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Isospin Symmetry Breaking Effects on Mirror Nuclei ^{43}Ti and ^{43}Sc

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Abstract

This work ia a theoretical study of the Mirror Energy Differences (MED) between analogue levels of the $T = \frac{1}{2}$ doublet ${}^{43}_{21}Sc$ and ${}^{43}_{22}Ti$, of positive and negative parity.
First, we will study the two nuclei in the shell model framework, and then find a good prediction for MED, modelling all the different contributions one by one.
Once the electromagnetic contributions to the MED have been estimated, it is possible to investigate the Charge Symmetry property of the nuclear interaction. It will be seen that an Isospin Non-Conserving (INC) contribution is needed and that it can be accounted for using a phenomenological model.

Contents

1 Introduction

The exchange symmetry between protons and neutrons has always been one of the pillars of nuclear physics. Such charge symmetry, along with the charge indipendence property of the nuclear interaction, led to the introduction of the so-called **Isospin Symmetry Principle**.
For a long time, it was thought that the only Isospin breaking interaction was the Coulomb one, which was expected to entirely account for the MED, the energy differences between analogue levels of mirror nuclei.
Nonetheless, it was found that, even estimating the finest electromagnetic contributions, theoretical predictions for MED were dramatically far from reproducing experimental values. This led researchers to think that such gap between theory and experiment could be filled introducing a **nuclear Isospin Non-Conserving (INC) effect**. In the last twenty years, many phenomenological models for such effect have been developed. Those models on which we will be focusing in this work, were first specific for the $f_{\frac{7}{2}}$ *shell* and then extended to the entire *pf* and *sd shells*. Some examples can be found in [1],[2] and [3].
Furthermore, in 2001 experimental data on nucleon-nucleon scattering clearly showed that **the charge symmetry of the free nucleon-nucleon interaction is broken** [4]. Nevertheless, the impact that such evidence has on nuclear structure is still being discussed and there is no clear idea of how to include it in nuclear effective interactions. Not even the connection with the previously mentioned phenomenological models is clear.
Apart from being a powerful tool for investigating Isospin Symmetry breaking effects, Mirror Energy Differences are interesting for many other reasons. They act as a **magnifing glass on the physics behind excited states** and reveal many subtle nuclear structure phenomena, such as correlations of pairs of particles, changes in the mechanism thorugh which the nucleus generates angular momentum, changes in radius and so on.
It is for those reasons that we drew our attention to the mirror nuclei ${}^{43}_{21}Sc$ and ${}^{43}_{22}Ti$ and attempted to build a good theoretical description of their MED.
First, in section 2, a general overview of shell model, the theoretical framework in which the two nuclei will be studied, is provided. Then, in section 3, the physical meaning of Mirror Energy Differences and their connection to Isospin Symmetry are clarified. Rigorous procedures for calculating the various contributions to the MED are shown as well. Finally, in section 4, all the theoretical results obtained in our study of ${}^{43}_{21}Sc$ and ${}^{43}_{22}Ti$ are discussed and compared to experimental data.

2 An Overview of Shell Model

A general overview of shell model will be provided, based on references [5], [6] and [7].

In principle, nuclear structure constitutes an **A-body problem** interacting via the effective nuclear force, which is different from the free nucleon-nucleon one. The hamiltonian of such problem, would be:

$$H = \sum_{i=1}^{A} T_i + \frac{1}{2} \sum_{i,j=1}^{A} V_{i,j} \tag{1}$$

where T_i is the kinetic energy of the nucleon and $V_{i,j}$ is the nucleon-nucleon potential. It is clearly evident that the complexity of such problem increases dramatically with A and makes it almost unsolvable even for a small number of particles. For such reason, in order to study nuclear structure, we need to use **approximate models**. One of those is the so-called *shell model*.
The main assumption behind shell model is the following:

To first order, each nucleon is moving in an indipendent way,
in a central average field

Hence, the hamiltonian of the A-body problem, can be read as the sum of two different terms:

$$H = H_0 + H_{residual} \tag{2}$$

where H_0 is the leading term containing only central potentials and $H_{residual}$ is the remaining part of the hamiltonian, which can be treated as a perturbation to H_0 and contains nuclear two-body potentials:

$$H_0 = \sum_{i=1}^{A} T_i + \sum_{i=1}^{A} U_i \qquad H_{residual} = \frac{1}{2} \sum_{i,j=1}^{A} V_{i,j} - \sum_{i=1}^{A} U_i, \tag{3}$$

where U_i is the central potential associated to each nucleon.

The idea of treating nucleons as indipendent particles in a central mean field is strongly supported by some **experimental evidences**, which are collected below:

- There are certain nuclei which are particularly stable. They are characterized by the fact that they either have a specific number of protons or neutrons:

  $$Z = 2, 8, 20, 28, 50, 82, 126 \quad or \quad N = 2, 8, 20, 28, 50, 82, 126$$

  Such numbers are called **magic numbers**.

- The **proton** and **neutron separation energies** follow a regular plot as function of respectively the number of neutrons and protons. This plot shows clear similarities with that of the electron ionisation energies in atomic physics. The maxima correspond to magic numbers.

- The **deviation of the experimental mass from that predicted with the liquid drop model**, follows a regular pattern as function of the number of protons and as a function of the number of neutrons. The minima in such pattern correspond to the magic numbers.

- The **first excitation energy in doubly even nuclei**, follows a regular pattern as function of neutron (proton) number. The peaks are located at the magic numbers.

Once it had been clear that a shell nuclear structure existed, the problem of finding a suitable central potential U_i, capable of reproducing experimental data and explaining magic numbers, had to be faced. The solution was found in 1950 - independently by Mayer and by Haxel, Jensen and Suess - and had such form:

$$U(r) = -U_0 + \frac{1}{2} m\omega^2 r^2 + D\ \vec{l}^2 - \frac{2}{\hbar}\alpha\ \vec{l} \cdot \vec{s} \tag{4}$$

where four different terms are summed:

- The term $-U_0$ represents a negative constant.
- The term $\frac{1}{2}m\omega^2 r^2$ represents a **harmonic oscillator potential**. Considering the potential $U(r) = -U_0 + \frac{1}{2}m\omega^2 r^2$, we may solve the eigenvalue problem with two different strategies:

  1. Decomposing the three dimensional harmonic oscillator, in three one dimensional harmonic oscillators. In this case, we find these eigenvalues:,

  $$E_N = \hbar\omega\left(N + \frac{3}{2}\right) \qquad for\ N = 0,1,2... \tag{5}$$

  where N is the principal quantum number.

  2. Solving the central problem. In this case, the eigenvalues are:

  $$E_{n,l} = (2(n-1) + l)\hbar\omega + \frac{3}{2}\hbar\omega - U_0, \tag{6}$$

  where l is the orbital angular momentum quantum number and n is the number of nodes in the wavefunction.

  Since $N = (2(n-1) + l)$, we could use N to identify the shells and (n,l) to find the shell degeneracy, which can be computed considering all the possible couples of integers (n,l), such that l is compatible with Pauli exclusion principle, and associating to each of those couples, $2(2l+1)$ particles. However, even in this case we fail at predicting magic numbers higher than 20.

- The term * $D\,\vec{l}^2$ describes an effect due to the **angular momentum**. It splits the degeneracy of E_N according to the various values for orbital angular momentum quantum number allowed by Pauli exclusion principle ($l = N, N-2, ...$):

  $$E_{n,l} = (2(n-1) + l)\hbar\omega + \frac{3}{2}\hbar\omega - U_0 + D\ l(l+1) \tag{7}$$

  Now, inside the shells identifed by the quantum number N, we find sublevels, which are labelled by the couple of quantum numbers (n,l). Still we are not able to predict magic numbers.

- The term $-\frac{2}{\hbar}\alpha\,\vec{l}\cdot\vec{s}$ is the so-called **spin-orbit potential**. The spin orbit term partially lifts the degeneracy of the eigenvalues found in equation (7) in this way:

  $$E_{n,l,j} = \underbrace{\overbrace{(2(n-1)+l)}^{N}\hbar\omega + \frac{3}{2}\hbar\omega - U_0}_{Negative\ Constant\ +\ Harmonic\ Oscillator} + \underbrace{Dl(l+1)}_{D\vec{l}^2\ Effect} + \underbrace{\alpha\begin{cases} -l & for\ j = l + \frac{1}{2} \\ l+1 & for\ j = l - \frac{1}{2} \end{cases}}_{Spin-Orbit} \tag{8}$$

  The reason why the spin-orbit term gives the right prediction for the magic numbers is that it lowers the energy of the orbit with the highest j value in a main shell.

To conclude, with the central potential $U(r)$ in equation (4), we are able to theoretically obtain the nuclear shell structure and give a satisfactory explanation for magic numbers.
Shells are identified by the principal quantum number N. Each shell contains in itself several orbits, which correspond to different energy levels and are identified by the triplet of quantum numbers (n,l,j). Every orbit has a degeneracy equal to $2j+1$.

Given that, protons and neutrons are fermions, in an indipendent particle view, they should be simply placed in the lowest possible orbits, compatible with the Pauli Exclusion Principle. Then, the total ground state energy will be the sum of the energies associated to each particle, and the total wave function will be the Slater determinant of all the single-particle wavefunctions.

The shell model structure of nuclei, in the indipendent particle view, is shown in figure 1.

*The Kinetic Energies in spherical coordinates already contain a term that is proportional to $\vec{l}^2$. Therefore some references do not include $D\,\vec{l}^2$ in the potential [5] [6], others do [7].

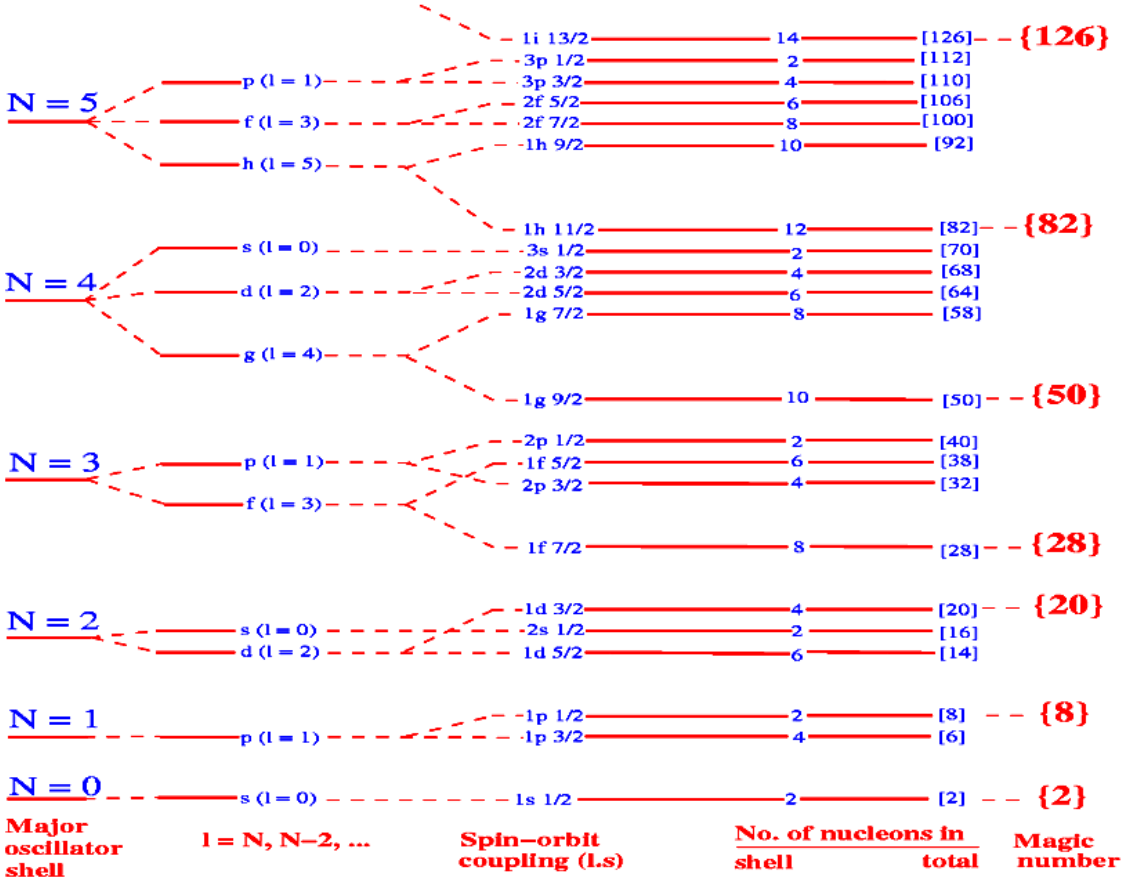


Figure 1: Shell Model. The Indipendent Particle View.

2.1 Interacting Shell Model

The indipendent particle shell model allows us to predict the magic numbers and the ground state energy of many nuclei, which has an order of magnitude of $\sim 10^3$ MeV. However, if we wish to describe fine details, such as the excitation energies, whose order of magnitude is ~ 1 MeV, the indipendent particle shell model generally fails.
On the one hand, the residual interactions among nucleons have to be considered, on the other, the computational complexity of finding the eigenvalues of the full hamiltonian dramatically increases with the number of nucleons.
It is for this reason that we should restrict our attention to a small portion of the entire Hilbert space $\mathcal{H}$ - the so-called **Model Space** $\mathcal{M}$ - and try to define the eigenvalue problem in $\mathcal{M}$ in a way which is mathematically equivalent but computationally easier. Hence, we can define the **Model Wavefunction** ψ', as the projection of the wavefuction in the full Hilbert Space ψ on the Model Space: $\psi' = \hat{P}\psi$. We now look for an **Effective Interaction**, requiring that it has on the Model Wavefunction, the same effect that the Residual Interactions have on the True Wavefunction.
To summarize, we are going to make the following steps:

$$\begin{aligned} Fulll\ Hilbert\ Space\ \mathcal{H} &\implies Model\ Space\ \mathcal{M} \\ True\ Wave\ Function\ \psi &\implies Model\ Wave\ Function\ \psi' \\ Hamiltonian\ H &\implies Effective\ Hamiltonian\ H_{eff} \\ Residual\ Interactions\ Potential\ V &\implies Effective\ Potential\ V_{eff} \end{aligned}$$

To be more specific, the full Hilbert space hamiltonian reads:

$$H = \underbrace{H_0}_{Indipendent\ Particle\ Hamiltonian} + \underbrace{V}_{Residual\ Interactions}, \tag{9}$$

where H_0 is the unperturbed hamiltonian, and admits a set of unperturbed eigenvectors in the full Hilbert Space $\mathcal{H}$:

$$H_0\psi_i^{(0)} = E_i^0\psi_i^{(0)} \qquad i = 1,2\cdots A \tag{10}$$

We ask for the existence of an Effective Hamiltonian H_{eff}, such that:

$$\langle\psi|H|\psi\rangle \iff \langle\psi'|H_{eff}|\psi'\rangle \tag{11}$$

Given $\hat{P}$, projector on $\mathcal{M}$, and $\hat{Q}$, projector on $\mathcal{H}/\mathcal{M}$, it can be proved that [5, page 303]:

$$(\underbrace{H_0 + V}_{H} - E)\psi = 0 \iff \hat{P}(\underbrace{H_0 + V_{eff}}_{H_{eff}} - E)\psi' = 0, \tag{12}$$

where V_{eff} is the Effective Potential and has this form:

$$V_{eff} = V + V\frac{\hat{Q}}{E - H_0}V + V\frac{\hat{Q}}{E - H_0}V\frac{\hat{Q}}{E - H_0}V + \cdots \tag{13}$$

Once proved that the definiton of an effective potential is theoretically admitted, we should face the problem of practically finding it. According to [6], three strategies have been explored up to now:

1. Finding directly **Two-Body Matrix Elements for** V_{eff}, starting from experimental data. In this case, no attempt is made to find the shape of the nuclear two-body potential V(1,2). Instead, the single-particle energies and the effective potential (V_{eff}) matrix elements are taken as free parameters. Then, starting from some random initial parameters, the iterative least square method is performed until there is good agreement with experimental data. Such procedure is the most feasible one. For this reason, effective matrix elements will be used to reconstruct the level scheme of ^{43}Sc and ^{43}Ti in section 4.

2. Bulding up V_{eff} from **Realistic Potentials for** V(1,2)
This strategy starts from the free nucleon-nucleon interaction in order to obtain the so-called *realistic potentials* for the nuclear two-body interaction V(1,2). Such realistic potentials have an analytic structure which is determined by general invariance principles, and contain some free parameters, which have to be found by fitting to the free nucleon-nucleon scattering observables. Such process is generally complicate.

3. Bulding up V_{eff} from **Schematic Interactions for** V(1,2).
Instead of bringing the features of the free nucleon-nucleon interaction into the nuclear two-body interaction, some very simple radial shapes are taken for the nuclear two-body interaction V(1,2) and the free parameters are determined in order to reproduce the measured energies for the excited states of the nuclei belonging to the mass region we wish to study. Some of the most common radial shapes are the Yukawa potentials ($\frac{e^{-\mu r}}{\mu r}$), the Gaussian potentials ($e^{-\mu r^2}$) and the Dirac potentials ($\delta(r)$).

Once the two-body matrix elements for V_{eff} have been determined, the solution to the eigenvalue problem in the Model Space can be found with a straightforward procedure.
First, we should find a basis for the Model Space: the most common and feasible choice is given by the eigenvectors of the single-particle part of the effective hamiltonian $(\psi_i^{(0)})_{i=1,2,\ \ldots\ dim\mathcal{M}}$. Then we can write the **eigenvalue problem** and find a suitable programme, such as the Antoine Code for Shell Model [8], to solve it:

$$\begin{bmatrix} \epsilon_1 + \left\langle\psi_1^{(0)}\middle|V_{eff}\middle|\psi_1^{(0)}\right\rangle & \cdots & \left\langle\psi_1^{(0)}\middle|V_{eff}\middle|\psi_{dim\mathcal{M}}^{(0)}\right\rangle \\ \vdots & \ddots & \vdots \\ \left\langle\psi_{dim\mathcal{M}}^{(0)}\middle|V_{eff}\middle|\psi_1^{(0)}\right\rangle & \cdots & \epsilon_{dim\mathcal{M}} + \left\langle\psi_{dim\mathcal{M}}^{(0)}\middle|V_{eff}\middle|\psi_{dim\mathcal{M}}^{(0)}\right\rangle \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_{dim\mathcal{M}} \end{bmatrix} = \lambda \begin{bmatrix} a_1 \\ \vdots \\ a_{dim\mathcal{M}} \end{bmatrix},$$

where ϵ_i are the single-particle energies in the model space, $\psi_i^{(0)}$ are the eigenvectors of the unperturbed problem and a_i are the coefficients of the linear combinations of the unperturbed eigenvectors representing the new eigenvector ψ_λ:

$$\psi_\lambda = \sum_{i=1}^{dim\mathcal{M}} a_i \psi_i^{(0)}, \tag{14}$$

Since the new eigenstate wavefunctions are linear combinations of the unperturbed single-particle eigenfunctions, in the new eigenstate particles will not occupy well defined orbits, but there will be a quantum superposition of single-particle states. Hence, orbits will have **fractional occupation numbers**.

2.2 Antoine: The Shell Model Code

The Antoine Code for Shell Model Calculations was developed by E.Caurier and F.Nowacki [8]. It works in the *m-scheme*, which means that the many body basis, which is constructed in order to diagonalize the Hamiltonian Matrix, has a fixed M, the quantum number associated to the total angular momentum projection along the z-axis .

The diagonalisation of the effective hamiltonian matrix is performed using the **Lanczos method** [7, section 3.A]. This method writes the hamiltonian matrix in a such a basis that it becomes tridiagonal.
To be more specific, taken a random pivot state $|1\rangle$, $|a_1\rangle = H|1\rangle$ is computed and is seen to be equal to:

$$|a_1\rangle = H_{11}|1\rangle + |2'\rangle \quad with\ \langle 1|2'\rangle = 0 \implies H_{11} = \langle 1|a_1\rangle = \langle 1|H|1\rangle \tag{15}$$

Then two other matrix elements are easily calculated:

$$|2\rangle = \frac{|2'\rangle}{\sqrt{\langle 2'|2'\rangle}} \implies H_{12} = \langle 1|H|2\rangle, \quad H_{22} = \langle 1|H|2\rangle. \tag{16}$$

We can iterate such method k times and and obtain the vector:

$$|a_k\rangle = H|k\rangle = H_{k,k-1}|k-1\rangle + H_{kk}|k\rangle + |k+1'\rangle, \tag{17}$$

and have the hamiltonian matrix in such form:

$$\begin{bmatrix} H_{11} & H_{12} & 0 & 0 & \cdots & 0 \\ H_{21} & H_{22} & H_{23} & 0 & \cdots & 0 \\ 0 & H_{32} & H_{33} & H_{34} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & H_{k,k-1} & H_{kk} \end{bmatrix}$$

The reason why such algorithm is adopted, is that in shell model calculations, few states of low energy are required and hamiltonian matrixes are really sparse. In fact the number of iterations required by the Lanczos algorithm, depends little on the matrix dimension but varies linearly with the number of non-zero elements of the initial matrix. It also depends on the number of converged states needed and on the choice of the initial pivot [7, section 3.A]. For those reasons, Lanczos algorithm, perfectly suits shell model calculations.

3 Mirror Nuclei and Mirror Energy Differences

3.1 Isospin symmetry

Two of the most relevant aspects of the nuclear two-body interaction are:

- **Charge Symmetry**, which implies that the proton-proton two-body interaction is equal to the neutron-neutron interaction:
$$V_{pp} = V_{nn}; \tag{18}$$
- **Charge Independence**, which implies that the neutron-proton two-body interaction is the average between the proton-proton and the neutron-neutron interaction:
$$V_{np} = \frac{V_{pp} + V_{nn}}{2}. \tag{19}$$

Such evidence led to the idea that proton and neutron could be considered as two different states of the same particle: the so-called *nucleon*. In order to distinguish protons from neutrons, the *Isospin* vector was introduced. It has the same algebra of the spin, and has a projection on the z-axis defined as follows:
$$t_z^{neutron} = \frac{1}{2} \qquad t_z^{proton} = -\frac{1}{2}. \tag{20}$$

For a nucleus made of N neutrons and Z protons, its Isospin vector is defined as the vectorial sum of the isospin vectors related to each nucleon. The projection along the z-axis is:
$$T_z = \frac{N - Z}{2}, \tag{21}$$

The module of the isospin vector, T, is not an observable but can be deduced from T_z, using the rule that $T \geq |T_z|$. For nuclei with the same number of particles, states with the same value of isospin module T, total angular momentum J and the same parity but different values of T_z, are called **Isobaric Analogue States (IAS)** and are completely degenerate in energy, if we consider only the nuclear two-body interaction and assume that it is charge-simmetric and charge-independent. This statement is known as the **Isospin Symmetry Principle**.
At the beginning of Nuclear Physics, it was believed that the only Isospin violating contribution to the nucleon-nucleon potential, was due to the Coulomb interaction between protons. However, models where the Coulomb interaction is the only responsible for Isospin Symmetry breaking effects, have not always succeeded in explaining them. Furthermore, it was found that the free nucleon-nucleon interaction is just approximately charge-independent and charge-symmetric ([9, section 2.2.1] and references there in). The scattering lengths of the free proton-proton and neutron-neutron interaction were measured and corrected in such a way that electromagnetic effects were not considered [4]. The obtained values are:
$$L_{\nu\nu} = -18.9 \pm 0.4 \text{ fm} \qquad L_{\pi\pi} = -17.3 \pm 0.4 \text{ fm}. \tag{22}$$

This provides clear evidence that the charge-symmetry of the free nucleon-nucleon interaction is slightly broken. However, how to take such experimental evidence into consideration in the nuclear effective interaction, remains an open question.

3.2 Energy Differences along Isobaric Multiplets

In order to study binding energy variations along an isobaric multiplet, we should consider the **Isobaric Multiplet Mass Equation (IMME)**, which is deduced - following the procedure used in [9, section 2.2] - under the two following assumptions:

- The charge-violating part of the Hamiltonian (H_{CV}) can be seen as a perturbation of the charge-conserving one (H_{CI});
$$H = H_{CI} + H_{CV}; \tag{23}$$

- H_{CV} is only due to the two-body interactions between nucleons, which means that it can be written as the sum of three tensors of rank, respectively, zero (*isoscalar component*), one (*isovector component*) and two (*isotensor component*):

$$H_{CV} = H^0_{CV} + H^1_{CV} + H^2_{CV}. \tag{24}$$

Hence, it can be shown that the perturbation to the binding energy due to H_{CV},

$$\Delta BE(T, T_z) = \langle \alpha T T_z | H_{CV} | \alpha T T_z \rangle \tag{25}$$

is equal to:

$$\Delta BE(T,T_z) = a + bT_z + cT_z^2 \tag{26}$$

where a, b and c are coefficients that depend on T and H_{CV}. More precisely, a depends on the isoscalar and the isotensor component of H_{CV}, b on the isovector component, and c on the isotensor one. Therefore, it yelds that b and c separately hold information respectively on the charge symmetry and on the charge independence of the nucleon-nucleon interaction.

3.3 Mirror Energy Differences

When studing an isobaric multiplet, one of the most important parameters is the **Mirror Energy Difference (MED)**, defined as the difference between the excitation energies related to the ground state, of analogue levels in two mirror nuclei of the same isobaric multiplet:

$$MED_{J,T} = E^*_{J,T,T_z=-|T_z|} - E^*_{J,T,T_z=|T_z|}. \tag{27}$$

It should be stressed that the energies of the two levels are normalised to the absolute binding energy of the ground states. This allows to cancel the bulk of the energy differences due to the Coulomb interaction and to study fine variations, that otherwise it would have been really difficult to appreciate.
An explicit expression for the MED can be obtained using the IMME formula. For example, in the $T = \frac{1}{2}$ pair, the MED can be written - see [9, section 2.2] - as follows:

$$MED_{J,T=\frac{1}{2}} = -\Delta b_J, \tag{28}$$

where Δb_J is the variation of the coefficient b as a function of the spin J, with respect to the value at the ground state.
As a consequence, not only does the MED shed light on fine variations of the energy differences as a function of the spin, but it enables us to study the charge symmetry violation separately from charge independence.
Hence, if we are able to predict all the possible contributions to the MED due to the electromagnetic interaction, then we can look at the difference between the predicted and the experimental value and estimate the impact of unknown **charge-symmetry violating effects**, such as the one due to the nucleon-nucleon interaction. Moreover, the MED provides information on the **evolution of nuclear structure properties** as a function of the total angular momentum.
To summarize, the MED works as a *magnifing glass* on the physics behind the excited states of mirror nuclei, improving our understanding of both charge-symmetry violating effects and nuclear structure phenomena as a function of the total angular momentum.

3.4 Origin of the energy differences between Mirror Nuclei

The main contribution to the MED is due to the Coulomb interaction, whose hamiltonian can be divided in two components: the *monopole term*, which takes into account single-particle and bulk effects due to the spherical field and the *multipole term*, which is related to all the other effects, in particular the correlation between valence nucleons. Isospin Non-Conserving Nuclear contributions to the MED might be included as well.
Therefore in our model for the MED, following [9, section 4], four different effects will be considered:

- The Multipole Coulomb field contribution;

- The Monopole Coulomb field contribution;
- The contribution due to some fine Corrections to Single-Particle Energies;
- The Isospin Non-Conserving Nuclear Interaction contribution.

3.4.1 Multipole Component of the Coulomb Field

The multipole Coulomb term is the one obtained considering the Coulomb contribution to the **two-body effective interaction** among nucleons of the valence space. The variation of this term with the angular momentum J outlines **the alignment of the spins of pairs of nucleons with a rotational angular momentum**.
To give an example, for the pair of mirror nuclei $^{49}Mg/^{49}Cr$, it was noted that the multipole contribution to the MED was really small for low spin states and had a rapid increase, when $J^\pi = \frac{17}{2}^+$ [9, section 4.1.1]. This enhancemnt of the MED was interpreted in terms of the alignment of nucleons along the rotational bands. In fact, it is known that two protons coupled in time reversed orbits have a stronger interaction than that of protons coupled in any other way. The intensity of the Coulomb interaction between aligned protons reaches its minimum when they are aligned at the maximum value (2j - 1) in a single j-shell. When, in a certain nucleus, a couple of protons gets aligned at the maximum value of spin, the excitation energy of the level decreases because the Coulomb interaction between protons is repulsive. But, in the corresponding mirror nucleus, two neutrons get aligned and there is no such effect: the result is a rapid increase or decrease in the MED, as it occurs at $J^\pi = \frac{17}{2}^+$ for the nuclei $^{49}Mg/^{49}Cr$.

3.4.2 Monopole Component of the Coulomb Field

The monopole contribution of the Coulomb Field to the MED takes into consideration the effect of the Coulomb spherical field obtained considering the nucleus as a charged sphere. It gives two contributions to the MED, which are related to:

- The **change of radius along the rotational band**, which is treated below;
- The **shift in proton single-particle energies**, caused by the interaction of the core, seen as a charged sphere, with valence protons, which will be described in section 3.4.3.

Thinking the nucleus as a charged sphere of radius R_C, its potential Coulombian energy is:

$$E_C = \frac{3}{5}\frac{Z(Z-1)e^2}{R_C}. \tag{29}$$

If we have two mirror nuclei, whose atomic numbers are $Z_>$ and $Z_<$, such that $Z_> = Z_< + n$, then the Coulomb energy difference of the ground states is:

$$\Delta E_C = E_C(Z_>) - E_C(Z_<) \simeq \frac{3}{5}\frac{n(2Z_> - n)e^2}{R_C}. \tag{30}$$

However, in the hypotesis that the nuclear radius does not change in the excited states, such effect vanishes when calculating the MED. Instead, if we consider the radius variations as function of the spin, $R_C(J) = R_C(J_{gs}) + \Delta R(J)$, then a monopole contribution to the MED will result:

$$\Delta_M \langle V_{Cr} \rangle = \Delta E_C(J) - \Delta E_C(J_{gs}) = -\frac{3}{5} n(2Z_> - n)e^2 \frac{\Delta R(J)}{R_C^2} \tag{31}$$

This formula has the advantage of providing us a simple expression to estimate the MED monopole contribution for every pair of mirror nuclei, but, at the same time, has the downside that it is hard to find the function $R(J)$.

In the specific case of two mirror nuclei in the *pf shell*, it happens that the radius changes when the occupations of the orbits $p_{\frac{3}{2}}$ and $p_{\frac{1}{2}}$ change as a function of the spin, because the p orbits have

a larger radius than the f orbits. A **phenomenological term for the radial effect on the MED in *pf shell* mirror nuclei**, can be easily estimated, following [9, section 4.2]:

$$\Delta_M \langle V_{Cr} \rangle = n\alpha_r \left(\frac{m_\pi(J_{g.s}) + m_\nu(J_{g.s.})}{2} - \frac{m_\pi(J) + m_\nu(J)}{2} \right), \tag{32}$$

where n is the difference between proton and neutron numbers in the two nuclei, m is the occupation number of the p orbits of a certain nucleon type in the state of angular momentum J, and α_r is a parameter, which has been estimated from experimental values. In the *pf shell*, α_r has the following value:

$$\alpha_r = 200 \text{ keV}. \tag{33}$$

3.4.3 Corrections to Single-Particle Energies

The single-particle energies are modified by two different effects:

- The **interaction of protons** in the valence space with the **monopole electromagnetic field** generated by the core,
- The **relativistic electromagnetic spin-orbit force**.

The first contribution affects only the single particle energies of protons and has been calculated by Duflo and Zuker [10], who found it to be proportional to the square of the orbital angular momentum of the protons:

$$E_{ll} = \frac{-4.5 Z_{closed\ shell} \left[2l(l+1) - N(N+3) \right]}{A^{\frac{1}{3}} \left(N + \frac{3}{2} \right)} \text{ keV}, \tag{34}$$

where N is the principal quantum number and l the orbital angular momentum of the proton shell.

The second contribution is due to the relativistic electromagnetic spin-orbit force (EMSO) which is related to the Larmor precession of nucleons in the nuclear electric field, and to the Thomas precession of protons.

The EMSO potential can be written as reported in [9, section 4.1.3]:

$$V_{ls} = (g_s - g_l) \frac{1}{2m_{nucleon}^2 c^2} \left(\frac{1}{r} \frac{dV_c}{dr} \right) \vec{l} \cdot \vec{s}, \tag{35}$$

where g_s and g_l are the gyromagnetic factors, respectively spin and orbital. If the core is modelled as a uniformly charged sphere, we get a simple expression for the the perturbation to single particle enrgies due to the EMSO force:

$$E_{ls} \simeq (g_s - g_l) \frac{1}{2m_{nucleon}^2 c^2} \left(-\frac{Ze^2}{R_C^3} \right) \langle \vec{l} \cdot \vec{s} \rangle, \tag{36}$$

In table 1, there are some approximate formulas for the EMSO single-particle energy shifts.

	$\pi \quad j = l + \frac{1}{2}$	$\pi \quad j = l - \frac{1}{2}$	$\nu \quad j = l + \frac{1}{2}$	$\nu \quad j = l - \frac{1}{2}$
E_{ls}	$-42\frac{Z}{A} l$ keV	$42\frac{Z}{A}(l+1)$ keV	$35\frac{Z}{A} l$ keV	$-35\frac{Z}{A}(l+1)$ keV

Table 1: EMSO shifts in single-particle energies
Table taken from [9, section 4.1.3]

It is important to stress out that the EMSO term differs from the nuclear spin-orbit. Nuclear spin-orbit effect must be always considered in shell model calculations and is of the order of several MeV, whereas EMSO gives birth to a second order effect, of about two order of magnitude smaller. When building up the energy level scheme of a nucleus, EMSO has a negligible impact on the final result. Nevertheless, in MED calculations, the EMSO force might have a significant influence, since it changes in different ways the proton and the neutron single-particle energies.
As an example, we can consider the shells $d_{\frac{3}{2}}$ and $f_{\frac{7}{2}}$ and see - using formulas in table 1 - that EMSO

brings protons $\sim$ 120 keV nearer, and enlarges by a similar amount the gap between neutrons. Therefore, in such case, the EMSO effect on MED will be stronger in states that are due to an only proton (only neutron in the mirror) excitation from $d_{\frac{3}{2}}$ to $f_{\frac{7}{2}}$, whereas it can be neglected when the excitation is due to a proton or a neutron with similar probabilities.

3.4.4 Isospin Non-Conserving Nuclear Interactions

In the hypothesis of isospin symmetry, the difference between the MED experimental value and its theoretical prediction made with all the Coulomb corrections described above, should be really tiny. However, such condition is not always observed. This leads to the hypothesis that the impact of **Isospin Non-Conserving Nuclear interactions (INC)** is not negligible. To give an example, this happens for many mirror nuclei of the *pf shell*, where, it is almost impossible to give a theoretical explanation for the MED based only on electromagnetic effects [3].

The most reasonable way to take into consideration the INC contribution would be that of building up an effective potential which contains also the Isospin Non-Conserving term. However, this task is very hard to achieve. For this reason, in many cases it seems more feasible to build, **phenomenological models** starting from experimental data.
One of such models was developed in 2002 by A.P. Zuker, S.M. Lenzi, G. Martinez-Pinedo and A. Poves [1] and aims at estimating the INC contribution to the MED for nuclei in the $f_{\frac{7}{2}}$ *shell*. The first mirror doublet in the $f_{\frac{7}{2}}$ *shell* which has been studied, was formed by ^{42}Ti and ^{42}Ca. It is clear, from table 2, that the MED predictions realised considering only electromagnetic effects fail at describing MED experimental values. As we can see, the main INC contribution to the MED appears at the state $J^\pi = 2^+$ and has an order of magnitude of 100 keV.

	$J=0$	$J=2$	$J=4$	$J=6$
Coulomb Contribution V_C (keV)	81.60	24.60	6.40	-11.40
$MED\left[^{42}Ti - ^{42}Ca\right] - V_C$ (keV)	5.38	92.55	4.57	-47.95

Table 2: Mirror Energy Differences in $^{42}Ti/^{42}Ca$ from [1]

Given that in the $f_{\frac{7}{2}}$ valence shells there are two protons for ^{42}Ti and two neutrons for ^{42}Ca, and that the excited states are mostly $f^2_{\frac{7}{2}}$ states, we infer that the leading term in the INC interaction is related to the coupling of two $f_{\frac{7}{2}}$ protons and two $f_{\frac{7}{2}}$ neutrons at $J = 2$.
Motivated by those reasons, we can construct a simple ansatz for the INC term, considering a difference of 100 keV for the matrix element of two protons in the$f_{\frac{7}{2}}$ shell coupled to $J = 2$ with respect to the two-neutron matrix element.

This ansatz has been applied to several other nuclei of the *pf shell* with masses different from $A = 42$, such as $A = 47,\ 49,\ 50,\ 51$ and gave succesful results.

In 2013, Kaneko, Sun, Mizusaski and Tazaki, proposed a different parametrisation for the INC term [2]: they considered a difference of - 100 keV for the matrix element of two protons in the $f_{\frac{7}{2}}$ shell coupled to $J = 0$ with respect to the two-neutron matrix element.
In 2015, Bentley, Lenzi, Simpson and Diget [3], studied the Mirror Energy Differences of a huge vairety of $f_{\frac{7}{2}}$ *shell* nuclei and proved the equivalence of the models developed in [1] and in [2]. According to them, the relevant aspect of the INC matrix elements is **the difference of** $\sim$ 100 keV **between the matrix element at J=2 and at J=0 in the** $f_{\frac{7}{2}}$ ***shell***, rather than the way such difference is distributed between the two matrix elements.
It was then shown that **the INC interaction defined in such way can be extended also to the other orbits of the *pf shell* and the *sd shell*.** For example, in [11], the INC interaction was extended to all the orbits of the *sd shell* and succesfully used to predict the MED of the mirror doublet formed by ^{23}Mg and ^{23}Na.

In [3], **the physical origin of the INC term** was discussed as well. It might seem that the INC term is directly connected to the breaking of the charge symmetry of the nucleon-nucleon interaction. Actually, it is possible to predict the matrix elements of the Isospin Non-Conserving part of such interaction starting from the free proton-proton and neutron-neutron scattering lengths, whose values were measured in [4] and corrected in such a way that electromagnetic effects are not considered: $L_{\nu\nu} = -18.9 \pm 0.4$ fm and $L_{\pi\pi} = -17.3 \pm 0.4$ fm. Hence, it was calculated that the matrix elements of the INC nuclear interaction should be around:

$$V_B^{J=0} \simeq 11 \text{ keV} \quad V_B^{J=2,4,6} = 0 \tag{37}$$

Such results do not agree, either in sign or value, with the INC matrix elements found in [3], suggesting that there might be some contribution of electromagnetic nature, which either has not been well estimated or has been neglected at all.

In section 4 we will apply the models found in literature to the negative (nautral) parity states and for the first time, for the positive (non-natural) parity states of mirror nuclei ^{43}Ti and ^{43}Sc. We adopt an isovector -100 keV in every orbit of the *pf* and *sd shell* for nucleons coupled to $J = 0$.

4 Study of the Mirror Nuclei $^{43}_{22}Ti$ and $^{43}_{21}Sc$

The mirror nuclei ^{43}Ti and ^{43}Sc can be studied consistently within the framework of the interacting shell model. In this work we are interested at the yrast states, which are the states with the lowest energy for every possible value of the total angular momentum.
Since ^{43}Ti and ^{43}Sc form a $T = \frac{1}{2}$ **doublet**, it is possible to investigate the **charge symmetry** property of the nucleon-nucleon effective interaction separately from charge independence, by simply looking at the Mirror Energy Differences (see section 3.3). Therefore, if we are able to build a fine theoretical prediction for the electromagnetic contribution to the MED, we can understand, from the analysis of the gap between theoretical and experimental values, whether **Isospin Non-Conserving nuclear forces** have a relevant impact or not.
Since the two nuclei have mass number $A = 43$, we may try to test on them the **phenomenological model for the INC contribution** which has been developed in [3].
Moreover, the energies of high spin positive parity yrast states of ^{43}Ti have not been measured. This work will give a theoretical prediction - which could be useful for future experiments - for the energies of such levels and the associated Mirror Energy Differences.

4.1 Negative Parity States

In order to study the yrast negative parity states, the model space which has been considered, is that of an inert $^{40}_{20}Ca$ core with a valence space, made up of the four orbits of the *pf shell*:

$$f_{\frac{7}{2}}, p_{\frac{3}{2}}, f_{\frac{5}{2}}, p_{\frac{1}{2}} \rightsquigarrow pf\ shell. \tag{38}$$

4.1.1 Level Scheme Reconstruction

Using the Antoine Code for Shell Model [8], we managed to build the **energy level scheme**. We used an **effective interaction**, called *kb3g.a42*, whose hamiltonian contains only the nuclear isospin conserving term [12]. Such interaction has been specifically developed for nuclei whose valence space is the *shell pf*. In our calculation, we allowed any possible excitation of the three valence nucleons within such shell.

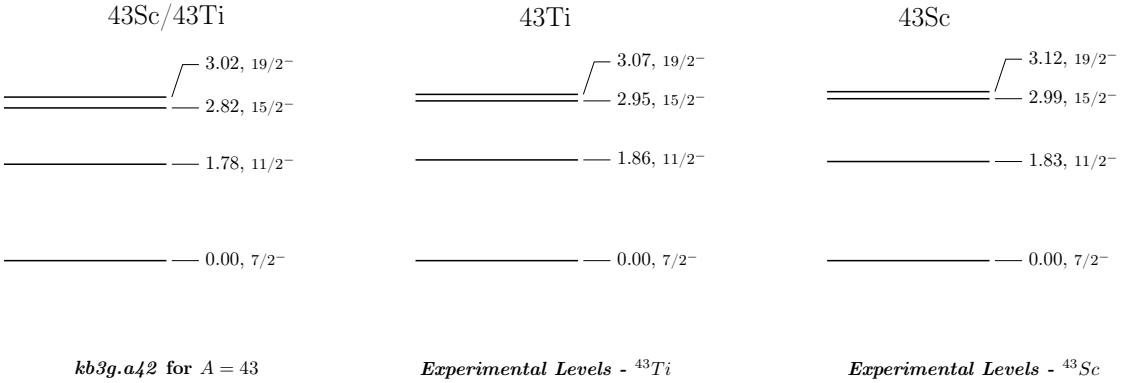


Figure 2: Energy levels (MeV)
Negative Parity Yrast States

In figure 2, the theoretical prediction for the level scheme, is compared to experimental data [13]. There is good agreement, since the theoretical values reproduce the correct level order and are almost equal to the experimental ones within the order of 100 keV.
It is important to note, that at this point, the prediction for the level schemes is the same for ^{43}Sc and ^{43}Ti, since we are neglecting all the isospn non-conserving contribution, either of Coulomb or nuclear nature.

4.1.2 Mirror Energy Differences

We proceeded to the calculation of **Mirror Energy Differences** for negative parity yrast states, considering all the contributions described in section 3.4

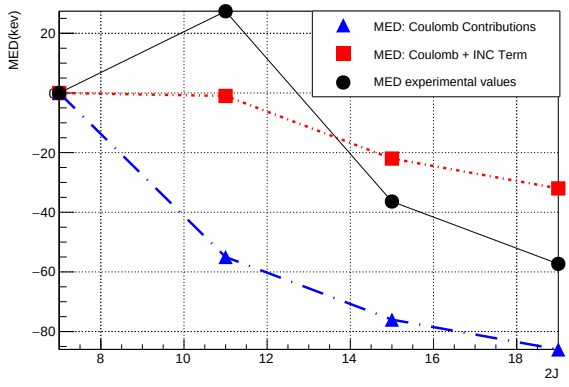
The graph in figure 3a compares the MED experimental values to two different theoretical predictions: one obtained using only Coulomb contributions and the other, adding the INC term to them. A quick glance tells us that **the addition of the INC term to the MED improves the predictions** and gives a better reproduction of the behaviour of experimental values.
In order to quantitavely evaluate how far the two predictions are from experimental data, we computed the associated root mean square (RMS) deviation.

	MED Prediction with Coulomb effects	MED Prediction with Coulomb and INC terms
RMS	56 keV	23 keV

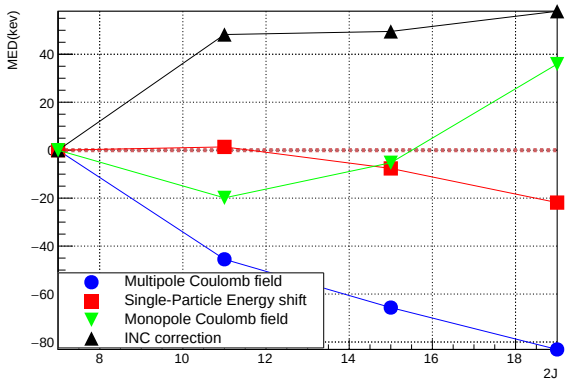
Table 3: Root Mean Square Deviation

It is clear that the addition of the INC term makes the RMS consistently smaller. Furthermore the RMS deviation obtained with the addition of the INC term is, as expected, of the same order of magnitude of the one obtained in the fit ($\sigma_{theo} \simeq 23$ keV) performed by Bentley and others in [3].
Figure 3b, instead, shows how every contribution affects the MED theoretical prediction, providing clear evidence that:

- The main contribution of electromagnetic origin comes form the multipole Coulomb field;
- The monopole Coulomb field and the single particle energy shifts give little corrections to the MED;
- The contribution of the INC term has a relevant value.



(a) *MED:Theoretical predictions*



(b) *Contributions to the MED Theoretical Prediction*

Figure 3: MED - $^{43}_{22}Ti$ and $^{43}_{21}Sc$
Negative Parity yrast States

4.2 Positive Parity States

The positive parity yrast states of mirror nuclei $^{43}_{22}Ti$ and $^{43}_{21}Sc$ cannot be obtained considering the *pf shell* as the valence space. In order to have positive values for parity, we should allow the **excitation of at least one particle from the core**. Here we will consider the excitation of only one nucleon from the highest energy orbit ($1d_{\frac{3}{2}}$) of the *sd shell* to the *pf shell*.

4.2.1 Level Scheme Reconstruction

In order to build a theoretical prediction for the positive parity level scheme, we used an **effective interaction**, called *sdpf* [14], which operates in the orbits of the two main shells:

$$1d_{\frac{5}{2}}, 2s_{\frac{1}{2}}, 1d_{\frac{3}{2}} \rightsquigarrow sd\ shell \tag{39}$$

$$1f_{\frac{7}{2}}, 2p_{\frac{3}{2}}, 1f_{\frac{5}{2}}, 2p_{\frac{1}{2}} \rightsquigarrow pf\ shell \tag{40}$$

Besides letting the particles free to move within the *pf shell*, the only permitted excitation in the *sd shell* was that of one nucleon from $1d_{\frac{3}{2}}$ to the orbits of the *pf shell*.
Hence, we calculated the energies of the levels using the *sdpf* interaction, which contains only the nuclear isospin conserving hamiltonian.

In figure 4, the predicted level scheme is compared to the known experimental levels [13]. The experimental energies of $^{43}_{22}Ti$ excited states with $J^\pi > \frac{9}{2}^+$ have not been measured yet.
The agreement between theory and experiment is acceptable but not as good as in the negative parity case: even if the correct level order has been reproduced, theoretical predictions differ from experimental values in some cases by 300/400 keV. A possible explanation for this result, is that the model where only one hole is made in the shell $1d_{\frac{3}{2}}$ is just an approximation, which is quite good but not completely faithful to the physics behind positive parity states.

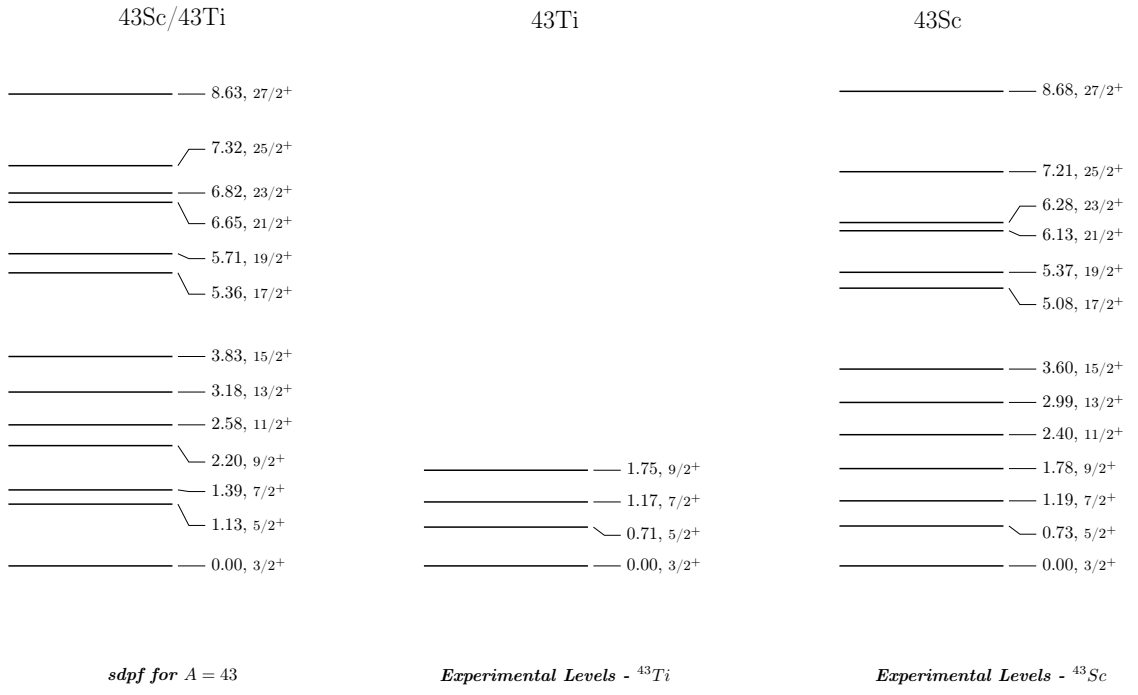


Figure 4: Energy levels (MeV)
Positive Parity yrast States

Finally, it should be observed that **the level energies are not normalised to the ground states** ($J^\pi = \frac{7}{2}^-$) of the two nuclei but to the lowest energy state ($J^\pi = \frac{3}{2}^+$) among those of positive parity. The reason for this choice is of practical nature: we do not have reliable predictions for the absolute energies of the ground state and of the $J^\pi = \frac{3}{2}^+$ state, beacause the inert core assumption made in our model is rather unjustified. Nevertheless, we have good predictions for the differences between absolute values of the energies - calculated using the same interaction - of different levels of the same nucleus. Therefore, given that we used different effective interactions for the negative and positive parity states, we chose to normalise the energies of the positive parity levels to the $J^\pi = \frac{3}{2}^+$ state.

4.2.2 Mirror Energy Differences

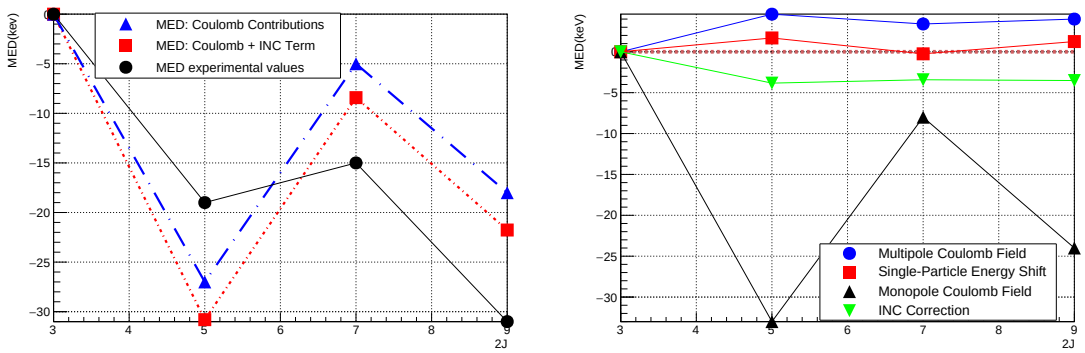
We proceeded to calculate the **Mirror Energy Differences**, following the protocol described in section 3.3. The results of our calculations can be seen in figures 5a and 6a, where two different theoretical predictions are shown: one where only electromagnetic contributions to the MED have been considered and the other where the INC term has been included as well.

Figure 5a shows the behaviour of the MED theoretical predictions for states with low angular momenta in comparison with experimental values. It can be seen that theoretical predictions agree well with data and that the MED value is almost entirely determined by the electromagnetic corrections. In order to quantitavely evaluate how far the two predictions are from experimental data, we computed the associated root mean square (RMS) deviation:

	MED Prediction with Coulomb effects	MED Prediction with Coulomb and INC terms
RMS	11 keV	10 keV

Table 4: Root Mean Square Error

It is clear that the INC correction has a very little effect on the final result.
Through figure 5b, it is possible to understand how the different corrections affect the final MED prediction. The INC correction and the single-particle energy shifts have almost no influence on the final result and the multipole Coulomb field contribution has a relatively little impact. The **term that dominates** over the others and explains the behaviour of experimental MED is the one due to **the change of radius along the rotational band**.



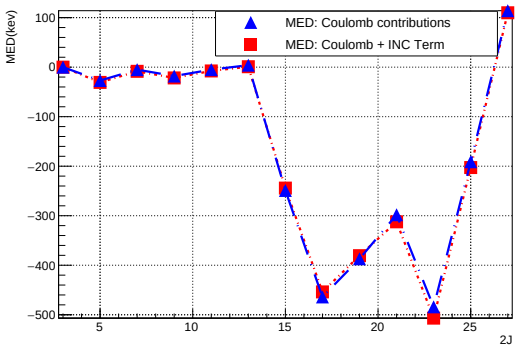
(a) *MED:Theoretical predictions vs Experimental Values* (b) *Contributions to the MED Theoretical Prediction*

Figure 5: MED - $^{43}_{22}Ti$ and $^{43}_{21}Sc$
Positive Parity States from $J^\pi = \frac{3}{2}^+$ to $J^\pi = \frac{9}{2}^+$

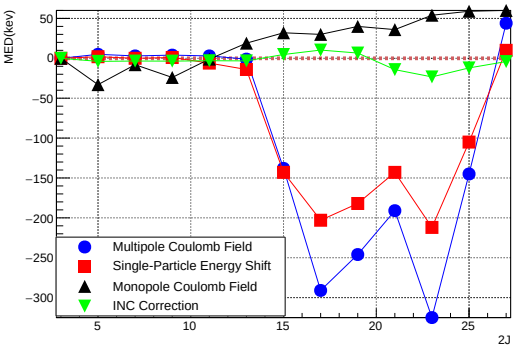
For the MEDs at higher values of spin, we have no experimental data to be compared with our predictions. Figure 6a shows the behaviour of the MED theoretical predictions, with and without the INC correction, along all the positive parity states. It can be seen that **the INC correction has an absolutely negligible impact** on the final result and that there is a **big decrease for those states with** $J^\pi > \frac{13}{2}^+$:

$$MED_{J^\pi > \frac{13}{2}^+} \ll MED_{J^\pi = \frac{3}{2}^+} = 0. \tag{41}$$

Figure 6b, instead, shows the influence that every contribution to the MED has on the final result: the two major effects come from the multipole Coulomb field and the single-particle energy corrections. This suggests that **the reason for the big decrease at** $J^\pi = \frac{13}{2}^+$ **has to be sought in the type of nucleon that in each state is excited from the orbit** $1d_{\frac{3}{2}}$ **to the *pf shell*.**



(a) *MED:Theoretical predictions*



(b) *Contributions to the MED Theoretical Prediction*

Figure 6: MED - ${}^{43}_{22}Ti$ and ${}^{43}_{21}Sc$
Positive Parity States from $J^\pi = \frac{3}{2}^+$ to $J^\pi = \frac{27}{2}^+$

In figure 7, we analyse how the $1d_{\frac{3}{2}}$ hole varies as a function of J: in the states with $J^\pi < \frac{13}{2}^+$, the hole is made up of only one type of nucleon, either a proton (${}^{43}_{21}Sc$) or a neutron (${}^{43}_{22}Ti$), whereas in the higher spin ones the hole is made up of both nucleons, in slightly equal percentages.

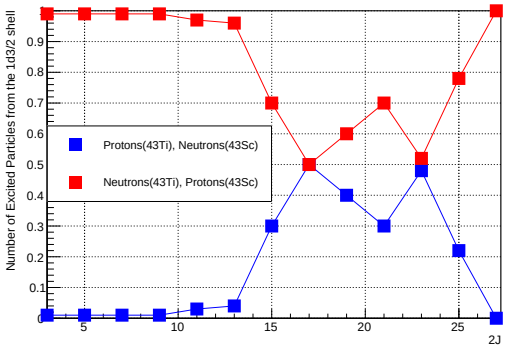


Figure 7: Hole in the orbit $1d_{\frac{3}{2}}$ as function of the momentum J

Hence, when we normalise all the states to $J^\pi = \frac{3}{2}^+$, which is not the ground state of the two nuclei, we cancel a big positive contribution to the MED, which is related to the fact that the hole at $J^\pi = \frac{3}{2}^+$ is a hundred percent made of, one proton for ${}^{43}Sc$ and one neutron for ${}^{43}Ti$. Then at $J^\pi = \frac{15}{2}^+$, the hole compositon becomes a mixture of protons and neutrons; this should bring the MED related to the ground state to small values, close to zero. But, in our calculation, the big positive contribution that had been cancelled when we normalised the MED to their value at $J^\pi = \frac{3}{2}^+$, appears as a big negative one when J^π reaches $\frac{15}{2}^+$.
When $J^\pi = \frac{27}{2}^+$, the two holes return to be a hundred percent formed by only one kind of nucleon. In fact, we observe a big positive jump of the MED value, such that:

$$MED_{J^\pi = \frac{27}{2}^+} \gg MED_{J^\pi = \frac{3}{2}^+} = 0. \tag{42}$$

This can be explained thinking that in low spin states there might be a big negative contribution, which is neglected when the MEDs are normalised to their value at $J^\pi = \frac{3}{2}^+$. This contribution, may disappear at high values of spin if we consider the MED normalised to the ground state, or equivalently, appear as big positive MED rise at $J^\pi = \frac{27}{2}^+$, if we consider the $J^\pi = \frac{3}{2}^+$ normalisation. However this is just a conjecture, that needs to be proved. One way to do it would be calculating the positive parity MED values related to the ground state. Unfortunately we did not manage to do this.

5 Conclusion and Future Directions

The predictions we obtained for the Mirror Energy Differences of the nuclei $^{43}_{21}Sc$ and $^{43}_{22}Ti$, can be considered reliable, and show **good agreement with experimental values**, when available. Such an agreement has undoubtedly been reached thanks to the addition of the INC term to the predicted MED.
For high spin positive parity Yrast States, there are no MED experimental values: we think that the theoretical predictions built in this work could be useful for researchers, who will attempt to measure high spin positive parity levels of $^{43}_{22}Ti$. The importance of seeing whether experiment and theory match for those states is due to the fact that the MED experimental values related to those states were excluded from the database which was used in [3] to obtain the INC term estimate. Hence, in this way the validity of such model for the INC term could be tested, even involving other orbits of the *pf* and *sd shells* different from $f_{\frac{7}{2}}$.

It should be said that we are still far from understanding the **physical nature of the INC term**. In [1], it was suggested that it could be related to the Isospin Non-Conserving part of the nuclear hamiltonian. However, in [3] it was shown that it did not match with the expected values for the INC term deduced from the free nucleon-nucleon scattering. This put into question the accuracy of our estimates for Coulomb contributions to the MED.
New approaches are being tried to model Isospin Non-Conserving nuclear interactions: one of those consists in including them in realistic potentials [11]. We hope that this will shed more light on the validity of the phenomenological model for the INC term and on its physical origin.
Such evidences clearly show that the **debate on the Charge Symmetry of nuclear two-body interactions still remains open** and is far from reaching an end.

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