single-particle excitations from the $p_{3/2}$ to the $f_{7/2}$ shell. The shell-model description of these nuclei is presently not as accurate as in the $f_{7/2}$ shell. This is partly due to the large dimensions of the matrices to be diagonalised – in particular for upper $sd$, $A \sim 30 - 40$, and lower $fp$, $A \sim 60$, nuclei. With the present computational capabilities, truncations are mandatory which introduce inaccuracies. The lack of appropriate and reliable residual interactions that, in some cases, have to take into account more than one main shell, also precludes a good description of the data. Aware of these limitations we have calculated the MED for some few examples as a preliminary theoretical approach to the description of the data.

In Fig. 2 we report some experimental data in comparison with shell model calculations obtained with the code ANTOINE [18]. For the negative-parity states in $A = 35$ and $A = 39$ the effective interaction $sdfp$ [14] in the reduced valence space $s_{1/2}d_{3/2}f_{7/2}p_{3/2}$ has been used, which has proven to give a rather good description of the spectroscopy of $^{34}$S [25]. The different contributions to the MED in these cases are the multipole Coulomb (VCM), calculated with equal single-particle energies for protons and neutrons, and the modified results when the single-particle energies are modified by the electromagnetic spin-orbit and the $E_{Cll}$ term. It is important to note that the two main contributions to the MED are due to the multipole Coulomb and the electromagnetic spin-orbit interactions, while the role of the orbital term is marginal. In the case of $A = 39$ these three terms fit the data while for $A = 35$ the theoretical curve follows qualitatively the experimental values but quantitatively overestimates them. While the monopole Coulomb interaction plays a minor role here, no parametrisations have been yet proposed for an eventual isospin-non-conserving nuclear component.

In the bottom panel of Fig. 2, the recently studied $A = 61$ mirror nuclei are shown in comparison with the shell model calculations using the GXPF1 [12] interaction and a truncation $t = 3$. It is clear from the figure that effect due to the $E_{Cll}$ single-particle term is very important in this mass region and preliminary calculations indicate a very important role played by the monopole radial Coulomb term that would bring theory in very good agreement with data.

Although the effective interactions in these mass regions are not completely reliable, and the valence spaces have to be truncated to cope with the present computational capabilities, the wave functions predicted by shell model calculations are consistent with the MED data: Those states that present large experimental MED values are predicted to have configurations with “pure” single-particle excitations and therefore, the single-particle effects show up.

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