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Effects of isospin symmetry breaking on doubly magic nuclei

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Sommario

Questo lavoro si concentra sulla rottura della simmetria di isospin nei nuclei doppiamente magici, studiando la differenza di energia tra i cosiddetti stati analoghi di nuclei isobari. Questi stati hanno lo stesso numero quantico di isospin e fanno parte di nuclei con il medesimo numero di massa A ma con diverso numero atomico Z.
La particolare simmetria esistente tra protone e neutrone, basata su varie osservazioni, tra le quali il fatto che abbiano massa quasi uguale e che gli spettri di nuclei specchio siano molto simili, è stata introdotta da Heisenberg nel 1932. Proprio tali considerazioni hanno portato ad introdurre il concetto di isospin e di simmetria di isospin, secondo cui le due particelle sono viste come due diversi stati di un più generale nucleone. Questa ha, tra le sue conseguenze, la simmetria e l'indipendenza dell'interazione nucleare dall'isospin, che non distingue protone e neutrone quando sono negli stessi stati quantici.
Il contributo maggiore alla rottura della simmetria di isospin è dato dal potenziale coulombiano. Perciò la differenza di energia tra stati analoghi, chiamata appunto *Coulomb Displacement Energy* (CDE), è dovuta prevalentemente a termini di origine elettromagnetica. In realtà, però, ci è resi contro che questo unico contributo non riesce a riprodurre con esattezza la CDE, ma rimane sempre una discrepanza tra i valori teorici e sperimentali di circa il 7%.
Con questo elaborato ci proponiamo di spiegare l'origine di questa discrepanza. La rottura della simmetria di isospin è già nota sperimentalmente, per esempio dagli esperimenti di scattering nucleone-nucleone, che mettono in luce i diversi valori delle lunghezze di scattering per protone-protone, neutrone-neutrone e protone-neutrone, e non riesce ad essere spiegata considerando solo effetti coulombiani. Noi siamo partiti da queste osservazioni per postulare la necessità di avere anche altri tipi di interazioni che rompano la simmetria di isospin, e che siano in grado di dar conto esattamente dei valori di CDE.
Ci siamo concentrati sugli stati isobarici analoghi di nuclei doppiamente magici, introducendo due interazioni: una che rompe la simmetria di carica e l'altra l'indipendenza di carica. Con l'utilizzo di entrambe contemporaneamente, i risultati mostrano un'accurata descrizione della CDE per lo ^{90}Zr, ^{114}Sn e il ^{208}Pb, per i quali otteniamo un differenza dai dati sperimentali di circa una decina di keV, cioè dello stesso ordine dell'errore sui risultati stessi.

Contents

Introduction

Symmetries in physical laws are a very powerful tool in the study of natural phenomena. Every symmetry is indeed correlated to the invariance of a physical quantity with respect to certain transformations of the system under consideration. In this way it is possible to simplify problems, to have a better understanding of the natural properties and to generalize the results to similar, but more complex, cases. For example in quantum mechanics the presence of symmetry is reflected in the existence of good quantum numbers.

Two principles at the base of nuclear physics are the symmetry under exchange of protons and neutrons and the independence of the strong interaction on the electric charge. This allows to depict neutrons and protons as the two states of a same particle, the nucleon, and to introduce the isospin formalism. In the absence of breaking of isospin symmetry we could identify multiplets of analogue states in isobaric nuclei, called *Isobaric Analogue States* (IAS), which would be degenerate in energy. The study of the energy differences between analogue states represents a resource for the analysis of the interaction terms that are not invariant under the exchange of protons and neutrons.

Symmetry and independence principles lead to the conclusion that energy differences between IAS are due to electromagnetic terms. Their contribution to the binding energy of the nucleus can be estimated, in first approximation, as the electrostatic energy of a uniformly charged sphere. Since, for equal mass number A, it depends only on the difference between the number of protons and neutrons, the energies of analogue

states of two isobaric nuclei differ by a quantity called *Coulomb Displacement Energy* (CDE). The problem highlighted by the work of Nolen & Shiffer [1] is that considering the Coulomb interaction as the only source of the CDE, a 7% discrepancy remains between the theory and the experimental data.

The CDE has been studied for many nuclei, but here we focused on nuclei that can be explained with mean-field approximations, which are used in nuclear physics for medium-heavy nuclei. We used a particular type of effective interaction having zero-range, the Skyrme interaction, to solve Hartree-Fock equations and to find single-particle states. In this representation we tried to introduce two new terms that break the isospin symmetry: charge symmetry and charge independence breaking interactions. The aim of the work is to try to understand the discrepancy between calculated and experimental values for doubly magic nuclei with the use of these isospin breaking interactions. Indeed experimental evidences suggest the existence of isospin breaking terms besides the Coulomb interaction, for example in the slight difference between proton and neutron masses or in the nucleon-nucleon scattering experiments, where there are different scattering lengths for proton-proton, neutron-neutron and proton-neutron.

The thesis is structured as follows. In Chapter 1, we present the Nolen-Shiffer anomaly and the isospin formalism, listing different types of isospin breaking forces. In Chapter 2, we recall the main theoretical elements needed to describe the nuclear systems. In Chapter 3, we introduce all the isospin breaking terms, calculating their contribution to the CDE. Chapter 4 is devoted to the presentation and the discussion of the results.

Chapter 1

Background

1.1 Isospin formalism

In nuclear physics the first experimental results, starting from the mass systematics and the mirror nuclei spectra, highlighted a particular symmetry between the behaviour of neutrons and protons: when electromagnetic interactions, which are much weaker than nuclear interactions, are not considered, the two body potential between two nucleons is independent from the fact that they are protons or neutrons, provided they are in the same quantum states. This is related to properties of charge independence and charge symmetry.
Charge independence (CI) implies that the forces between the nucleons have to be independent of the charge and we can write it as

$$\frac{V_{pp} + V_{nn}}{2} = V_{np} \tag{1.1}$$

On the other hand charge symmetry (CS) means that proton-proton interaction V_{pp} is equivalent to neutron-neutron interaction V_{nn}:

$$V_{pp} = V_{nn} \tag{1.2}$$

Neglecting all the electromagnetic interactions, charge symmetry and charge independence can be seen in the almost identical spectra of mirror nuclei, with the same total nucleons number but different proton and neutron number.

These ideas have led to the introduction of a new quantum number: the isospin (T) that stands for the length of isospin vector **T** and whose projection is defined as $T_z = \frac{N-Z}{2}$. In this view neutron and proton can be interpreted as the two up and down states of a single particle, the nucleon, having isospin value $T = \frac{1}{2}$. In this work we will use $T_z = -\frac{1}{2}$ for the proton and $T_z = \frac{1}{2}$ for the neutron.
When there is invariance under some transformation there is always a conserved quantity: as in the case of absence of a preferred direction in space we have rotational invariance, that leads to angular momentum conservation, in the same way the inability to distinguish between up and down states in isospin space implies that nuclear forces are invariant under rotations in this space. This last thing means that the isospin is conserved in strong interactions. As long as only the strong nuclear force is present, the isospin vector can point in any direction so that

$$[H_s, \mathbf{T}] = 0 \tag{1.3}$$

where H_s stands for the strong Hamiltonian. On the contrary electromagnetic interactions are not isospin conserving, because the coupling with the charge allows us to distinguish between proton and neutron.
The value of T can be determined knowing that it behaves as an angular momentum, therefore obeying to the same laws. In particular it must be $|T_z| \leq T$ and $T_z = T, T-1, ..., -T$. Let us take for example a two particle system, i.e. *pp*, *nn* or *np*. The z isospin component is respectively $-1, 1, 0$, thus we have possible isospin values equal to 0 and 1. Every state that can be built for *pp* (or *nn*) has to exist also in *np* system, but the converse is not true, because we could have states in *np* that are prohibited in *pp* and *nn* for Pauli principle. The one which is only allowed in the *np* case is $T = 0$ (since $T_z = 0$), while every state in *nn* system, as in the *pp* one, has to have $T = 1$, since the isospin projection are respectively $+1$ and -1. However since a $T = 1$ state can also have $T_z = 0$, then this state have to exist in the *np* system too. These three state corresponding to $T = 1$ in *nn*, *np* and *pp* systems (i.e. with $T_z = -1, 0, 1$) form a so called *isospin triplet*.
The above reasoning can be extended to multi-particle systems. Low energy states, as the ground state, have $T = T_z$. This is the minimum possible value, since it is more expensive in terms of energy to create a state with isospin greater than T_z . States with the same T which are part of a set of nuclei with different T_z form a *isospin multiplet*, or *isobaric multiplet*, and these states are called *Isobaric Analogue*

States (IAS). Without Coulomb effects, or any isospin symmetry breaking interaction, these states have to be degenerate.
The simplest example of an isobaric multiplet is a pair of mirror nuclei where the number of pp interactions in one member is equal to the number of nn interactions in the other. Hence only charge symmetry of the nucleon-nucleon interaction is required to provide isospin symmetry in a mirror pair (this is not the case for any set of IAS). If we look at the isobaric triplet of mass $A = 22$ formed by the $N = Z$ nucleus ^{22}Na and the two mirrors ^{22}Mg and ^{22}Ne in Fig. 1.1, we see that the ground state of ^{22}Na is a $T = 0$ and the first $T = 1$ states lies at 657 keV excitation energy. This state is the isobaric analogue of the ground states of ^{22}Mg and ^{22}Ne.

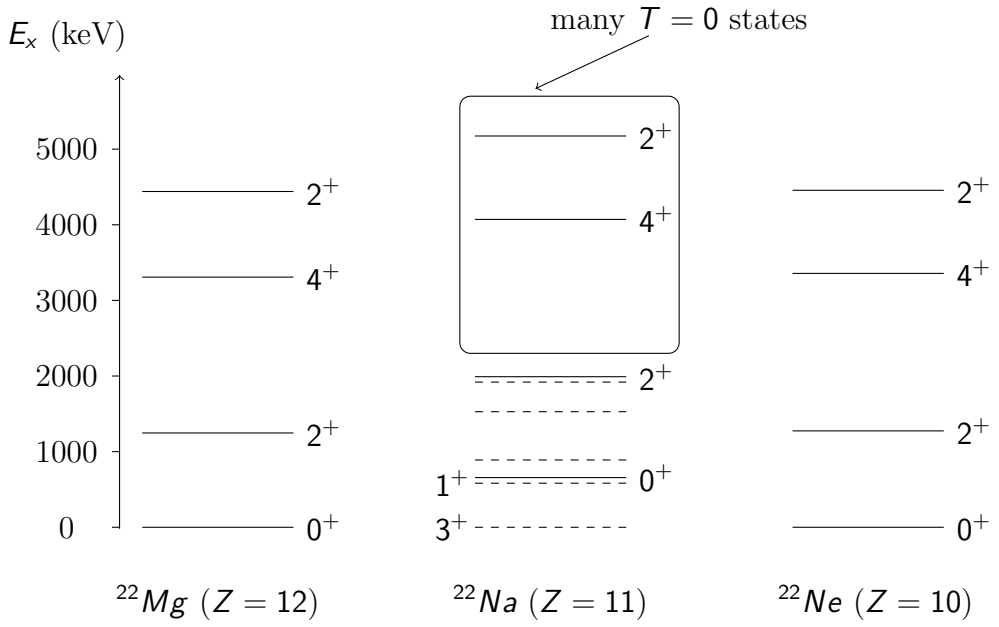


Figure 1.1 – The isobaric triplet A=22. The dashed lines (and the boxed area) stand for $T = 0$ states, while the continuos lines for $T = 1$ states. Due to Pauli principle the $N = Z$ nucleus has more excited states than the other member of the triplet. (Values from [2]).

The small differences between the excitation energy are due to the isospin symmetry breaking terms of the interaction, so once this effects are taken into account, the size of the remaining differences is a test of the charge independence of the nuclear interaction.

1.2 Coulomb Displacement Energy

Symmetry and independence principles lead to the conclusion that the eventual binding energy differences between analogue states of two nuclei from the same isobaric multiplet are due only to electromagnetic effects (since this is the most important contribution) or other isospin breaking terms. For this reason this difference is famous as *Coulomb Displacement Energy* (CDE).
The effects of the Coulomb interaction on the nuclear structure have been discussed for the first time by Bethe & Bacher [3] in 1936. To compute the Coulomb energy they made the assumption that the nucleus can be treated as a uniformly charged sphere of radius R. The calculation was concerned with the form of the Coulomb term in the semiempirical mass formula:

$$E_{binding} = a_V A - a_S A^{2/3} - a_C \frac{Z(Z-1)}{A^{1/3}} - a_A \frac{(A-2Z)^2}{A} + \delta(A,Z). \tag{1.4}$$

This leads to a Coulomb energy difference Δ_D between a nucleus with Z protons and its isobaric analogue with atomic number $Z+1$ equal to

$$\Delta_D = \frac{a_C}{R}[((Z+1)Z - (Z-1)Z] = a_C \frac{2Z}{R} \tag{1.5}$$

where, remembering that $R = r_0 A^{1/3}$,

$$a_C = \frac{3e^2}{5r_0} \tag{1.6}$$

is obtained by the comparison with the potential energy of a uniformly charged sphere, given by

$$E_C = \frac{3}{5}\frac{e^2 Z(Z-1)}{R}. \tag{1.7}$$

But this is only the direct term of the Coulomb interaction. Indeed since indistinguishable particles are symmetrical under exchange, the ground-state wave function needs to be antisymmetric and it is then necessary the introduction of an exchange term. Thus the total Coulomb Displacement Energy is given by the sum of the two terms:

$$\Delta = \Delta_D + \Delta_{exch} \tag{1.8}$$

where Δ_{exch} has been estimated to be of the order of hundreds of keV. The major contribution is given by the direct term, so in the end the overall Δ is between 1 and

20 MeV [1].

As we said before electromagnetic terms are the only ones that contribute to the *Coulomb Displacement Energy*; however, even if they are actually dominant, they are not sufficient to reproduce the CDE trend. Indeed a 7% shift remains between theoretical and experimental values, famous as Nolen-Shiffer anomaly. A possible explanation could be the omission of some, previously neglected, corrections to the calculated Coulomb-energy shift, as the contributions of charge and independence breaking terms to the strong interaction.

1.3 Charge Independence and Symmetry Breaking

The first evidence of charge symmetry and independence breaking (CSB and CIB) comes from proton and neutron masses. Indeed if charge symmetry were exact, the proton and the neutron would have the same mass. But it is known that there is a little difference

$$m_p = 938.28 \text{ MeV}/c^2 \qquad m_n = 939.57 \text{ MeV}/c^2 \tag{1.9}$$

due to the different quarks, that are the internal constituent of the nucleons[1]. If charge symmetry is broken, the isospin invariance and charge independence are broken too, but the converse is not true (as we can see from Equation (1.2)) .
Another evidence of CSB and CIB is the difference in proton-proton and neutron-neutron scattering lengths, of which we will talk briefly in 1.3.2.

1.3.1 Classification of forces

Charge dependence and asymmetry of nuclear forces can be characterized according to their isospin dependence, since we have seen that the two concepts are strictly correlated. The discussion by Henley & Miller's [4] listed four classes of forces between two nucleons, i and j.

[1]Protons are made up of one d quark and two u quarks, while neutrons have the opposite composition.

- Class I: Interactions which are isospin or charge independent. Such forces have either no isospin dependence or their dependence is proportional to $\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j$ (because they are the only scalar operators), where $\boldsymbol{\tau}_i$ is the Pauli isospin operator for nucleon i. Thus they obey $[V_I, \mathbf{T}] = 0$ and have the general form

$$V_I = a + b\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j \tag{1.10}$$

  where a and b are Hermitian isospin-independent operators. Class I interactions dominate the nuclear force.

- Class II: Forces which maintain charge symmetry but break charge independence. These can be written as

$$V_{II} = c[\tau_i^z \tau_j^z - \frac{1}{3}\boldsymbol{\tau}_i \cdot \boldsymbol{\tau}_j] \tag{1.11}$$

  with c space and spin operator.

- Class III: Forces which break charge symmetry (and therefore necessarily charge independence), but that are symmetric under the interchange $i \leftrightarrow j$ in isospin space,

$$V_{III} = d[\tau_i^z + \tau_j^z], \tag{1.12}$$

  where d is a Hermitian operator that is symmetric under the interchange $\boldsymbol{\sigma}_i \leftrightarrow \boldsymbol{\sigma}_j$. A Class III force differentiates between nn and pp systems, but vanishes in the np system.

- Class IV: Forces that break charge symmetry and charge independence and are antisymmetric under the interchange $\boldsymbol{\tau}_i \leftrightharpoons \boldsymbol{\tau}_j$ (in other words they causes isospin mixing). These forces are proportional to

$$\begin{aligned} V_{IV} = e[\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j] \cdot \boldsymbol{L}[\tau_i^z - \tau_j^z] + \\ + f[\boldsymbol{\sigma}_i \times \boldsymbol{\sigma}_j] \times \boldsymbol{L}[\boldsymbol{\tau}_i \times \boldsymbol{\tau}_j]^z \end{aligned} \tag{1.13}$$

  where e and f are spin-independent operators.

For example the Coulomb force between two nucleons contains Class I, II and III parts, but no Class IV terms. This topic will be dealt with more detail in Chapter 3.

1.3.2 Nucleon-Nucleon scattering lengths

In this section we will discuss how the NN scattering in ${}^1S_0$ channel can be related to the breaking of charge symmetry and independence, as described in [5].
The scattering length is defined in terms of the low-energy limit of the cross section:

$$\lim_{E\to 0} \sigma = 4\pi a^2, \tag{1.14}$$

and even if both σ and a have dimension, respectively, of a surface and a length, they represent the strength of the scattering. For further details see [6].
Charge independence implies the equality of the NN scattering lengths

$$a_{pp} = a_{nn} = a_{np} \tag{1.15}$$

However, we need to correct these values accounting for electromagnetic effects: these are discussed in [7]. The experimental results [8][9] are as follows:

$$\begin{aligned} a_{pp}^N &= -17.3 \pm 0.4 \text{ fm} \\ a_{nn}^N &= -18.8 \pm 0.3 \text{ fm} \\ a_{np}^N &= -23.77 \pm 0.09 \text{ fm} \end{aligned} \tag{1.16}$$

in which the subscript N represent the "nuclear" effect obtained after the electromagnetic corrections have been made. The differences among these scattering lengths represent CIB and CSB.
For nucleons of mass M and two different potentials ($\Delta V = V_1 - V_2$), manipulating the Schrödinger equation we obtain that the scattering lengths, a_1 and a_2 are related by:

$$\frac{\Delta a}{a} = -aM \int_0^\infty dr\ u_1(r) u_2(r) \Delta V(r) \tag{1.17}$$

where $\Delta a = a_2 - a_1$, $a^2 = a_1 a_2$ and u_i is the corresponding zero-energy wave function, normalized to approach $1 - r/a$ as r approach ∞ and $u_i(0) = 0$. The effects of changing the potential on the wave function are very small, so we can use $u_1(r)^2$ or $u_2(r)^2$ in (1.17) instead of their product; the error made with this approximation is less than 2% in Δa [10].
In Ref. [11] has been shown that

$$\frac{\Delta a}{a} = -(10 - 15)\frac{\Delta V}{V} \quad \text{[MeV]} \tag{1.18}$$

where a simple shape for V_1, V_2 is chosen, for example an exponential or a Yukawa potential.
For

$$\Delta a_{CIB} \equiv \frac{1}{2}(a_{pp}^N + a_{nn}^N) - a_{np}^N = 5.7 \pm 0.3 \text{ fm} \tag{1.19}$$

$\Delta V/V$ is estimated to be approximately 2.5% and for

$$\Delta a_{CSB} \equiv a_{pp}^N - a_{nn}^N = 1.5 \pm 0.5 \text{ fm} \tag{1.20}$$

$\Delta V/V$ amounts to approximately a 0.6% effect.

Chapter 2

Nuclear Hartree-Fock

2.1 Mean field model

A many body system is very difficult to solve exactly, because an exact solution of the Schrödinger equation does not exist for more than two or three particles. Thus the mean field model replaces the n-body system with a one-body problem with a chosen effective potential. It considers every particle as independent from the others, and consists of an interaction acting on the single particle, that is the average of the interactions of all the other particles of the system. In this way the problem is reduced to the simpler one-body problem in which a particle, in this case a nucleon, feels a potential and moves according to that. Thus the main idea is to replace all interactions among all bodies with an average or an effective interaction, namely the mean field potential.
The idea that nucleons inside the nucleus can be described as independent particles in a mean potential is supported by the experimental evidence, coming from scattering experiments, of their large mean free path, namely of the order of, or larger than, the nuclear radius [12]. This may seem to disagree with the strong repulsive part of the nucleon-nucleon interaction at short range, but the solution to this problem lies in the fact that the nucleus is not a very dense system. The nuclear radius is

$$R = r_0 A^{1/3} \qquad \text{with } r_0 = 1.2 - 1.3 \text{ fm} \tag{2.1}$$

Thus the volume per nucleon is

$$\frac{V}{A} = \frac{\frac{4}{3}\pi R^3}{A} \approx 4r_0^3 \tag{2.2}$$

and the average distance between the nucleons is of the order of ≈ 2 fm; this means that they remain at a large distance from one another enough to not feel the repulsive part of the NN interaction, that has a range of ≈ 0.7 fm, for most of the time [6]. Moreover, experiments show that the density is approximately constant inside the nucleus, about 0.16 fm^{-3}, while outside the nucleus both the density and the potential drop, as the figure shows:

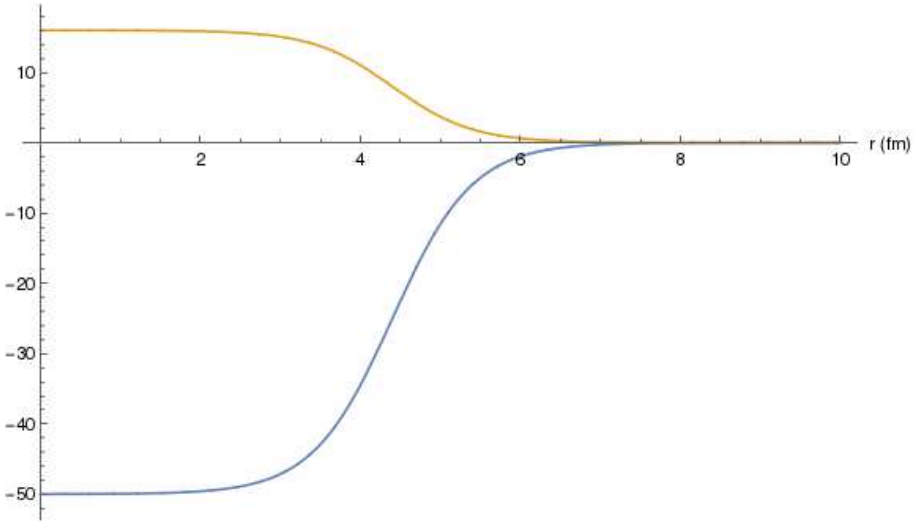


Figure 2.1 – Schematic representation of a Woods-Saxon potential, in blue, with parameters $V_0 = -50$MeV and $a = 0.5$fm, and a Fermi function for the nuclear density ($\cdot 100$), in orange, with the same parameters as before. The dimensions of measure are MeV for the first and fm^{-3} for the second.

Furthermore looking at the binding energies we notice that they have a systematic trend similar to the atomic one: in nuclei with a particular number (*magic number*) of neutrons or protons, the binding energy has a sharp change going form a nucleus to the next one, becoming smaller than usual; this means that this kind of nuclei are more stable that the others.
This similar trend can be seen in all nuclear phenomenology, not only for what concerns the binding energy; for example also in the behaviour of nuclear radii and excitation

energies. These considerations suggest a correspondence with electrons in atoms: thus in analogy with the atomic shell model has been introduced the nuclear shell model. Since shells exist for neutrons and protons separately, we can speak about *magic nuclei* if one of the two types reaches a *magic number* and about *doubly magic nuclei* when both of them reach that numbers. The main difference is that the atomic shells are mainly governed by an external interaction (the Coulomb attractive potential of the nucleus), while nuclear shells emerge from the complicated behaviour of self-interacting particles.
At this point we can use phenomenological potentials that describe well the essential proprieties of nuclei, as the Woods-Saxon potential for spherical nuclei, to solve the Schrödinger equations. Otherwise we can use of the eigenfunctions of these phenomenological potential as the starting point for a self-consistent variational method, called Hartree-Fock method, of which we make use in the present work.

2.2 Hartee-Fock method

The main aim of the Hartree-Fock theory is to go from a microscopic model, in which the nucleon interactions are described as two particle interactions, to a single particle mean field potential.
Let us start writing the Hamiltonian of the multi particle system as

$$H = T + V \tag{2.3}$$

where T is the sum of single particles kinetic energy

$$T = \sum_i t_i = \sum_i -\frac{\hbar^2}{2m}\nabla_i^2 \tag{2.4}$$

and V is a two-body potential between nucleons

$$V = \frac{1}{2}\sum_{ij} v(\mathbf{r}_i, \mathbf{r}_j) \tag{2.5}$$

If we take an eigenfunction Ψ, the Schrödinger equation is $H|\Psi\rangle = E|\Psi\rangle$ and it can be shown [13] to be equivalent to the variational equation

$$\delta E = 0 \tag{2.6}$$

Because of all the correlations between particles, the expression for Ψ is very difficult to find, thus we restrict to an Hilbert subspace in which we choose a particular shape for the system eigenfunction. We can express the total wave function of A nucleons as the totally anti-symmetric product of single-particle wave function $\phi_i(x_j)$, where x denotes the set $\mathbf{r}$,σ,τ of space, spin and isospin coordinates, through the so-called *Slater Determinant*:

$$\phi(x_1, x_2, ..., x_A) = \frac{1}{\sqrt{A!}} \det |\phi_i(x_i)| \tag{2.7}$$

For the sake of simplicity we here omit spin and isospin dependence.
At this point we can calculate the Hamiltonian expectation value $E = \langle\Psi|H|\Psi\rangle$ and solve the Equation (2.6), writing that the total energy E is stationary with respect to individual variations of the single-particle states ϕ_i (or on ϕ_i^*) with the condition of orthonormality of the wave function[1]

$$\frac{\delta}{\delta\phi_i}\left(E - \lambda \int d\mathbf{r}\ \phi_i^*(\mathbf{r})\phi_i(\mathbf{r})\right) = 0 \tag{2.8}$$

Thus once we have calculated the expectation value as

$$\begin{aligned}\langle\Psi|H|\Psi\rangle = \sum_{i=1}^{A} -\frac{\hbar^2}{2m}\int d\mathbf{r}\ \phi_i^*(\mathbf{r})\nabla^2\phi_i(\mathbf{r}) + \\ + \frac{1}{2}\sum_{ij}\int d\mathbf{r}d\mathbf{r}'\phi_i^*(\mathbf{r})\phi_j^*(\mathbf{r}')v(\mathbf{r},\mathbf{r}')\phi_i(\mathbf{r})\phi_j(\mathbf{r}') + \\ - \frac{1}{2}\sum_{ij}\int d\mathbf{r}d\mathbf{r}'\phi_i^*(\mathbf{r})\phi_j^*(\mathbf{r}')v(\mathbf{r},\mathbf{r}')\phi_i(\mathbf{r}')\phi_j(\mathbf{r})\end{aligned} \tag{2.9}$$

we can apply the variational principle obtaining the Hartree-Fock equations

$$\begin{aligned}-\frac{\hbar^2}{2m}\nabla_i^2\phi_i(\mathbf{r}) + \sum_{j=1}^{A}\int d\mathbf{r}'\phi_j^*(\mathbf{r}')v(\mathbf{r},\mathbf{r}')\phi_j(\mathbf{r}')\phi_i(\mathbf{r}) + \\ -\sum_{j=1}^{A}\int d\mathbf{r}'\phi_j^*(\mathbf{r}')v(\mathbf{r},\mathbf{r}')\phi_j(\mathbf{r})\phi_i(\mathbf{r}') = \epsilon_i\phi_i(\mathbf{r})\end{aligned} \tag{2.10}$$

where we have turned the Lagrange multiplier λ in ϵ_i because the above set of equations has the form of a set of Schrödinger equations, thus here λ assumes the physical role of single-particle eigenvalue.

[1] condition reached adding a Lagrange multiplier λ

We can rewrite the above equation putting in evidence the density distribution of the A nucleons $\rho(\mathbf{r}) = \sum_{j=1}^{A} |\phi_j(\mathbf{r})|^2$

$$-\frac{\hbar^2}{2m}\nabla_i^2\phi_i(\mathbf{r}) + \left(\int d\mathbf{r}'\rho(\mathbf{r}')v(\mathbf{r},\mathbf{r}')\right)\phi_i(\mathbf{r}) - \sum_{j=1}^{A}\int d\mathbf{r}'\phi_j^*(\mathbf{r}')v(\mathbf{r},\mathbf{r}')\phi_j(\mathbf{r})\phi_i(\mathbf{r}') = \epsilon_i\phi_i(\mathbf{r}) \tag{2.11}$$

The terms on the left after the kinetic one are called Hartree and Fock terms. The first of these has a local nature and represent the interaction of the i-th nucleon with the the other nucleons, whose distribution is given by ρ. The Fock term comes from the fermionic nature of nucleons, it is non-local and gives to Eq. (2.11) the integro-differential structure.

The method to solve this equation is iterative and self-consistent: we start with a potential (that we know to be similar to what we are looking for), we find the eigenfunction associated to this potential, we put them into Eq. 2.11 and solve it for ϕ_i. The solutions found are then used to calculate the new potential and to calculate again the Hartree and Fock terms. This procedure is repeated until the difference between single-particle levels between an iteration and the next one is lower than a certain precision.

The binding energy in this model is equivalent to the energy given by Eq. (2.9). Thus we will use the notation

$$E = \sum_i \langle i|\, t\, |i\rangle + \frac{1}{2}\sum_{ij}\langle ij|\, v\, |ij\rangle_{AS} \tag{2.12}$$

with

$$\langle i|\, t\, |i\rangle = -\frac{\hbar^2}{2m}\int d\mathbf{r}\ \phi_i^*(\mathbf{r})\nabla^2\phi_j(\mathbf{r}) \tag{2.13}$$

for the matrix elements of the kinetic energy and

$$\langle ij|\, v\, |ij\rangle_{AS} = \int d\mathbf{r}d\mathbf{r}'\phi_i^*(\mathbf{r})\phi_j^*(\mathbf{r}')v(\mathbf{r},\mathbf{r}')\left[\phi_i(\mathbf{r})\phi_j(\mathbf{r}') - \phi_i(\mathbf{r}')\phi_j(\mathbf{r})\right] \tag{2.14}$$

for the antisymmetrized matrix elements of the two-body potential.

2.3 Skyrme interaction

A way to solve Hartree-Fock equations is by means of effective interactions, i.e. interactions built *ad hoc* to reproduce well the major part of the ground-state nuclear properties. These are constructed with some free parameters, generally about ten, that are fitted with experimental data of properties of tens of nuclei, but they reproduce $10^2 - 10^3$ nuclei. These interactions have to be short-range ones, with a dependence on spin and isospin and must be such that the attractive and repulsive terms balance each other to reach nuclear saturation.
In this work we have used the Skyrme interaction, that is an effective interaction proportional to a Dirac delta function, $\delta(\mathbf{r} - \mathbf{r}')$. In this way the Fock term loses its non locality and the integro-differential equations turn into differential ones, becoming easier to solve. Even if it is a contact interaction, the finite range is simulated using a moment dependence and the demonstration is given in [13] or in the article of Vautherin and Brink [14]. The original form of Skyrme's interaction can be written as a potential

$$V = \sum_{ij} v_{ij}^{(2)} + \sum_{ijk} v_{ijk}^{(3)} \tag{2.15}$$

where v_{ij} is a two-body part and v_{ijk} a three-body part. The first term can be expressed as

$$\begin{aligned} v_{12} = {} & t_0 \left(1 + x_0 P_\sigma\right) \delta(\mathbf{r}_1 - \mathbf{r}_2) + \frac{1}{2} t_1 \left[\delta(\mathbf{r}_1 - \mathbf{r}_2) k^2 + k'^2 \delta(\mathbf{r}_1 - \mathbf{r}_2)\right] + \\ & + t_2 \mathbf{k}' \cdot \delta(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{k} + i W_0 (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot \mathbf{k}' \times \delta(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{k} \end{aligned} \tag{2.16}$$

where $\mathbf{k} = (\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2)/2i$ is the operator acting on the right, $\mathbf{k}' = -(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2)/2i$ is the operator acting on the left, σ_1 σ_2 are the Pauli spin matrices, $P_\sigma = \frac{1}{2}(1 + \sigma_1 \cdot \sigma_2)$ is the operator exchanging the spin of particles 1 and 2, t_0 is the parameter for the central component of the potential, t_1 and t_2 are the parameters for the non local terms and W_0 is the parameter for the spin-orbit component.
For the three-body force Skyrme also assumed a zero-range force

$$v_{123}^{(3)} = t_3 \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_2 - \mathbf{r}_3) \tag{2.17}$$

that for even-even nuclei ground state can be mapped[2] as a two-body interaction depending on the density:

$$v_{12} = \frac{1}{6}t_3(1 + x_3P_\sigma)\delta(\mathbf{r}_1 - \mathbf{r}_2)\rho\left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2}\right) \tag{2.18}$$

From Eq. (2.12) the expectation value of the total energy should be

$$E = \sum_i \langle i|\, t\, |i\rangle + \frac{1}{2}\sum_{ij} \langle ij|\, v_{12}\, |ij\rangle_{AS} + \frac{1}{6}\sum_{ijk} \langle ijk|\, v_{123}\, |ijk\rangle_{AS} \tag{2.19}$$

but the presence of a three-particle term that depends on the density makes the above equation no longer valid. In this case we have to consider also a *rearrangement* term, that is given by [14]:

$$E_R = -\frac{1}{12}\sum_{ijk} \langle ijk|\, v_{123}\, |ijk\rangle_{AS} = -\frac{1}{8}t_3 \int \rho_n(\mathbf{r})\rho_p(\mathbf{r})\rho(\mathbf{r})d^3r \tag{2.20}$$

Thus the real total binding energy is given by

$$E = \frac{1}{2}\sum_i (t_i + \epsilon_i) + E_R \tag{2.21}$$

that we can write as a function of the energy density as

$$E = \int H(\mathbf{r})d^3r. \tag{2.22}$$

$H(\mathbf{r})$ depends locally on the nucleon densities ρ_q, the kinetic energy τ_q and spin densities J_q (where q stands for proton or neutron) and it can be split into the sum of terms associated to different parts of the interaction:

$$H = K + H_0 + H_3 + H_{eff} + H_{fin} + H_{so} + H_{sg} + H_C \tag{2.23}$$

where K is the kinetic term, H_0 is the central term, H_3 is the three-body term, H_{eff} is an effective mass term, H_{fin} is a finite range term, H_{so} is the spin-orbit term, H_{sg} a term due to the tensor coupling with spin and gradient and H_C is the Coulomb term. They are all listed in [15] and here we report only H_0, H_3 and H_C to give to the reader an idea of how their shape is. For even-even nuclei we can take advantage of the fact

[2]The demonstration can be found in [14]

that if a single particle state is occupied, also its time-reversed state is occupied, and as a consequence the expectation value of operators as $\sigma_1 \cdot \sigma_2$ is zero. Thus we have:

$$\begin{aligned} H_0 &= \frac{1}{4}[(2+x_0)\rho^2 - (2x_0+1)(\rho_p^2+\rho_n^2)] \\ H_3 &= \frac{1}{24}t_3\rho^\alpha[(2+x_3)\rho^2 - (2x_3+1)(\rho_p^2+\rho_n^2)] \end{aligned} \tag{2.24}$$

where ρ_q is the protons or neutrons local density and ρ is the total local density.
The Coulomb potential requires an additional approximation for the exchange contribution in order to keep it local (the Coulomb interaction, unlike the Skyrme force, has a non-zero range). We used the Slater approximation [16] to express the Coulomb exchange contribution to the Coulomb potential and, with the direct term, it becomes

$$V_C(\mathbf{r}) = e^2 \left[\int \frac{\rho_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d^3r' - \left(\frac{3}{\pi}\rho_p\right)^{\frac{1}{3}} \right] \tag{2.25}$$

and the corresponding contribution to the energy density is given by

$$H_C = \frac{1}{2} V_C(\mathbf{r})\rho_p(\mathbf{r}). \tag{2.26}$$

The expressions of the terms in (2.23) are derived explicitly in the Appendix of [14] and in the next chapter we will make use of the same technique to find the energy density for the CSB and CIB terms.
Applying now the variational principle (Eq.(2.8)) we find that the single-particle wave functions ϕ_i have to satisfy the following set of equations:

$$-\left[\boldsymbol{\nabla} \cdot \frac{\hbar^2}{2m_q^*(\mathbf{r})}\boldsymbol{\nabla} + U_q(\mathbf{r}) + \mathbf{W}_q(\mathbf{r}) \cdot (-i)(\boldsymbol{\nabla} \times \boldsymbol{\sigma})\right]\phi_i = \epsilon_i \phi_i. \tag{2.27}$$

From now on we assume spherical symmetry. In the above equation i is the set of quantum numbers $\{n, l, j, m\}$, q stands for the charge of the single-particle state i and m^* is the effective mass which depends on the density only:

$$\frac{\hbar^2}{2m_q^*(\mathbf{r})} = \frac{\hbar^2}{2m} + \frac{1}{4}(t_1+t_2)\rho + \frac{1}{8}(t_2-t_1)\rho_q. \tag{2.28}$$

U_q is the nuclear central field, given by the functional derivative of the energy density respect to the density (of protons or neutrons), and W_q is the spin-orbit potential [15]. For spherical doubly magic nuclei HF equations simplify into a set of one-dimensional

differential equations in the radial coordinate r. In the end we can find the HF radial equations:

$$\frac{\hbar^2}{2m_q^*(r)}\left[-u_i'' + \frac{l(l+1)}{r^2}u_i\right] + V_q(r)u_i - \left(\frac{\hbar^2}{2m_q^*}\right)u_i' = \epsilon_i u_i \tag{2.29}$$

where the HF potential $V_q(r)$ is the sum of central, Coulomb and spin-orbit terms. Now the Hartree-Fock equations can be easily solved numerically.

2.4 Short introduction to the program

In this work we have performed Hartree-Fock calculations using the "`skyrme_rpa`" program [17]. It starts from an assumed form of nuclear effective interaction (the Skyrme forces) and solves the Hartree-Fock equations on a radial mesh, using a Numerov algorithm. The solutions are iterated until self-consistence is achieved, and is possible to build the mean field of a given nucleus. The main restrictions are related to the request of spherical symmetry and absence of pairing correlations.
There is the possibility to choose between different type of Skyrme interactions, each of them characterized by a different set of parameters. In particular we have used SLy5 [15] and LNS [18] forces:

	SLy5	LNS
t_0	-2484.88	-2484.97
t_1	483.13	266.735
t_2	-549.40	-337.135
t_3	13763	14588.2
x_0	0.778	0.06277
x_1	-0.328	0.65845
x_2	-1	-0.95382
x_3	1.267	-0.03413
W_0	126	96
α	0.1666666	0.1666666

Table 2.1 – Parameters for SLy5 and LNS interactions.

Chapter 3

Isospin symmetry breaking

3.1 CSB and CIB potentials

As we have seen in Section 1.3, a term that breaks charge symmetry is given by the sum of the isospin third components of the interacting particles.
We have chosen a Yukawa function as a short-range potential that describes well the nuclear interaction and we did the limit for the range of this interaction going to zero, obtaining $4\pi\delta$. This means that we can consider a delta function instead of a Yukawa one because they behave in a similar way due to their short range. If a delta function representation has proven to be effective for most of the nucleon-nucleon interactions, this holds even stronger for this small part. For these reasons, for the two-body CSB interaction we took a potential with the following structure:

$$v(\mathbf{r}, \mathbf{r}') = t_4(\tau_1^z + \tau_2^z)(1 + x_4 P_\sigma)\delta(\mathbf{r} - \mathbf{r}') \tag{3.1}$$

where t_4 and x_4 are free parameters that whose values will be discussed later on. We can write τ as $2t$ so that the isospin third component acts by giving -1/2 or 1/2 respectively for a proton and a neutron.
Now following the same procedure described in [14] to find the expectation value of (3.1), we antisymmetrize the matrix elements of the zero-range force using the trick to multiplicate the potential by the quantity $(1 - P_{12})$, where P_{12} is the operator switching particles 1 and 2, given by the product $P_r P_\sigma P_\tau$ (that are the three operator

exchanging position, spin and isospin respectively)

$$E_4 = \frac{1}{2}\sum_{ij}\langle ij|v(\mathbf{r},\mathbf{r}')|ij\rangle_{AS} = \frac{1}{2}\sum_{ij}\langle ij|v(\mathbf{r},\mathbf{r}')(1-P_rP_\sigma P_\tau)|ij\rangle \tag{3.2}$$

For a delta-force like (3.2) P_r is 1. P_σ is given by $\frac{1+\sigma_1\sigma_2}{2}$ and P_τ has a similar form. Furthermore, since there is not charge mixing in Hartree-Fock states, the effect of P_τ is only to introduce a factor δ_{q_i,q_j}:

$$\begin{aligned}
E_4 &= \frac{1}{2}\sum_{ij}\left\langle ij|2t_4(t_1^z+t_2^z)(1+x_4P_\sigma)\delta(\mathbf{r}-\mathbf{r}')(1-P_\sigma\delta_{q_i,q_j})\right|ij\right\rangle \\
&= t_4\sum_{ij}\langle ij|\,\delta(\mathbf{r}-\mathbf{r}')(t_1^z+t_2^z)(1+\frac{1+\sigma_1\sigma_2}{2}x_4-\frac{1+\sigma_1\sigma_2}{2}\delta_{q_i,q_j}-x_4\delta_{q_i,q_j}\,|ij\rangle \\
&= t_4\sum_{ij}\langle ij|\,\delta(\mathbf{r}-\mathbf{r}')(t_1^z+t_2^z)\left(1+\frac{1}{2}x_4-\left(\frac{1}{2}+x_4\right)\delta_{q_i,q_j}+\frac{1}{2}(x_4-1)(\sigma_1\sigma_2)\right)|ij\rangle
\end{aligned} \tag{3.3}$$

Because terms containing Pauli matrices do not contribute to the mean value we arrive at the following expression:

$$\begin{aligned}
E_4 &= t_4\int d^3r\left(1+\frac{x_4}{2}\right)2\rho(r)\left(\frac{1}{2}\rho_n(r)-\frac{1}{2}\rho_p(r)\right)-\left(\frac{1}{2}+x_4\right)(\rho_n^2-\rho_p^2) \\
&= t_4\int d^3r\frac{1}{2}(1-x_4)(\rho_n^2-\rho_p^2)
\end{aligned} \tag{3.4}$$

this means that the contribution to the energy density is given by:

$$H_4 = \frac{t_4}{2}\left[(1-x_4)(\rho_n^2-\rho_p^2)\right] \tag{3.5}$$

Therefore the proton and neutron mean-field is:

$$\begin{aligned}
U_p &= \frac{\partial H_4}{\partial\rho_p} = -t_4(1-x_4)\rho_p \\
U_n &= \frac{\partial H_4}{\partial\rho_n} = t_4(1-x_4)\rho_n.
\end{aligned} \tag{3.6}$$

Following the same reasoning than before we can introduce the CIB potential with the structure:

$$v(\mathbf{r},\mathbf{r}') = t_5(\tau_1^z\tau_2^z)(1+x_5P_\sigma)\delta(\mathbf{r}-\mathbf{r}'), \tag{3.7}$$

whose expectation value is given by Eq. (3.2). The calculation can be performed with the same technique as above and we arrive at the final expression:

$$E_5 = t_5 \int d^3r \left[\frac{1}{4}(1-x_5)(\rho_n^2+\rho_p^2) - 2(2+x_5)\rho_n\rho_p\right] \tag{3.8}$$

Thus the contribution to the energy density is

$$H_5 = \frac{t_5}{4}\left[(1-x_5)(\rho_n^2+\rho_p^2) - 2(2+x_5)\rho_n\rho_p\right] \tag{3.9}$$

and the protons and neutrons mean fields are

$$\begin{aligned} U_p &= \frac{\partial H_5}{\partial \rho_p} = \frac{t_5}{2}\left[(1-x_5)\rho_p - (2+x_5)\rho_n\right] \\ U_n &= \frac{\partial H_5}{\partial \rho_n} = \frac{t_5}{2}\left[(1-x_5)\rho_n - (2+x_5)\rho_p\right]. \end{aligned} \tag{3.10}$$

We want to specify that these formula are consistent with the CDE calculation, and give an idea of the origin of the CDE, that comes, in fact, from the change in energy on single-particle levels. Indeed the introduction of the CSB and CIB potentials make the nucleons feel a different force than that described in Eq. (2.29), and to take into account these new effects we have to add to the standard HF potential the mean fields (3.6) and (3.10).

3.2 Contributions to the CDE

Let us consider two nuclei with atomic number Z and $Z+1$. The wavefunction of the first nucleus, called parent nucleus, having both isospin and isospin third component equal to T_0, is given by the antisymmetrized product of the single particle eigenfunctions of the Z protons and N neutrons. The analogue of this nucleus, called daughter nucleus, is formed by changing one of the $N-Z$ excess neutrons in the parent nucleus into a proton, and has the same isospin value T_0 but the z-projection equal to T_0-1. The *Coulomb Displacement Energy* between a nucleus and its isobaric analogue can be computed as

$$\Delta E = \langle T_0, T_0-1|H|T_0, T_0-1\rangle - \langle T_0, T_0|H|T_0, T_0\rangle \tag{3.11}$$

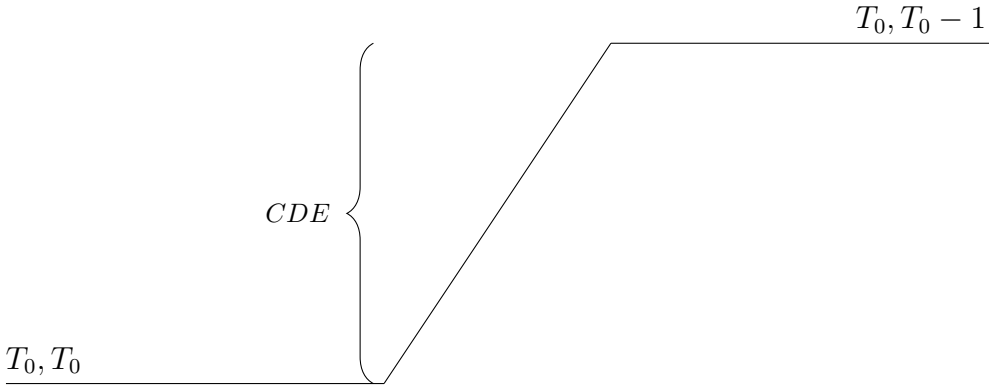


Figure 3.1 – Schematic representation of the Coulomb Displacement Energy between the ground state levels of a nucleus (on the left) and its isobaric analogue (on the right).

As it has been done for the angular momentum we can introduce also in this case the ladder operators defined by:

$$T^{\pm} |T, T_z\rangle = \sqrt{T(T+1) - T_z(T_z \pm 1)}\, |T, T_z \pm 1\rangle \,. \tag{3.12}$$

Acting on a state where the third component of the isospin is equal to the isospin itself, we obtain:

$$\begin{aligned} T^{-} |T_0, T_0\rangle &= \sqrt{T_0(T_0+1) - T_0(T_0-1)}\, |T_0, T_0 - 1\rangle \\ &= \sqrt{2T_0}\, |T_0, T_0 - 1\rangle \end{aligned} \tag{3.13a}$$

$$\begin{aligned} T^{+}T^{-} |T_0, T_0\rangle &= \sqrt{2T_0}\sqrt{T_0(T_0+1) - T_0(T_0-1)}\, |T_0, T_0\rangle \\ &= 2T_0\, |T_0, T_0\rangle \,, \end{aligned} \tag{3.13b}$$

and thus we can write the (3.11) as

$$\begin{aligned} \Delta E &= \frac{1}{2T_0} \left\langle T_0, T_0 | T^{+} H T^{-} \right| T_0, T_0 \rangle - \langle T_0, T_0 | H | T_0, T_0 \rangle \\ &= \frac{1}{2T_0} \left\langle T_0, T_0 | T^{+} (H T^{-}) \right| T_0, T_0 \rangle - \frac{1}{2T_0} \left\langle T_0, T_0 | T^{+} (T^{-} H) \right| T_0, T_0 \rangle \\ &= \frac{1}{2T_0} \left\langle T_0, T_0 | T^{+} [H, T^{-}] \right| T_0, T_0 \rangle \end{aligned} \tag{3.14}$$

The Hamiltonian of the system can be written as:

$$H = H_N + V_C + V_{CSB} + V_{CIB} \tag{3.15}$$

where V_C is the Coulombian interaction, V_{CSB} is the *Charge Symmetry Breaking* potential and V_{CIB} is the *Charge Independence Breaking* interaction, while H_n is the sum of the kinetic energy and the nuclear potential, that commutes with the isospin. The only terms breaking isospin symmetry, and then they give a not zero contribute for the commutator, are V_C, V_{CSB} and V_{CIB}, that we are going to study now.

3.2.1 Coulomb term

The Coulomb interaction as a function of the isospin can be written as:

$$V_C = \frac{1}{2}\sum_{ij}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}\left(\frac{1}{2} - t_i^z\right)\left(\frac{1}{2} - t_j^z\right) \tag{3.16}$$

where t_i^z e t_j^z are the third components of single particle isospin.
Defining the total lowering operator of the isospin of the nucleus as the sum of the operator of single particle

$$T^- = \sum_k t_k^- \tag{3.17}$$

we can calculate the commutator:

$$\begin{aligned}
[V_C, T^-] &= \frac{1}{2}\sum_{ij}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}\sum_k\left[\left(\frac{1}{2} - t_i^z\right)\left(\frac{1}{2} - t_j^z\right), t_k^-\right] \\
&= \frac{1}{2}\sum_{ij}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}\left[\left(\frac{1}{2} - t_i^z\right)\delta_{jk}\left[t_k^-, t_j^z\right] + \delta_{ik}\left[t_k^-, t_i^z\right]\left(\frac{1}{2} - t_j^z\right)\right] \\
&= \frac{1}{2}\sum_{ij}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}\left[\left(\frac{1}{2} - t_i^z\right)t_j^- + t_i^-\left(\frac{1}{2} - t_j^z\right)\right] \\
&= \frac{1}{2}\sum_{ij}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}\left(t_j^- - 2t_i^z t_j^-\right),
\end{aligned} \tag{3.18}$$

where in the last step we have renamed the indexes using the fact that the interaction is symmetrical for the exchange of the two particles $i \leftrightarrow j$. Now using Eq. (3.14), for the Coulomb term we obtain:

$$\Delta E_C = \frac{1}{4T_0}\sum_{ij}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}\langle ij|\, t_j^+ t_j^- - 2t_j^+ t_i^z t_j^-\, |ij\rangle\,. \tag{3.19}$$

Operator t_j^- acts on the j-th neutron changing it into a proton and t_j^+ acts on the same particle bringing it back from proton to neutron; t_i^z extracts the value of the isospin

third component, that is 1/2 for neutrons and -1/2 for protons. Going from the wave functions to the densities we have:

$$\begin{aligned}\Delta E_C &= \frac{1}{4T_0}\int\int d^3r_1 d^3r_2 \frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\left[\rho(\mathbf{r}_1)\rho_{ex}(\mathbf{r}_2) - (\rho_n(\mathbf{r}_1)-\rho_p(\mathbf{r}_1))\,\rho_{ex}(\mathbf{r}_2)\right] \\ &= \frac{1}{2T_0}\int\int d^3r_1 d^3r_2 \frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\rho(\mathbf{r}_1)\rho_{ex}(\mathbf{r}_2),\end{aligned} \tag{3.20}$$

where $\rho(\mathbf{r}_1)$ comes from the first term of (3.19) that does not act on the i-th particle and ρ_{ex} is the excess neutron density, in other words neutrons that occupy higher orbitals not occupied by protons.
The integral of (3.20) is non-local and we can simplify it making a multipole expansion

$$\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} = \sum_{lm}\frac{r_<^l}{r_>^{l+1}}\left(\frac{4\pi}{2l+1}\right)Y_{lm}(\theta_1,\phi_1)Y^*_{lm}(\theta_2,\phi_2) \tag{3.21}$$

and remembering that in spherical symmetry densities just depend on the absolute value of the distance: $\rho(\mathbf{r}) = \rho(r)$. Developing the calculations and using spherical harmonics properties we obtain an expression easy to integrate:

$$\Delta E_C = \frac{(4\pi e)^2}{N-Z}\left(\int_0^{+\infty} dr_1 r_1^2\rho_p(r_1)\int_0^{+\infty} dr_2\frac{r_2^2}{r_>}\rho_{ex}(r_2)\right) \tag{3.22}$$

where the outer integral can be broken depending on which is the greater distance:

$$\int_0^{+\infty} dr_2\frac{r_2^2}{r_>}\rho_{ex}(r_2) = \int_0^{r_1} dr_2\frac{r_2^2}{r_1}\rho_{ex}(r_2) + \int_{r_1}^{+\infty} dr_2 r_2\rho_{ex}(r_2). \tag{3.23}$$

This is the direct part of the Coulomb term, but we have also a contribution from the exchange term. We take it into account using the approximate expression from [19]:

$$\Delta E_{exch} = -900\frac{Z}{A}\ \text{keV}. \tag{3.24}$$

3.2.2 CSB term

We calculate now the contribution to the CDE due to the potential (3.1). Remembering that $\tau = 2t$, the procedure is similar to that of the Coulomb term, starting from the commutator

$$\begin{aligned}\left[V_{CSB}, T^-\right] &= 2t_4(1+x_4P_\sigma)\delta(\mathbf{r}_1-\mathbf{r}_2)\sum_3\left[t_1^z+t_2^z,\ \ t_3^-\right] \\ &= 2t_4(1+x_4P_\sigma)\delta(\mathbf{r}_1-\mathbf{r}_2)(-2t_1^-)\end{aligned} \tag{3.25}$$

but is more complicated due to the presence of the antisymmetrization of the two-body potential matrix elements:

$$\Delta E_{CSB} = -\frac{2}{4T_0}\sum_{ij}\langle ij|\, T^+ t_4(1+x_4P_\sigma)\delta(\mathbf{r}_1-\mathbf{r}_2)(-2t_1^-)\,(1-P_rP_\sigma P_\tau)\,|ij\rangle \tag{3.26}$$

with $P_r = 1$ as in (3.2). To simplify the computation we can observe that $(1+x_4P_\sigma)$ commutes with the other operators, that allows us to take it after t_1^- and do at once

$$(1+x_4P_\sigma)\,(1-P_\sigma P_\tau) = (1+x_4P_\sigma - P_\sigma P_\tau - x_4P_\tau) \tag{3.27}$$

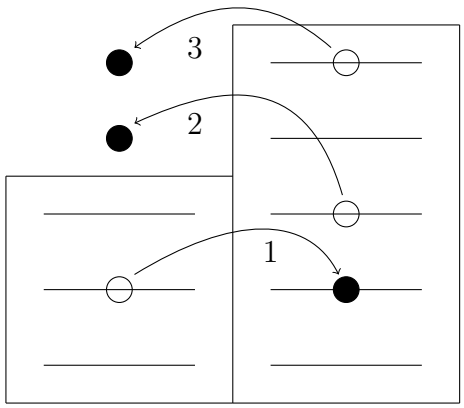
and writing P_τ as

$$P_\tau = \frac{1}{2}\,(1+\tau_1\tau_2) = \frac{1}{2}\,(1+4t_1t_2) = \frac{1}{2}\left(1+4t_1^zt_2^z+2t_1^+t_2^- +2t_1^-t_2^+\right) \tag{3.28}$$

we arrive at the following expression

$$\begin{aligned}\Delta E_{CSB} = -\frac{2t_4}{2T_0}\sum_{ij}\langle ij|\,\delta(\mathbf{r}_1-\mathbf{r}_2)T^+t_1^-\cdot \\ \cdot\left[1+\frac{x_4}{2}-\left(\frac{1}{2}+x_4\right)\left(\frac{1}{2}+2t_1^zt_2^z+t_1^+t_2^-+t_1^-t_2^+\right)\right]|ij\rangle\end{aligned} \tag{3.29}$$

where we have already considered that the expectation value for $\sigma_1\sigma_2$ is zero in even-even nuclei.
Looking at $\langle ij|\, T^+t_1^-t_1^+t_2^-\,|ij\rangle$ and $\langle ij|\, T^+t_1^-t_1^-t_2^+\,|ij\rangle$, every time we act with this operators we change the charge state of particles 1 and 2 and if the final state is different from the initial one, the expectation value will be zero. Thus the only way to have a value different from zero is to bring back both particles in the same initial conditions. But this is not possible. In fact we can not change a proton into a neutron because of Pauli principle, since all the neutron shells are occupied; moreover an intermediate state cannot be different from the starting one (i.e. if we want to change a neutron of the $1s$ shell, it has to become a $1s$ shell proton), because we assume that there is not isospin impurity, so the wavefunctions have to be identical. The following figure shows what we just said:



3 → see below

2 → not possible because wavefunctions are different

1 → not possible because of Pauli principle

Figure 3.2 – Schematic representation of proton and neutron shells (see text above). Empty circles are holes left by the tranformation of a particle into one of the other kind (black circles).

Summarizing $\langle ij|\, T^+ t_1^- t_1^- t_2^+ \,|ij\rangle$ is zero because t_1^- acts two times and we do not have two t_1^+ to return to the initial charge state, and $\langle ij|\, T^+ t_1^- t_1^+ t_2^- \,|ij\rangle$ is zero too because t_1^+ acts first (since $t_1^- t_1^+$ do not commute) changing a proton into a neutron, but all neutron shells are complete.
This forces T^+ to be t_1^+ if we want an expectation value different from zero. Thus in the end we have:

$$\begin{aligned}\Delta E_{CSB} &= -\frac{2t_4}{2T_0}\sum_{ij}\langle ij|\,\delta(\mathbf{r}_1-\mathbf{r}_2)t_1^+t_1^-\left[1+\frac{x_4}{2}-\left(\frac{1}{2}+x_4\right)\left(\frac{1}{2}+2t_1^zt_2^z\right)\right]|ij\rangle \\ &= -\frac{2t_4}{N-Z}\int d^3r\left[\frac{3}{4}\rho_{ex}(r)\rho(r)-\left(\frac{1}{4}+\frac{x_4}{2}\right)\rho_{ex}(r)\rho_{ex}(r)\right]\end{aligned} \tag{3.30}$$

where ρ_{ex} arises from the fact that the only neutrons that can be changed into protons are the excess ones (arrow 3 in Figure 3.2), as explained before for the Coulomb term. Now let us try to understand the formula (3.30). When we move a neutron as in figure 3.2 we will have that all protons and neutrons interact between them in a different way than before. So an excess proton interacts with both the other protons and the other neutrons, minus the missing excess neutron that interacts with both the other neutrons and the other protons; schematically:

$$V^{pp} + V^{pn} - V^{nn} - V^{np} \tag{3.31}$$

pp, *pn* e *nn* interactions have a different weight; in particular in this interaction that acts as $v(t_1^z + t_2^z)$, where v is an average value of the space and spin parts, if one of the two particles is a proton and the other one a neutron we do not have contributions, so the two terms V^{pn}, V^{np} are zero. For the remaining terms the *pp* interaction goes as -2 and the *nn* one as +2, so we can write

$$\begin{aligned} &\langle ex, p| \, v \, |ex, p\rangle + \langle ex, n| \, v \, |ex, n\rangle = \\ &= \int d^3r(\psi_{ex}^\dagger \psi_p^\dagger) v(\psi_{ex}\psi_p) + \int d^3r(\psi_{ex}^\dagger \psi_n^\dagger) v(\psi_{ex}\psi_n) \end{aligned} \tag{3.32}$$

and passing to the densities we finally have an expression with the structure

$$\rho_{ex}\rho_p + \rho_{ex}\rho_n = \rho_{ex}\rho \tag{3.33}$$

This is only the direct term. Indeed in this reasoning we have not considered the exchange term, though in the computation to arrive to (3.30) we hold into consideration the exchange of particles 1 and 2. In (3.30) we have $(-\rho_{ex}\rho_{ex})$ because there are exchange terms only if the neutron is part of the excess (we cannot change the proton with the excess because the expectation value would be zero).
Let us look at the factors now. We know that the delta function can be written in multipole expansion, and the multipole component ahead is independent from L, which represents the exchanged angular momentum in the corresponding multipole term:

$$\delta(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{lm} \frac{\delta(r_1 - r_2)}{r_1^2} Y_{lm}^\dagger(\theta_1, \phi_1) Y_{lm}(\theta_2, \phi_2) \tag{3.34}$$

in this way a zero-range force has no angular dependence. For this reason we can restrict to the channel $L = 0$ without loss of generality. Here we can have $S = 0$ and $T = 1$, that would mean to have $x_4 = -1$, or $S = 1$ and $T = 0$, i.e. $x_4 = 1$. In the first case we have 3/4 for the direct term and 1/4 for the exchange one and since $T = 1$, we have the interactions *pp*, *pn* and *nn*, corresponding to $T_z = -1, 0, 1$; so it is makes sense that the direct term is the triple of the other. In the second case we have -3/4 for the exchange term.
In the interaction (3.1) only particles of the same types interact, and they are in the subspace $T = 1$, so it would not be reasonable having a $T = 0$ state, that would lead to having also *pn* interactions.
If we make the limit $\rho_{ex} \to \rho$, in which we have neutrons as the single type of particle,

what we obtain is 3/4+1/4=1 for the $S = 0$ channel and 3/4-3/4=0 for the $S = 1$ channel (this last thing is reasonable because $T = 0 \Rightarrow T_z = 0$ correspond to have a proton and a neutron, but this contribution can not exist in a system made up of neutrons only).
As explained so far, we think it is reasonable to use an interaction with $x_4 = -1$.

3.2.3 CIB term

The last commutator we have to calculate is given by the CIB potential (Eq. (3.7)) and is equal to:

$$\begin{aligned}\left[V_{CIB}, T^-\right] &= 4t_5(1 + x_5 P_\sigma)\delta(\mathbf{r}_1 - \mathbf{r}_2) \sum_3 \left[t_1^z t_2^z,\ \ t_3^-\right] \\ &= 4t_5(1 + x_5 P_\sigma)\delta(\mathbf{r}_1 - \mathbf{r}_2)(-2t_1^- t_2^z)\end{aligned} \tag{3.35}$$

Using Eqs. (3.27) and (3.28) we find the CIB contribute to the *Coulomb Displacement Energy*:

$$\begin{aligned}\Delta E_{CIB} = -\frac{4t_5}{2T_0} \sum_{ij} &\langle ij|\, \delta(\mathbf{r}_1 - \mathbf{r}_2) T^+ t_1^- t_2^z \cdot \\ &\cdot \left[1 + \frac{x_4}{2} - \left(\frac{1}{2} + x_4\right)\left(\frac{1}{2} + 2t_1^z t_2^z + t_1^+ t_2^- + t_1^- t_2^+\right)\right] |ij\rangle\end{aligned} \tag{3.36}$$

where no contribution arises from the last two terms $t_1^+ t_2^-$ and $t_1^- t_2^+$ for the same reason explained for the CSB term in the previous section. Thus in the end we have:

$$\begin{aligned}\Delta E_{CIB} &= -\frac{4t_5}{2T_0} \sum_{ij} \langle ij|\, 2\delta(\mathbf{r}_1 - \mathbf{r}_2) t_1^+ t_1^- t_2^z \left[1 + \frac{x_4}{2} - \left(\frac{1}{2} + x_4\right)\left(\frac{1}{2} + 2t_1^z t_2^z\right)\right] |ij\rangle \\ &= -\frac{2t_5}{N - Z} \int d^3r \left[\frac{3}{4}\rho_{ex}(r)\rho_{ex}(r) - \left(\frac{1}{4} + \frac{x_5}{2}\right)\rho_{ex}(r)\rho(r)\right]\end{aligned} \tag{3.37}$$

We see that it has the same structure of the CSB term, but with interchanged dependence on the densities in the direct and exchange terms. And also in this case we can give an interpretation of this structure. An excess proton interacts with both the other protons and the other neutrons, minus an excess neutron that interacts with both the other neutrons and the other protons:

$$V^{pp} + V^{pn} - V^{nn} - V^{np}. \tag{3.38}$$

Since this interaction acts as $t_1^z t_2^z$ all the terms in the above equation give their contribution, specifically V_{pp} as $\rho_{ex}\rho_p$, V_{pn} as $-\rho_{ex}\rho_n$, V_{nn} as $\rho_{ex}\rho_n$ and V_{np} as $-\rho_{ex}\rho_p$. So in the end we have a direct term that goes as $(\rho_p - \rho_n)\rho_{ex}$, exactly as the first term of Eq. (3.37) if we write $(\rho_p - \rho_n)$ as $-\rho_{ex}$.
Also here the choice of $x_5 = -1$ is justified by the need to be in the channel $T = 1$ (which implies $S = 0$ for a delta force), since CIB acts between pp, nn and pn.

Chapter 4

Results

In this chapter we will discuss the effects of the introduction of CSB and CIB terms calculated in Chapter 3. These terms should exist in every formulation, since experimental evidences (as those presented in the first chapter) show the existence of isospin symmetry breaking effects.
We have tested in the beginning three doubly magic nuclei: ^{48}Ca, ^{90}Zr and ^{208}Pb. In reality ^{90}Zr has 50 neutrons and 40 protons, then it is not a doubly magic nucleus but only magic. However, the last proton shell is far enough from the others so that it can be considered doubly magic. For these nuclei the *Coulomb Energy Differences* to reproduce are the following:

	CDE (MeV)	Experimental error (keV)
^{48}Ca	7.175 [20]	15
^{90}Zr	11.90 [21]	12
^{208}Pb	18.87 [22]	15

Table 4.1 – Experimental Coulomb Displacement Energy for the three nuclei.

The CDE values listed above are obtained studying compound-nucleus resonances in ^{48}Sc, ^{90}Nb and ^{208}Bi, formed by bombarding targets of ^{47}Ca, ^{89}Zr and ^{207}Pb with a proton. Normally in these reaction there is a lot of background and many large states which merge with each other, but the analogue states display a sharp peak and, so,

are easy to indentify. For this reason this energy has a small error (of about 15 keV), and this is the result of isospin symmetry, in the sense that the IAS of the daughter nucleus has the same isospin T_0 of the parent nucleus and couples weakly with the other states that are a mix of mainly states with the same isospin of the ground state, $T_0 - 1$.

4.1 Sensitivity Study

First of all it is necessary to study the sensitivity of the CDE due to CSB and CIB depending on the variation of the parameters t_4 and t_5. And we did this for the two interactions presented in Table 2.1 of Chapter 2: one more empirical (SLy5) and the other more microscopic (LNS), observing that the second is not suitable for the description of our nuclei.

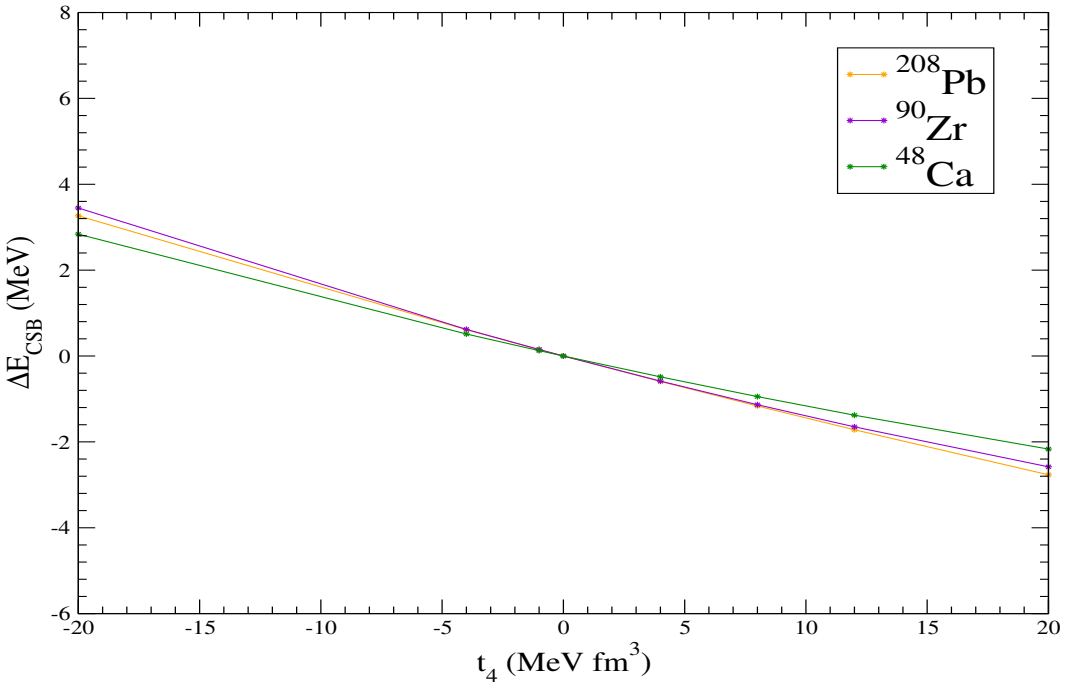


Figure 4.1 – ΔE_{CSB} in function of t_4 with SLy5 interaction.

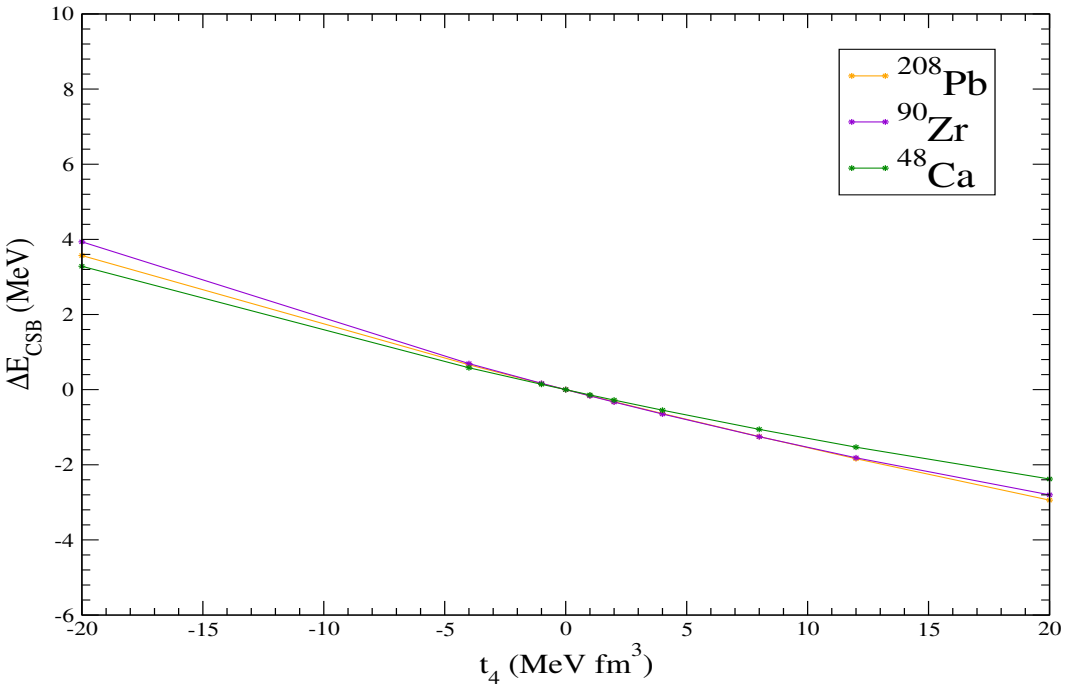


Figure 4.2 – ΔE_{CSB} in function of t_4 with LNS interaction.

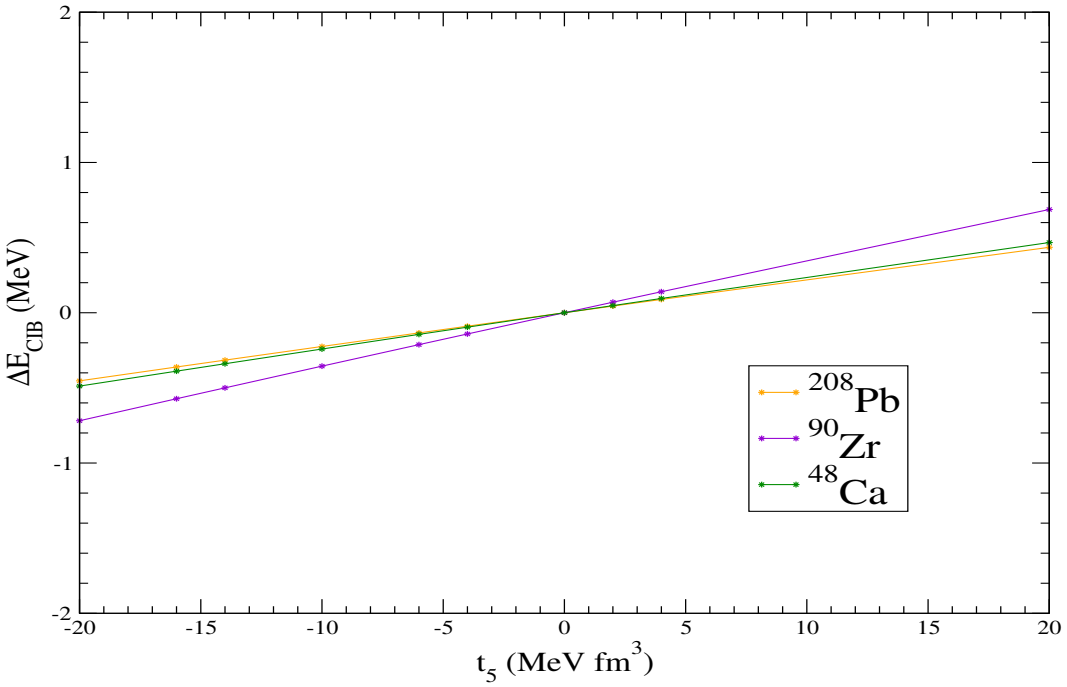


Figure 4.3 – ΔE_{CIB} in function of t_5 with SLy5 interaction.

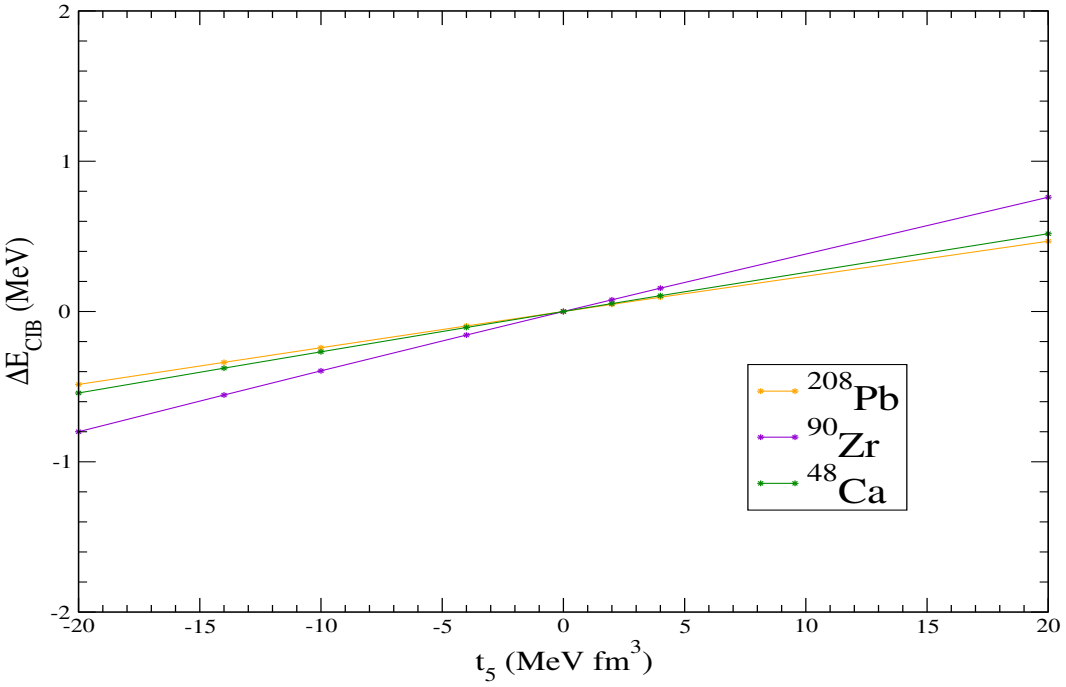


Figure 4.4 – ΔE_{CIB} in function of t_5 with LNS interaction.

Both ΔE_{CSB} and ΔE_{CIB} have a linear trend that is very similar between the two types of interaction, in particular in the central zone, and this is linked to the fact that they behave essentially as a perturbation.
Looking at the binding energies and the nuclear charge radii for the two interactions we see that they are both not well described in the case of LNS:

	BE experimental (MeV)	BE SLy5 (MeV)	BE LNS (MeV)
^{48}Ca	416.001	416.000	420.747
^{90}Zr	783.893	783.461	771.988
^{208}Pb	1636.430	1636.441	1569.450

Table 4.2 – Binding energy for the three nuclei.

Since the error for the masses must be within 1.5-2 MeV to be in agreement, for typical Skyrme forces, with the experimental data, we can see immediately that the LNS interaction gives results very far from that value (of the order of tens of MeV for all the three nuclei), while the binding energies win the case of SLy5 are always well

reproduced with an error of tens of keV.
For the radii, where the error is of 0.05 fm, we have the same situation in which the LNS values differers in the first digit from the experimental data:

	rms experimental (fm)	rms SLy5 (fm)	rms LNS (fm)
^{48}Ca	3.477	3.541	3.392
^{90}Zr	4.269	4.296	4.137
^{208}Pb	5.501	5.507	5.324

Table 4.3 – Radii for the three nuclei.

In fact the parameters of the SLy5 are fitted on as many as possible experimental nuclear data of finite nuclei, while the aim of the LNS is not to fit experiments but a more microscopic theory applied to the infinite matter. Thus we have decided to use only the SLy5 interaction to calculate the contribution to the CDE from the charge symmetry and charge independence breaking.
In the case of the radii we observe that also ^{48}Ca with SLy5 is not consistent with the experimental value. We will take into account this consideration in the next section, where we will determine the t_4 and t_5 parameters.

4.2 Parameters determination

The calculated values for the CDE with the SLy5 interaction are obtained from (3.22) for the direct term and (3.24) for the exchange term:

	CDE direct (MeV)	CDE exchange (MeV)	CDE total (MeV)
^{48}Ca	7.230	-0.375	6.855
^{90}Zr	12.270	-0.400	11.870
^{208}Pb	19.417	-0.355	19.062

Table 4.4 – Calculated Coulomb Displacement Energy for the three nuclei

The deviation of the data of the last column from the experimental ones in Table 4.1 has been evaluated using the root-mean-square error (RMSE), and this is equal to 216

keV, that must to be compared with the experimental error of 14.1 keV. To see now if the introduction of the CSB or the CIB term is able to remove this difference between calculated and experimental values we looked for the best values for the parameters with a fit that minimizes the RMSE.
Let us start from considering only the breaking of charge symmetry, that is a stronger request than the breaking of charge independence. In this case the RMSE is minimized by $t_4 = -0.2$ MeV fm^3, that corresponds to an error of 213 keV. The values for the CDE obtained for the three nuclei are shown in the following figure:

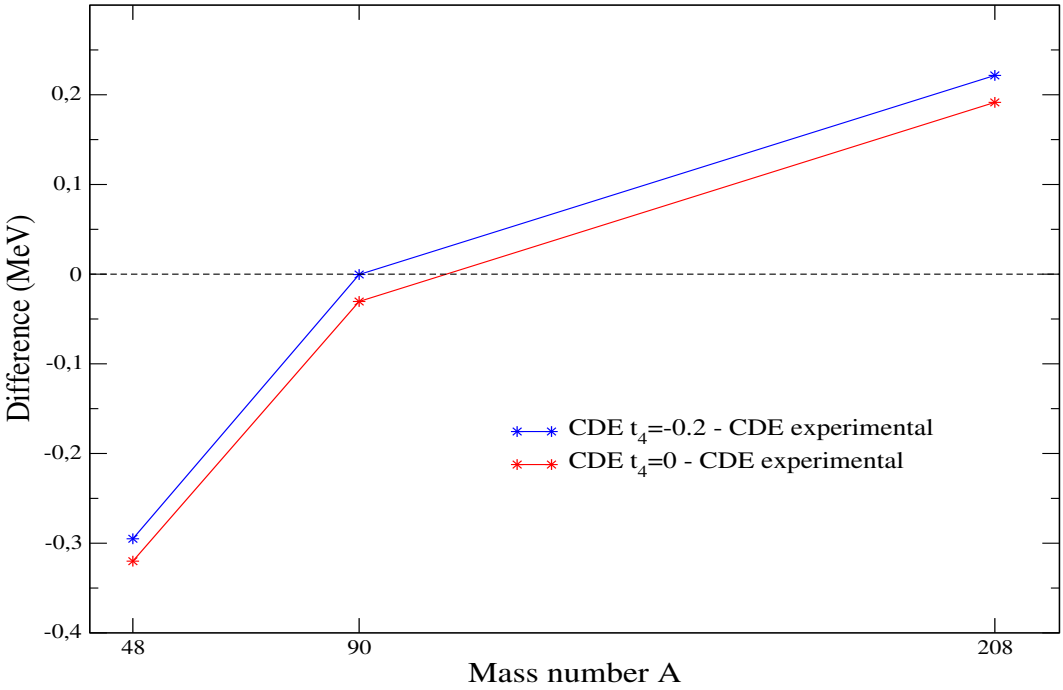


Figure 4.5 – The red stars are the difference between the CDE calculated without the introduction of the CSB term and the experimental values. The blue stars represent the difference between the CDE calculated with the introduction of the CSB term, with the parameter that minimizes the error, and the experimental values.

We see from the above figure an improvement of the CDE for ^{48}Ca and ^{90}Zr, while ^{208}Pb moves away from the experimental value. Even if the error is slightly less than before, is however too big to describe satisfactorily the CDE, in particular that of ^{48}Ca that remains very far from the expected value. So we try to use the CIB term instead the CSB to see how it acts on the CDE and if it is able to describe with a better precision these energy differences.

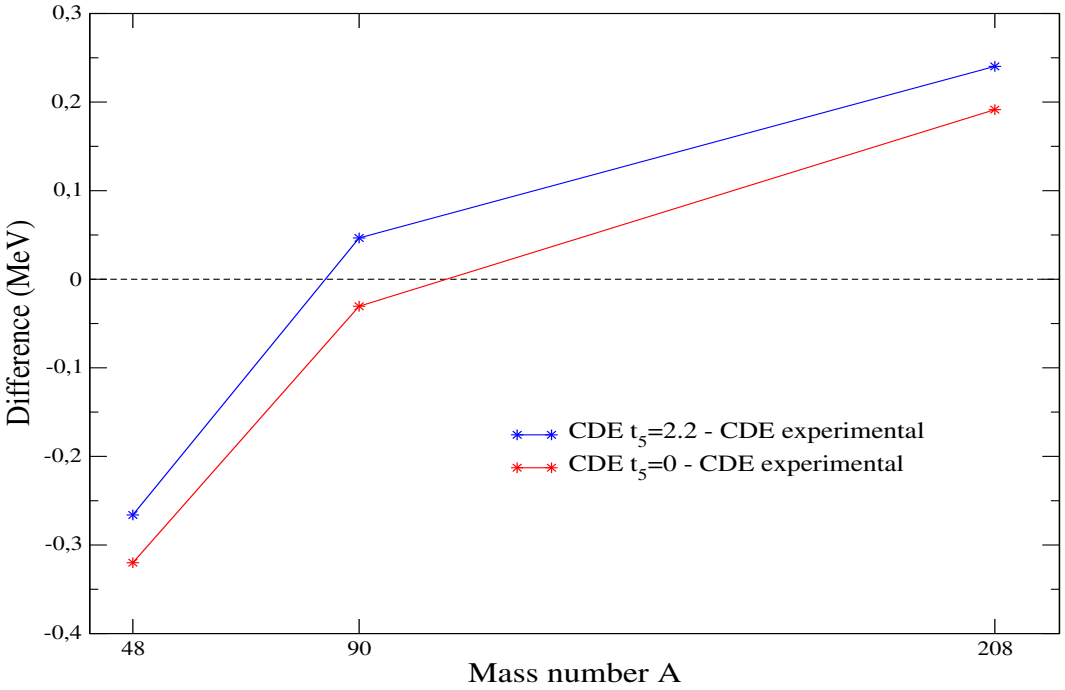


Figure 4.6 – The red stars are the difference between the CDE calculated without the introduction of the CIB term and the experimental values. The blue stars represent the difference between the CDE calculated with the introduction of the CIB term, with the parameter that minimizes the error, and the experimental values.

In this case the agreement is better than the previous one, since the RMSE is equal to 208 keV instead of 213 kev, but also here the theory is far from describing well the experimental results.

The failure in describing well the experimental CDE with these two methods can be explained looking at Fig. 4.1 and Fig. 4.3: we see that to correct the initial CDE values separately with the CSB term and CIB term we need effects of hundreds of keV, that means small parameters in both cases, that give quite the same ΔE values for the three nuclei considered (indeed it begins to differ from one nucleus to another starting from t_4=20 MeV fm^3 for CSB and t_5 about 10 MeV fm^3 for CIB). Furthermore the corrections for the three nuclei go all in the same direction (looking at the two Figs. 4.5 and 4.6 they increase the CDE) because for a fixed parameter the positivity or negativity of the ΔE_{CSB} and ΔE_{CSB} is independent from the nucleus (see Eqs. (3.30)

and (3.37) considering that always is $N > Z$). So, since is necessary to increase the CDE of ^{48}Ca and ^{90}Zr while that of ^{208}Pb has to be decreased to reach the experimental values, we have decided to introduce both the parameters at the same time. Considering that CSB goes like $N - Z$, while CIB like $(N - Z)^2/4$, we have a stronger dependence on the nucleus considered. In this way we obtain the following figure:

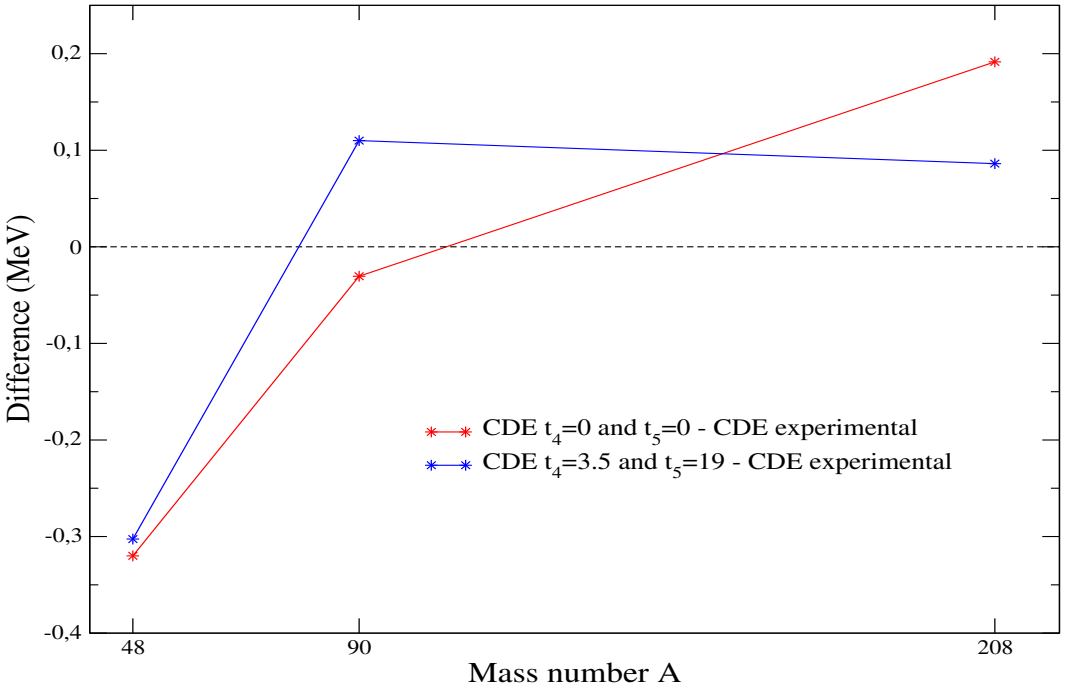


Figure 4.7 – The red stars are the difference between the initial CDE and the experimental values. The blue stars represent the difference between the CDE calculated with the introduction of the CSB and CIB terms, with the parameters that minimize the error, and the experimental values.

We have a RMSE equal to 192 keV, which means that the calculated CDE are not yet compatible with the experimental data.
Looking at Figs. 4.5, 4.6 and 4.7 we see that in particular we fail in a good representation of ^{48}Ca in all the three cases presented. It can be that this nucleus is too light to be well described by Skyrme parameters that are usually fitted on medium and heavy nuclei. So we decided to concentrate only on the other two nuclei, fitting the experimental CDE of ^{90}Zr and ^{208}Pb with t_4 and t_5 and finding the results in the following Table:

	computed CDE (MeV)	experimental CDE (MeV)	difference (MeV)
^{90}Zr	11.8970	11.90	-0.0030
^{208}Pb	18.8734	18.87	0.0034

Table 4.5 – CDE values compared with the experiment.

These values are obtained using $t_4 = 3.7$ and $t_5 = 16.5$. The RMSE in this case is of 3.2 keV, in perfect agreement with the experimental results.

To confirm that these parameters works also for other nuclei in the region with A between 90 and 208, and that effectively ^{48}Ca is to light to be taken into account, we looked for others experimental data of the CDE. Most of them are, however, for deformed nuclei or for odd neutron or proton numbers (which we cannot use since our formulas for the CDE have been obtained considering a mean value equal to zero for terms proportional to $\sigma_1\sigma_2$, that can be done only for even-even nuclei). In the end the only available nucleus to test and to compare with the experimental result is ^{114}Sn, with 50 protons and 64 neutrons.

	CDE experimental (MeV)	CDE computed (MeV)
^{114}Sn	13.91	13.94

Table 4.6 – Coulomb Displacement Energy experimental and computed before the introduction of the CSB and CIB terms.

Looking at the figure below we see that also the CDE of ^{114}Sn can be described well within this model, with a total RMSE equal to 11.4 keV, contained in the experimental error of 15.76 keV.

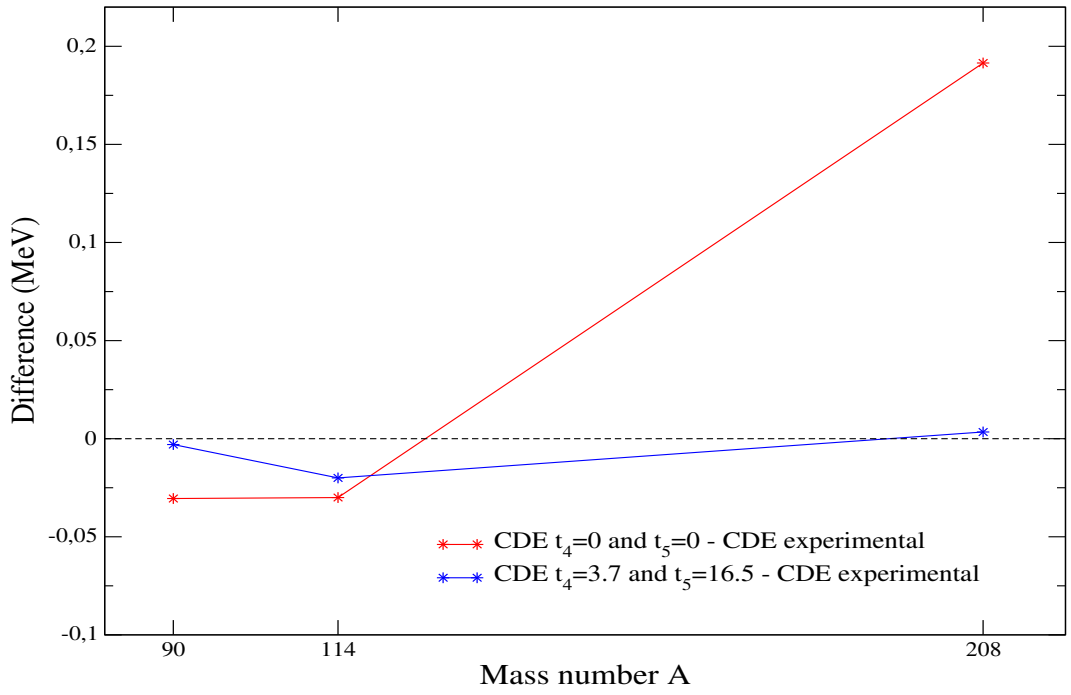


Figure 4.8 – The red stars are the difference between the initial CDE and the experimental values. The blue stars represent the difference between the CDE calculated with the introduction of the CSB and CIB terms, using the parameters in figure, and the experimental values.

4.3 Mean-field potentials and single-particle levels

The following section has the purpose to show to the reader how the introduction of the charge symmetry and charge independence breaking terms affects the mean field of protons and neutrons.
Looking at Eq. (3.6):

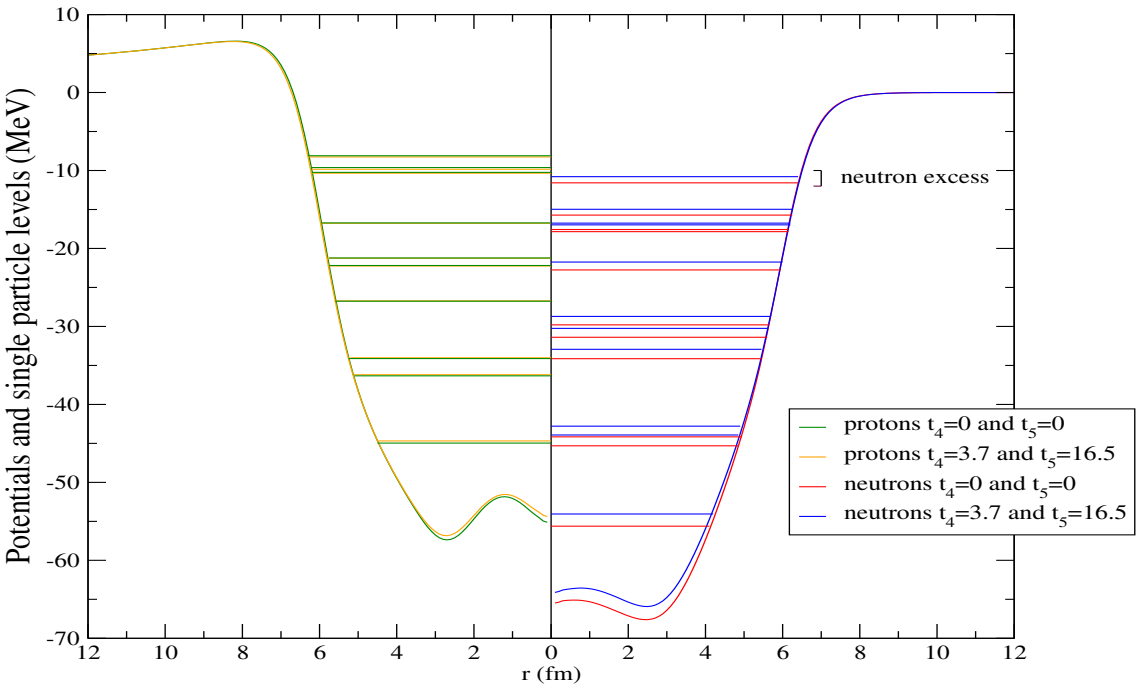
$$\begin{aligned} U_p &= \frac{\partial H_4}{\partial \rho_p} = -t_4(1-x_4)\rho_p \\ U_n &= \frac{\partial H_4}{\partial \rho_n} = t_4(1-x_4)\rho_n, \end{aligned} \tag{4.1}$$

we see that the introduction of the CSB term with positive t_4 and $x_4 = -1$ increases the depth of the proton potential and lowers that of the neutrons and looking at

Eq.(3.10):

$$\begin{aligned} U_p &= \frac{\partial H_5}{\partial \rho_p} = \frac{t_5}{2}\left[(1-x_5)\rho_p - (2+x_5)\rho_n\right] \\ U_n &= \frac{\partial H_5}{\partial \rho_n} = \frac{t_5}{2}\left[(1-x_5)\rho_n - (2+x_5)\rho_p\right], \end{aligned} \tag{4.2}$$

the introduction of the CIB term with positive t_5 and $x_5 = -1$ lowers the depth of both proton and neutron potentials. Hence considering their action at the same time we will expect a higher potential (and thus higher single particle energy levels) for the neutrons, and for the protons a small displacement from the initial potential depending on which of the two effects (CSB or CIB) will prevail. Since t_5 is much bigger than t_4 we will have a little shift upward of the potential and of the single particle levels, but it is so small that they overlap almost completely the initial data, as represented in the following figures for the three different nuclei:



(a) ^{90}Zr

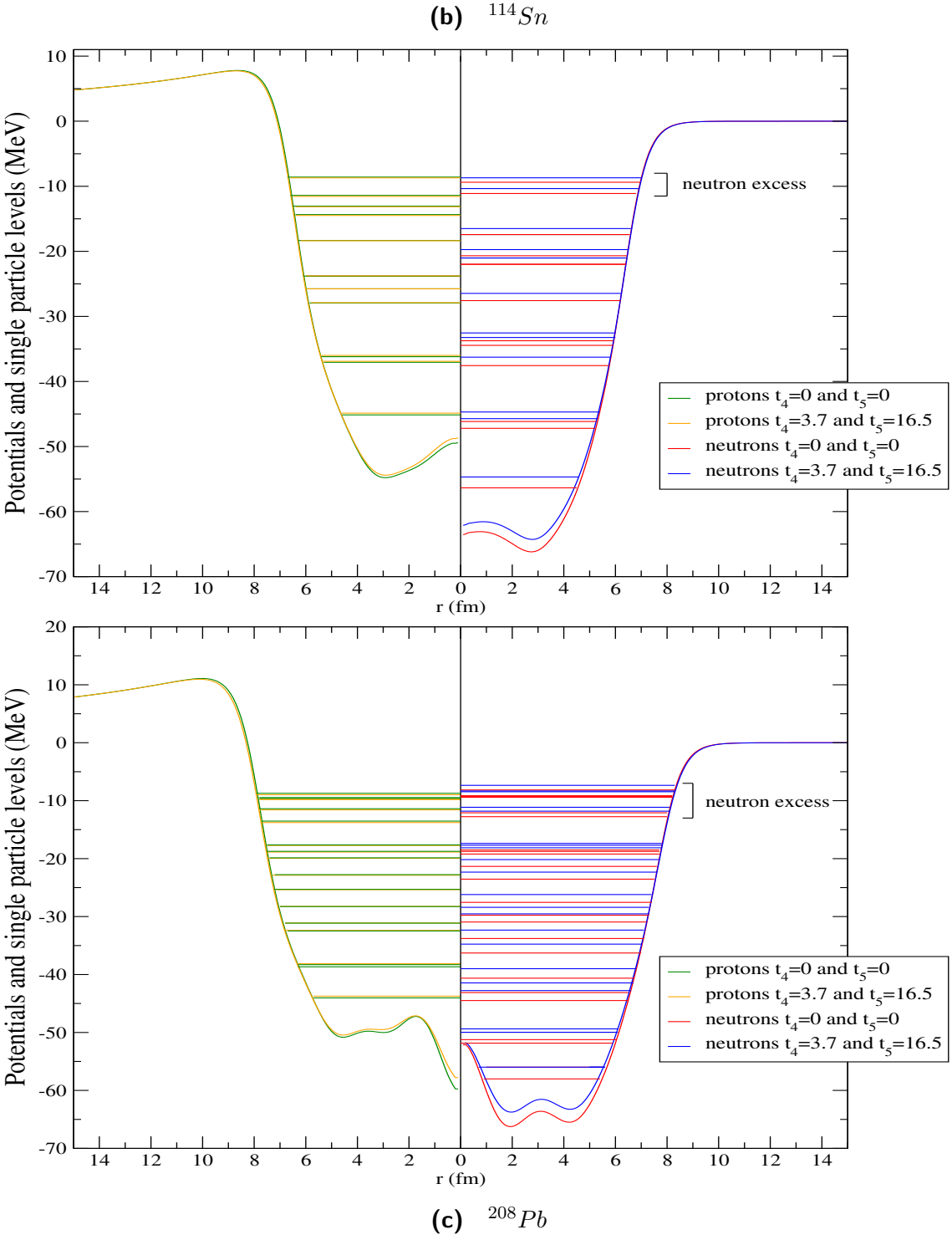


Figure 4.10 – In **(a)**, **(b)** and **(c)** are presented the potentials and single particle energy levels of protons on the left and neutrons on the right for the three nuclei analysed. The green color represents the situation of the protons before the introduction of the CSB and CIB terms, while the orange color is the after. The red color represents the situation of the neutrons before the introduction of the CSB and CIB terms, while the blue color is the after. The difference between before and after is very small, particularly for the protons, in fact in many point the lines overlap; while for the neutrons the energy increase for the potential and, thus, for the particle levels can be seen quite well.

Chapter 5

Conclusions

Most of the nuclear interaction conserves isospin, while this is broken by the Coulomb force. The experimental energy difference between analogue states in neighbouring nuclei is sensitive to isospin breaking, but present models cannot explain very accurately this difference. Thus in this work we proposed a theory based on the breaking of the isospin symmetry in nuclei to try to explain the experimental energy differences, called *Coulomb Displacement Energy*, between analogue states of nuclei which are part of the same isobaric multiplet. We have introduced two new types of two-body interactions: the first (CSB) depending on the sum of the isospin third components of the two particles, that breaks the charge symmetry, while the second (CIB) breaks the charge independence symmetry and has a structure depending on the product of the isospin third components.

Our starting point has been the mean-field formalism, where we used existing Skyrme interactions to solve the Hartree-Fock equations and to find single-particle states. In this scheme we have added to the Skyrme interaction the two new potentials which break charge symmetry and charge independence, and we have calculated the contribution to the *Coulomb Displacement Energy* from all the isospin symmetry breaking terms (Coulomb, CSB and CIB) for the three nuclei ^{48}Ca, ^{90}Zr and ^{208}Pb. We started studying the sensitivity of the CSB and CIB terms taking into account the two types of Skyrme interaction SLy5 and LNS, but we noticed that the second was not able to describe well charge radii and binding energies, so we concentrated only on the

first. Continuing the investigation with the SLy5 interaction we noticed that it was not possible to describe the three nuclei at the same time using only one of the new isospin symmetry breaking terms introduced, because we obtain only a shift of the curve (up or down) but the trend does not change. So we decided to use both the terms together to allow the CDE to vary independently from one nucleus to another. Once put ^{48}Ca aside, since we supposed it to be too light to be well described by Skyrme parameters, which are usually fitted on medium and heavy nuclei, we were actually able to describe the experimental CDE. To find a confirmation of the soundness of our theory we calculated also the CSB and CIB contribution to the CDE for the ^{114}Sn (between the ^{90}Zr and ^{208}Pb), finding that is in agreement with the previous result for the other two nuclei.

In conclusion we found that the effects of isospin symmetry breaking succeed in reproducing the shift between the calculated and experimental values for the nuclei ^{90}Zr, ^{114}Sn and ^{208}Pb, failing instead with the lighter ^{48}Ca. A further development of this theory would be the extension to non magic even-even nuclei (in which would be sufficient the introduction of pairing terms), and then to odd-even and odd-odd nuclei, so that the terms depending on the spin can also be considered and benchmarked, and so that it is possible to compare the theory with more experimental data.

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