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Isospin Symmetry Breaking in Nuclear Masses

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Contents

Introduction

In this work we concentrate on the study of nuclear Isospin Symmetry Breaking effects. The motivations are the following. In the early studies about nuclear interaction, a particular symmetry between protons and neutrons has been observed: in good approximation, the strong nuclear interaction does not distinguish different nucleons. This, and the fact that nucleons have almost equal masses, made them be considered as two states of the same particle. Thus, it was introduced the concept of *isospin* (T), which is a good quantum number whose z-projection distinguishes proton ($T_z = -1/2$) from neutron ($T_z = 1/2$). This implies that, if we neglect electromagnetic interaction, the energy spectrum of nuclei with the same total isospin (for example nuclei with the number of neutrons and protons interchanged) would be perfectly identical. We say that the nuclear Hamiltonian is invariant under a rotation of the isospin, in good approximation.

Yet, there are some evidences of a breaking of these isospin-symmetries. Of course, the main isospin symmetry breaking effect is due to the Coulomb field, which act on protons only, and it is obviously known. But the difference between the binding energies between the *isobaric analogue states* (the so-called Coulomb Displacement Energy CDE), that are nuclei in the same isospin multiplet, cannot be described by electromagnetic force alone, as studied in details by Nolen and Schiffer [1]. There is always a discrepancy between the experimental and theoretical CDE, even if one adds all the possible corrections to the electromagnetic interaction, such as the exchange energy, the vacuum polarization, the nucleons finite size correction, the electromagnetic spin-orbit, and the proton-neutron mass difference [2]. This is called *Nolen-Schiffer anomaly*.

Different values for the pp, nn and pn scattering lengths measures suggest that these particles interact with different intensity. These evidences suggest that one should introduce some nuclear forces that break *charge symmetry* ($V_{nn} \neq V_{pp}$) and *charge independence* ($V_{np} \neq (V_{nn} + V_{pp})/2$). In this work we make use of Skyrme effective interaction solved at the mean field approximation to calculate the binding energies of nuclei. We extend the Skyrme model, which does not breaks isospin symmetry, to account for the above mentioned effects. We will try to explain the Nolen-Schiffer anomaly through a self-consistent method, based on

an effective microscopic interaction. We shall concentrate on the energy difference between a particular kind of isobaric analogue states, the mirror nuclei, to find a description of the so-called Mirror Displacement Energy.

The thesis is organized as follows: in the first chapter we recall the theoretical background: Hartree-Fock theory, Skyrme interaction and pairing interaction. In the second chapter we introduce two nuclear interactions that break isospin symmetry: one (Charge Symmetry Breaking) depends on the sum of the isospins of the particles, and the other (Charge Independence Breaking) that depends on their product. Then we discuss the effects of different contributions to the Coulomb Displacement Energy, while in the third chapter we show the results of the fit of the experimental Mirror Displacement Energy. In the last chapter we discuss about an astrophysical application, that is the effects of the ISB interactions on the equation of state of infinite matter and on mass and radius of neutron stars.

Chapter 1

Mean field and Skyrme interaction

1.1 Hartree-Fock method

A nucleus is a many-body system, bound by the nuclear interaction. We can not solve the Schrödinger equation exactly for many particles, so we have to use some approximations. Experimental evidences, such as the occurence of magic numbers, support the shell model and show the existence of a mean field. This means that we can substitute the interacting many-body problem with a set of one-body problems, which describe the motion of independent particles moving in a mean field made up by the particles themselves.

The main problem in nuclear physics is that we do not know exactly the nucleon-nucleon interaction. That is why to solve many-body problem we use effective interactions (e.g. Skyrme, which we will discuss later), which have been shown to successfully describe bulk properties of nuclei such as binding energies (within the % accuracy), charge radii (also within the % accuracy) and the excitation energy and sum rules of nuclear collective excitations (within the few % accuracy).

Hartree-Fock theory gives a microscopic explaination to a mean field approach. Starting from a variational principle, it gives a Scrödinger equation, obtained by minimizing the expectation value of the Hamiltonian H on a state $|\Psi\rangle$, which is written as a total antisymmetric combination of a set of single-particle states $|\phi_i\rangle$, with respect to these states. The total wavefunction need to be antisymmetric under any exchange of the A particles, as the nucleons are fermions, according to Pauli principle. The simplest way of writing an antisymmetric wave function is the *Slater determinant*:

$$|\Psi\rangle = \frac{1}{\sqrt{A!}} \det |\phi_i(j)\rangle \tag{1.1}$$

Particles in a nucleus are non-relativistic, in fact the kinetic energy ($\epsilon_F \simeq 36$

MeV) is much lower than their mass ($m \simeq 940$ MeV). So the Hamiltonian is $H = T + V$, where

$$\begin{aligned} T &= \sum_{i=1}^{A} \frac{-\hbar^2}{2m} \nabla_i^2 \\ V &= \frac{1}{2} \sum_{ij} v(i,j) \end{aligned} \tag{1.2}$$

are kinetic and potential energy (in coordinates representation). The variational principle states:

$$\delta E = \delta \Big[\langle \Psi | H | \Psi \rangle - \sum_{ij} \lambda_{ij} \int \mathrm{d}^3 r \phi_i^\star(\vec{r}) \phi_j(\vec{r}) \Big] = 0 \tag{1.3}$$

where we imposed an orthonormality constraint on the wavefunctions ϕ_i (λ_{ij} are Lagrange's multipliers). This leads to the *Hartree-Fock equations* [3]:

$$\begin{aligned} -\frac{\hbar^2}{2m} \nabla_i^2 \phi_i(\vec{r}) + \sum_j \int \mathrm{d}^3 r' \phi_j^\star(\vec{r'}) v(i,j) [\phi_i(\vec{r}) \phi_j(\vec{r'}) - \phi_j(\vec{r}) \phi_i(\vec{r'})] = \\ = \sum_j \lambda_{ij} \phi_j(\vec{r}) = \epsilon_i \phi_i(\vec{r}) \end{aligned} \tag{1.4}$$

These have the form of Schrödinger equations. The first term in the left hand side of the equation is the kinetic one, the second is the Hartree potential term, which is the local mean field, and the third one is the *nonlocal* Fock contribution, which is related to the fermionic nature of nucleons. Fock term can be justified saying that, as a particle interacts with the mean field, which is made by all the particles, we have to subtract the interaction with itself. In the right hand side there are the energy eigenvalues ϵ_i, called also *single-particle energies*, obtained with a unitary transformation in the last step.

We should note that the potential terms depends on the wave functions, thus these equations need to be solved by iteration: we start chosing a potential (with a Wood-Saxon shape) and we find its solutions. Then we calculate a new potential with these wave functions and repeat the procedure until self-consistence is achieved, that is when the difference between consecutive solutions is smaller than a chosen value. The total Hartree-Fock energy (the expectation value of H) is not the sum of the single-particle levels, otherwise the potential term would be counted twice, but it is

$$E = \frac{1}{2} \sum_i \Big(\epsilon_i + \frac{\hbar^2 k_i^2}{2m} \Big) \tag{1.5}$$

Actually, we apply a correction to Eq. (1.5), called center of mass correction. We subtruct the kinetic energy of the center of mass, just multiplying m for a factor $\frac{A}{A-1}$ [4].

For a nucleus we shall generalize the Hartee-Fock equations, reminding to add isospin as an extra degree of freedom, so that $\phi_i = \phi_{qi}(\vec{r_i}, \vec{\sigma}_i)$, where q stays for neutron or proton. We consider no isospin impurity, that means the isospin is well defined on a state ϕ_{qi}. The mass of the nucleons is as usually approximated to their average value. In the present form, the Hamiltonian is isospin symmetric except for the Coulomb interaction, that would introduce the main difference between neutrons and protons in nuclei.

To solve these equations we need a model for the effective interaction v_{ij}, as we discuss in the following section.

1.2 Skyrme interaction

In this work we solved Hartree-Fock equations using the Skyrme interaction [5]. It is a contact force, because it is proportional to a delta function, so that it acts only when the positions of the i-th and j-th particles coincide in the same point of space. The usual expression is:

$$\begin{aligned} v(i,j) = \quad & t_0\delta(\vec{r_i}-\vec{r_j})(1+x_0P_\sigma^{ij}) \\ & + \frac{1}{2}t_1\delta(\vec{r_i}-\vec{r_j})(1+x_1P_\sigma^{ij})(k^2+k'^2) \\ & + t_2\,\delta(\vec{r_i}-\vec{r_j})(1+x_2P_\sigma^{ij})\vec{k'}\cdot\vec{k} \\ & + \frac{1}{6}t_3\delta(\vec{r_i}-\vec{r_j})(1+x_3P_\sigma^{ij})\rho^\alpha(\tfrac{\vec{r_i}+\vec{r_j}}{2}) \\ & + iW_0\delta(\vec{r_i}-\vec{r_j})(\vec{\sigma}_i+\vec{\sigma}_j)\cdot(\vec{k'}\times\vec{k}) \end{aligned} \tag{1.6}$$

The first term in Eq. (1.6) is the central one, as it only depends on the difference of the positions. The second and the third ones depends on the relative momuntum, as $\vec{k} = \frac{1}{2i}(\vec{\nabla}_i - \vec{\nabla}_j)$ and $\vec{k'}$ its conjugate, which acts on the left state. They mimic the finite range of the interaction [6]. The fourth one is a density dependent term, inspired by a 3-particles interaction $v_{ijk} \propto \delta(\vec{r_i}-\vec{r_j})\delta(\vec{r_j}-\vec{r_k})$ integrated over one variable. The last term represents the spin-orbit interaction and it depends on spins and momenta. The interactions are symmetric under the exchange of the spins, so they are proportional to factors $(1 + xP_\sigma^{ij})$, where $P_\sigma^{ij} = (1 + \vec{\sigma}_i \cdot \vec{\sigma}_j)/2$. $t_0, t_1, t_2, t_3, x_0, x_1, x_2, x_3, \alpha$ and W_0 are free parameters, fitted in order to reproduce the nuclear masses and other fundamental properties.

If i and j are protons, then we add the Coulomb interaction $v(i,j) = e^2/|\vec{r_i}-\vec{r_j}|$, which is the main source of isospin symmetry breaking and that is local only for

the Hartree term. The non-local Fock term is customary approximated by using the Slater approximation which is local.

The delta shape of the interaction simplifies the Schrödinger equations, so that also the Fock (exchange) part of the potential becomes local, and we can write the expectation value of H as an integral of the energy density $\mathcal{H}(\vec{r})$ over the space:

$$E = \int \mathcal{H}(\vec{r})\, \mathrm{d}^3 r \tag{1.7}$$

Actually $\mathcal{H}(\vec{r})$ depends on the particles, kinetic and spin-orbit density, respectively defined as:

$$\begin{cases} \rho_q(\vec{r}) := \sum\limits_{i\vec{\sigma}} \left|\phi_{qi}(\vec{r},\vec{\sigma})\right|^2 \\ \tau_q(\vec{r}) := \sum\limits_{i\vec{\sigma}} \left|\vec{\nabla}\phi_{qi}(\vec{r},\vec{\sigma})\right|^2 \\ \vec{J}_q(\vec{r}) := -i \sum\limits_{i\vec{\sigma}\vec{\sigma}'} \phi^{\star}_{qi}(\vec{r},\vec{\sigma}) \left[\vec{\nabla}\phi_{qi}(\vec{r},\vec{\sigma}') \times \left\langle \vec{\sigma}\middle|\hat{\vec{\sigma}}\middle|\vec{\sigma}'\right\rangle\right] \end{cases} \tag{1.8}$$

We find that $\mathcal{H} = \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_{eff} + \mathcal{H}_{fin} + \mathcal{H}_3 + \mathcal{H}_{so} + \mathcal{H}_{sg}$ is the sum of many energy density terms, each one is shown in details in Ref. [7, 6].

Following Vautherin and Brink [6], the variational principle (Eq. (1.3)) leads to the equation:

$$\left\{-\vec{\nabla}\frac{\hbar^2}{2m^{\star}_q(\vec{r})}\cdot\vec{\nabla} + U_q(\vec{r}) + \delta_{q,proton}V_C(\vec{r}) - iW_q(\vec{r})\cdot(\vec{\nabla}\times\vec{\sigma}) - \epsilon_i\right\}\phi_{qi}(\vec{r},\vec{\sigma}) = 0 \tag{1.9}$$

where $i = 1,\ldots,A$. The kinetic term depends now on an effective mass $m^{\star}$, since it has absorbed kinetic density dependent Hamiltonian. The effective mass $\hbar^2/2m^{\star}_q$, the mean field $U_q(\vec{r})$ and $W_q(\vec{r})$ are defined as the functional derivative of $\mathcal{H}$ respect to τ_q, ρ_q and $\vec{J}_q$, respectively. We added the Coulomb field, which only acts on protons, and its expression is:

$$V_C(\vec{r}) = V_C^{Direct}(\vec{r}) + V_C^{Exchange}(\vec{r}) = e^2\int \frac{\rho_p(\vec{r'})}{|\vec{r}-\vec{r'}|}\,\mathrm{d}^3 r' - e^2\left(\frac{3}{\pi}\right)^{1/3}\rho_p^{1/3} \tag{1.10}$$

where the second term in the rhs is the Slater approximation to the exchange term [8], which is very convenient since it does not break locality.

The Coulomb energy density is

$$\mathcal{H}_C = \frac{1}{2}V_C^{Direct}\rho_p - \frac{3}{4}e^2\left(\frac{3}{\pi}\right)^{1/3}\rho_p^{4/3} \tag{1.11}$$

One can solve Hartree-Fock and find the binding energy of a nucleus. Actually we have to add a *rearrengement* term [6] to Eq. (1.5), because of density dependence of the three-body interaction and the Slater approximation of Coulomb exchange term, so that:

$$\begin{aligned} E &= \frac{1}{2}\sum_i \Big(\epsilon_i + \frac{\hbar^2 k_i^2}{2m_q}\Big) + E_R \\ E_R &= -\frac{t_3}{8}\int \rho_n(\vec{r})\rho_p(\vec{r})\rho^\alpha(\vec{r})\,\mathrm{d}^3r - \int \frac{e^2}{4}\Big(\frac{3}{\pi}\Big)^{1/3}\rho_p^{4/3}\,\mathrm{d}^3r \end{aligned} \tag{1.12}$$

Once we find the solutions ϕ_{qi}, we can calculate the densities ρ_q, τ_q, $\vec{J}_q$ and so the energy density $\mathcal{H}$. The integral of $\mathcal{H}$ is useful to know the contribution of each term of the Hamiltonian to the total energy and it should not be corrected by rearrangement terms. Also, it may be a test to verify the good implementation of Hartree-Fock equation, since E calculated by using Eq. (1.12) must coincide with $\int \mathcal{H}\,\mathrm{d}^3r$.

Numerical solution for spherical nuclei

We restrict our calculation to spherical nuclei, so that we can make use of spherical symmetry. We can define the eigenfunctions as a product between a radial function and a spherical harmonic, and the spin part:

$$\phi_i(r,\Omega,\vec{\sigma}) = \frac{R_{nl}(r)}{r}\mathcal{Y}_{ljm}(\Omega)\chi_m(\vec{\sigma}) \tag{1.13}$$

where $i = \{n, l, j, m\}$ is the usual set of good quantum numbers defining the state, and $\Omega = (\vartheta, \varphi)$ are the angular coordinates. Then, from the definition 1.8, we find the expression for the densities in function of r, using the properties of spherical harmonics:

$$\begin{cases} \rho_q(r) = \dfrac{1}{4\pi r^2}\displaystyle\sum_i (2j+1)R_{nl}^2(r) \\ \tau_q(r) = \dfrac{1}{4\pi}\displaystyle\sum_i (2j+1)\Big[\Big(\frac{\mathrm{d}}{\mathrm{d}r}\frac{R_{nl}}{r}\Big)^2 + \frac{l(l+1)}{r^4}R_{nl}^2\Big] \\ J_q(r) = \dfrac{1}{4\pi r^3}\displaystyle\sum_i (2j+1)\Big[j(j+1) - l(l+1) - \frac{3}{4}\Big]R_{nl}^2(r) \end{cases} \tag{1.14}$$

The Schrödinger equation 1.9 can be reduced to a 1-dimension equation, making use of:

- $-\vec{\nabla}\cdot\dfrac{\hbar^2}{2m^\star(r)}\vec{\nabla} = -\dfrac{\mathrm{d}}{\mathrm{d}r}\dfrac{\hbar^2}{2m^\star(r)}\dfrac{\mathrm{d}}{\mathrm{d}r} - \dfrac{\hbar^2}{2m^\star(r)}\dfrac{1}{r}\dfrac{\mathrm{d}^2}{\mathrm{d}^2r}r + \dfrac{\hbar^2}{2m^\star(r)}\dfrac{L^2}{r^2}$

- $-i\vec{W}_q(\vec{r})\cdot\vec{\nabla}\times\vec{\sigma} = -iW_q(\vec{r})\dfrac{\vec{r}}{r}\cdot\vec{\nabla}\times\vec{\sigma} = \dfrac{1}{r}W_q(r)\vec{L}\cdot\vec{\sigma}$

where $\vec{L} = -i\vec{r}\times\vec{\nabla}$ is the orbital angular momentum, in units of $\hbar$. Then the radial Hartree-Fock equation is:

$$-\frac{\hbar^2}{2m_q^\star}\Big[R_i'' + \frac{l(l+1)}{r^2}R_i\Big] - \frac{\mathrm{d}}{\mathrm{d}r}\frac{\hbar^2}{2m_q^\star}\Big[R_i' - \frac{R_i}{r}\Big] + \\ + \Big\{U_q + V_C + \frac{1}{r}W_q[j(j+1) - l(l+1) - 3/4]\Big\}R_i = \epsilon_i R_i \quad (1.15)$$

This equation is already implemented in the program in Ref. [4], which we used and we added all the corrections we need for our scope, that are discussed in Chapter 2.

1.3 Pairing interaction

Pairing correlation plays an important role as in superconducting solids as in open-shell nuclei, and it can be treated in reasonable approximation with the *Bardeen-Cooper-Schrieffer* (BCS) approximation [3, 9].

Among the experimental evidences of pairing effects, there is the *odd-even staggering*, firstly. That is the fact that the binding energy of an odd nucleus is smaller than the average of its even-even neighbours. This implies the characteristic staggering of the binding energy. Secondly, there is the *energy gap*, that is the fact that the excitation spectrum of even-even open-shell nuclei shows a gap of about 1-1.5 MeV between the ground state and the first excited state. For odd nuclei the spectrum is very different, in fact it shows many excited states in the same energy interval. These two evidences can be seen in Fig. 1.1, that shows the first excited states of some tin isotopes.

The energetically most stable configuration in a Hartree-Fock description is the one with all the particles paired in the lowest energy shells. Particles in a pair have opposite projection of angular momentum J_z, that is why even-even nuclei ground states have total angular momentum $J = 0$. Because of the short range of nuclear force, and because particles in the same orbital with same $|J_z|$ have the same spatial distribution, there exist a strong correlation between these two particles. This implies that in order to excite even-even nuclei we have to break at least one couple, and this explains qualitatively the gap in the excitation spectrum between even-even and odd nuclei.

The gap in the excitation spectrum is analogous to superconductive metals. We can study pairing correlation applying the superconductivity theory, the BCS approximation, to nuclei. Like the Hartree-Fock method, BCS equations can be

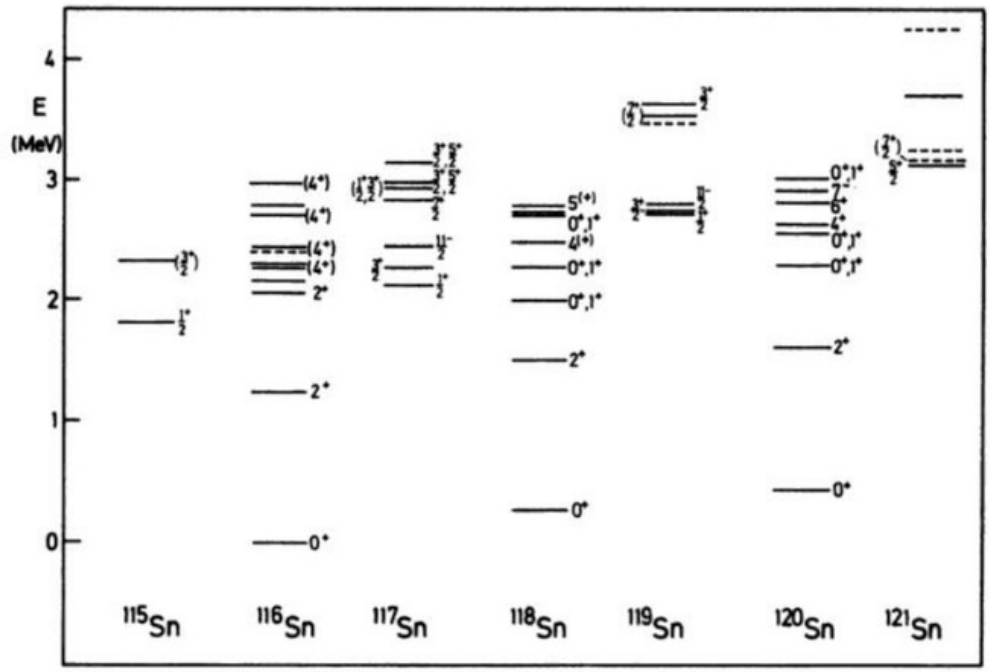

Figure 1.1: Excited spectra of some tin isotopes. Note the odd-even staggering of the ground states and the energy gap between the ground state and the first excited state of even isotopes, which are discussed in the text. The figure is taken from Ref. [3]

derived from a variational principle too. The main difference is that in Hartree-Fock theory particles are distributed to fill all the lowest energy states, up to the Fermi energy. Instead, BCS theory assumes a ground state which is not made with all the lowest levels completely full, but each level, below or over the Fermi energy, have an *occupation probability* that can be different from 1 or 0. In fact, the energy necessary to excite a couple from Hartree-Fock ground state is balanced by the binding energy of the couple. In second quantization formalism:

$$|BCS\rangle = \prod_{k>0} (u_k + v_k a_k^+ a_{\tilde{k}}^+) \, |-\rangle \tag{1.16}$$

where $|-\rangle$ is the vacuum state, $k, \tilde{k}$ label particles in the same state with opposite spin, and $\{|u_k|^2, |v_k|^2\}$ are the probabilities that the paired state is empty and occupied, respectively. Minimizing the expectation value of the Hamiltonian on this state (respect to the occupation probabilities), with the constraint that the number of particles is fixed, one can find the BCS equations [3]. These equations show that the minimum energy necessary to make an excitation in an even-even nucleus is finite and it depends on a model for the interaction.

Many studies show that a density dependent delta interaction provides good agreement with experiments [10]. The model we used here for the pairing strength is the following two body interaction:

$$V_{pairing}(i,j) = V_0\left(1 - \frac{\rho}{\rho_0}\right)^{\gamma} \delta(\vec{r}_i - \vec{r}_j) \tag{1.17}$$

where V_0 and γ are constants to adjust phenomenologically, while $\rho_0 = 0.16\,\mathrm{fm}^{-3}$ is the *saturation density* (for symmetric nuclear matter, that is when $\rho_p = \rho_n$).

We look for an observable which is sensitive to the pairing correlation, so that we can compare it with our calculations. Unfortunately the pairing gap is not directly accessible in experiments, but the observable with the closest relation to the pairing correlation is the odd-even staggering, as previously discussed. We can use this to fit the pairing strength. We can extract information on the pairing gap from some combinations of adjacent mass values, called *finite difference formulae*. These combinations are found with a Taylor expansion of nuclear mass in nucleons number difference. In first order of approximation the pairing gap can be estimated as the separation energy, but this is not good to fit the pairing strength, as explained in Ref. [11]. We then consider the second order of approximation, that is called *three-point formula*:

$$\Delta_q^{(3)}(N_0) := \frac{\pi_{N_0}}{2}\Big[E(N_0 - 1) - 2E(N_0) + E(N_0 + 1)\Big] \tag{1.18}$$

where $\pi_{N_0} = (-1)^{N_0}$, and N_0 can be protons or neutrons number.

In this work we will fit the binding energy of some open-shell nuclei (see Chapter 3). Our purpose will be to find a pairing constant V_0 in Eq. (1.17) which is good enough to reproduce $\Delta_q^{(3)}$ when the experimental values for E are used, by solving BCS equations.

Chapter 2

Isospin symmetry breaking

In this work we study the Isospin-Symmetry Breaking (ISB) corrections due to the nuclear interaction.

If we could switch off all the ISB effects, Coulomb field too, then the binding energy of mirror nuclei (nuclei with the number of protons and neutrons exchanged) would be exactly the same. In general, the energy of all the *Isobaric Analogue States* (IASs), that are states with the same total isospin T, would be the same as well. In this case we say that the Hamiltonian commutes with total isospin ($[H, \mathrm{T}] = 0$), or that it is invariant under any rotation in the isospace (i.e. changing the z-projection T_z of isospin).

Yet, experimental results show that there is a difference in energy between adjacent IASs. This difference is called *(Coulomb) Displacement Energy* (DE), because in a nucleus the main source of ISB effects is the Coulomb field, which acts on protons only. But this field alone is not sufficient to describe the DE, in fact calculations show that Coulomb energy usually contributes with about 90% to the DE. This is known as *Nolen-Schiffer anomaly*[1]. Neither the *Mirror Displacement Energy* $\quad \mathrm{MDE} := BE(T, -T_z) - BE(T, T_z) \quad$ can be described by Coulomb field alone.

Also, the difference in the nucleon-nucleon scattering length implies that neutrons and protons interact with different strength [12]. In fact, they are two distinct particles, with different mass and inner structure.

All these considerations suggest that we should add some Isospin Symmetry Breaking corrections to the standard nuclear Hamiltonian. In this chapter we will discuss many terms which break isospin symmetry: first of all, the Charge Independence Breaking and Charge Symmetry Breaking nuclear forces, then some electromagnetic corrections, such as the exact Coulomb exchange (no Slater approximation), the finite size correction, the vacuum polarization, the electromagnetic spin-orbit and, at last, the mass difference between nucleons. We will evaluate which terms are significant and which ones are negligible for our scope.

2.1 Isospin-Symmetry Breaking in nuclear Hamiltonian

We distinguish two kinds of ISB nuclear interactions: the one that breaks charge independence (CIB) and the one that breaks charge symmetry (CSB). CIB forces mean that $v_{np} \neq \frac{1}{2}(v_{nn} + v_{pp})$, while CSB forces mean that $v_{nn} \neq v_{pp}$. In fact, experiments show that v_{nn} is about 1% stronger than v_{pp}, and v_{np} is about 2.5% stronger than the average of v_{nn} and v_{pp} [12].

We add to the standard Skyrme interaction (Eq. (1.6)) the following CIB and CSB potentials, defined in an analogous form:

$$v_{\mathrm{CIB}}(i,j) := \frac{1}{2}\,\tau_z(i)\tau_z(j)\,\delta(\vec{r_i} - \vec{r_j})\cdot \tag{2.1a}$$
$$\left\{u_0(1 + z_0 P_\sigma^{ij}) + \frac{1}{2}u_1(1 + z_1 P_\sigma^{ij})(k^2 + k'^2) + u_2(1 + z_2 P_\sigma^{ij})\vec{k'}\cdot\vec{k}\right\}$$

$$v_{\mathrm{CSB}}(i,j) := \frac{1}{4}\,[\tau_z(i) + \tau_z(j)]\,\delta(\vec{r_i} - \vec{r_j})\cdot \tag{2.1b}$$
$$\left\{s_0(1 + y_0 P_\sigma^{ij}) + \frac{1}{2}s_1(1 + y_1 P_\sigma^{ij})(k^2 + k'^2) + s_2(1 + y_2 P_\sigma^{ij})\vec{k'}\cdot\vec{k}\right\}$$

where $u_{0,1,2}$, $z_{0,1,2}$, $s_{0,1,2}$ and $y_{0,1,2}$ are free parameters, which one can find with a fit to experimental data. We remind that $\tau_z = 1(-1)$ for neutrons (protons). The first terms in Eqs. (2.1) are central forces, as they depend on spatial coordinates only, while the others depend on the momenta.

The energy densities associated to these interactions are the following (the detailed calculations can be found in the Appendix A):

$$
\begin{aligned}
\mathcal{H}_{\mathrm{CSB}} =& \frac{s_0}{8}(1-y_0)(\rho_n^2-\rho_p^2) \\
&+ \frac{3}{64}\{-s_1(1-y_1)+s_2(1+y_2)\}(\rho_n\nabla^2\rho_n-\rho_p\nabla^2\rho_p) \\
&+ \frac{1}{16}\{s_1(1-y_1)+3s_2(1+y_2)\}(\rho_n\tau_n-\rho_p\tau_p) \\
&+ \frac{1}{32}\{s_1(1-y_1)-s_2(1+y_2)\}(J_n^2-J_p^2)
\end{aligned} \tag{2.2a}
$$

$$
\begin{aligned}
\mathcal{H}_{\mathrm{CIB}} =& \frac{u_0}{8}[(1-z_0)(\rho_n^2+\rho_p^2)-2(2+z_0)\rho_n\rho_p] \\
&+ \frac{3}{64}\{-u_1(1-z_1)+u_2(1+z_2)\}(\rho_n\nabla^2\rho_n+\rho_p\nabla^2\rho_p) \\
&+ \frac{1}{64}\{3u_1(2+z_1)-u_2(2+z_2)\}(\rho_n\nabla^2\rho_p+\rho_p\nabla^2\rho_n) \\
&+ \frac{1}{16}\{u_1(1-z_1)+3u_2(1+z_2)\}(\rho_n\tau_n+\rho_p\tau_p) \\
&- \frac{1}{16}\{u_1(2+z_1)+u_2(2+z_2)\}(\rho_p\tau_n+\rho_n\tau_p) \\
&+ \frac{1}{32}\{u_1(1-2z_1)-u_2(1+2z_2)\}(J_n^2+J_p^2) \\
&+ \frac{1}{32}\{u_1z_1+u_2z_2\}J^2
\end{aligned} \tag{2.2b}
$$

From the definitions of the effective mass, the mean field and the spin-orbit:

$$
\begin{cases}
\dfrac{\hbar^2}{2m_q^\star} := \dfrac{\delta\mathcal{H}}{\delta\tau_q} \\
U_q := \dfrac{\delta\mathcal{H}}{\delta\rho_q} = \dfrac{\partial\mathcal{H}}{\partial\rho_q} - \vec{\nabla}\cdot\dfrac{\partial\mathcal{H}}{\partial(\vec{\nabla}\rho_q)} + \nabla^2\dfrac{\partial\mathcal{H}}{\partial(\nabla^2\rho_q)} \\
\vec{W}_q := \dfrac{\delta\mathcal{H}}{\delta\vec{J}_q}
\end{cases} \tag{2.3}
$$

we can find now the contribution of the ISB interactions:

$$\frac{\hbar^2}{2m_q^\star} = \frac{1}{16}\{u_1(1-z_1)+3u_2(1+z_2)\}\rho_q - \frac{1}{16}\{u_1(2+z_1)+u_2(2+z_2)\}\rho_{q'} + \frac{1}{16}\{\pm s_1(1-y_1)\pm 3s_2(1+y_2)\}\rho_q \tag{2.4a}$$

$$\begin{aligned} U_q = {} & \frac{u_0}{4}\{(1-z_0)\rho_q-(2+z_0)\rho_{q'}\}\pm\frac{s_0}{4}(1-y_0)\rho_q \\ & \frac{3}{32}\{-u_1(1-z_1)+u_2(1+z_2)\}\nabla^2\rho_q+\frac{1}{32}\{3u_1(2+z_1)-u_2(2+z_2)\}\nabla^2\rho_{q'} \\ & +\frac{1}{16}\{u_1(1-z_1)+3u_2(1+z_2)\}\tau_q-\frac{1}{16}\{u_1(2+z_1)+u_2(2+z_2)\}\tau_{q'} \\ & +\frac{3}{32}\{\mp s_1(1-y_1)\pm s_2(1+y_2)\}\nabla^2\rho_q+\frac{1}{16}\{\pm s_1(1-y_1)\pm 3s_2(1+y_2)\}\tau_q \end{aligned} \tag{2.4b}$$

$$\begin{aligned} \vec{W}_q = {} & \frac{1}{16}\{u_1(1-z_1)-u_2(1+z_2)\}\vec{J}_q+\frac{1}{16}\{u_1z_1+u_2z_2\}\vec{J}_{q'} \\ & +\frac{1}{16}\{\pm s_1(1-y_1)\mp s_2(1+y_2)\}\vec{J}_q \end{aligned} \tag{2.4c}$$

where the first (second) sign is for neutrons (protons) and $q \neq q'$ label different particles.

We add these corrections to Eq. (1.15) and we will discuss some results in Sec. 2.5.

2.2 Exact Coulomb exchange

The standard treatment of Coulomb exchange term is the *Slater approximation* [8], which makes it local and easy to compute. In this procedure one approximates exchange potential to that of a free particle gas with the same charge density. This approximation is reasonable for the description of nuclear masses but becomes insufficient for the description of the Mirror Displacement Energy and other observables where small corrections due to ISB are important. For that reason, we will explain here how we correct for such an effect.

The Slater and the exact exchange potentials are:

$$\begin{cases} U_{ex}^{\text{Slater}}\phi_i(\vec{r}) &= -e^2\left(\frac{3}{\pi}\right)^{1/3}\rho_{\text{ch}}^{1/3}\phi_i(\vec{r}) \\ U_{ex}^{\text{Exact}}\phi_i(\vec{r}) &= -e^2\sum_j\int \mathrm{d}^3r'\frac{\phi_j^\star(\vec{r'})\phi_j(\vec{r})}{|\vec{r}-\vec{r'}|}\phi_i(\vec{r'}) \end{cases} \tag{2.5}$$

The Slater approximation solutions are reasonable for most of low-energy nuclear physics studies, as they well reproduce the density of the nucleus and the total binding energy (with a precision around 3-6% [13] with respect to the exact value of the Coulomb exchange). So we can treat the exchange potential in a pertubative way. This means to solve Hartree-Fock equations within the Slater approximation and then correct the protons energy levels like:

$$\tilde{\epsilon}_i = \epsilon_i + \int \mathrm{d}^3r\,\phi_i^\star(\vec{r})[U_{ex}^{\text{Exact}} - U_{ex}^{\text{Slater}}]\phi_i(\vec{r}) \tag{2.6}$$

and we sum them like in Eq. (1.12). In this case no Coulomb rearrangement term is needed.

Knowing that the wave function can be written in spherical symmetry as Eq. (1.13), and knowing that the Coulomb interaction can be decomposed as a sum of spherical harmonics like

$$\frac{e^2}{|\vec{r}-\vec{r'}|} = e^2\sum_{lm}\frac{4\pi}{2l+1}\mathcal{Y}_{lm}^\star(\Omega')\mathcal{Y}_{lm}(\Omega)\frac{r_<^l}{r_>^{l+1}} \tag{2.7}$$

where $r_{<(>)}$ is the lowest (greatest) between r and r', and also with the properties of the spherical harmonics, we find that the first term in the integral (2.6) is [14]:

$$\begin{aligned}\int \mathrm{d}^3r\,\phi_i^\star(\vec{r})U_{ex}^{\text{Exact}}\phi_i(\vec{r}) = -e^2\sum_{l\,l_j}\frac{\left\langle l_i\tfrac{1}{2}l0\middle|l_j\tfrac{1}{2}\right\rangle^2}{2l_j+1}\Big[\int_0^\infty \mathrm{d}r\int_0^r dr'\,\frac{r'^l}{r^{l+1}} \\ + \int_0^\infty \mathrm{d}r'\int_0^{r'}\mathrm{d}r\,\frac{r^l}{r'^{l+1}}\Big]R_i^\star(r)R_j^\star(r')R_j(r)R_i(r')\end{aligned} \tag{2.8}$$

where $\left\langle l_i\frac{1}{2}l0\middle|l_j\frac{1}{2}\right\rangle$ is a Clebsh-Gordan coefficient.

For the exact Coulomb exchange correction, we do not have an expression for the contribution to the energy density $\mathcal{H}$. So we just add the perturbation calculated with the sum of eigenvalues $\Delta E = E_{Exact} - E_{Slater}$ to the integral of the energy density in Eq. (1.7), in order to find consistent results between the energy calculated by using Eq. (1.12) and the direct integration of $\mathcal{H}$.

2.3 Finite proton size

In Hartree-Fock theory nucleons are treated as point-like particles. This means that the square modulus of the eigenfunctions gives the probability density to find point-like charges. In fact, they have a finite dimension, and an inner structure. We are interested to find a better approximation of the charge distribution, and to use that to calculate the Coulomb energy.

We define the *charge density* as the convolution product between the protons density and an effective electromagnetic factor form G for protons:

$$\rho_{\mathrm{ch}}(\vec{r}) := \int \mathrm{d}^3 x\, G(\vec{r}-\vec{x})\rho_p(\vec{x}) \tag{2.9}$$

One should in principle consider also the electromagnetic form factor of neutrons, since neutrons have finite size too, and so they have a charge distribution, as it is shown in Ref. [15], yet we neglect their contribution beacause it is small for our purposes.

We chose a gaussian form factor G with width $\mu = 0.65\,\mathrm{fm}$, which represents the finite size of the particles, and an amplitude such that it is normalized. Once we find ρ_{ch}, we just substitute it in the Coulomb potential 1.10, and we obtain the total electromagnetic energy:

$$E_C = \frac{e^2}{2}\int \frac{\rho_p(\vec{r'})\rho_{\mathrm{ch}}(\vec{r})}{|\vec{r}-\vec{r'}|}\mathrm{d}^3 r' \mathrm{d}^3 r - \frac{3}{4}e^2\left(\frac{3}{\pi}\right)^{1/3}\int \rho_{\mathrm{ch}}^{1/3}(\vec{r})\rho_p(\vec{r})\mathrm{d}^3 r \tag{2.10}$$

For a distribution of charge ρ_{ch} the right expression for the Coulomb energy would be like Eq. (2.10) with ρ_{p} substituted by ρ_{ch}. But Hartree-Fock states are single-particle eigenstates, and this implies that, by integrating Hartree-Fock equations, we obtain Eq. (2.10), since $\rho_{\mathrm{p}}(\vec{r}) = \sum_{i\vec{\sigma}} |\phi_{\mathrm{p}i}(\vec{r},\vec{\sigma})|^2$ (see Eq. (1.8)). So we decide to solve Hartree-Fock equations in a perturbative way: once we calculate ρ_{ch}, we substitute ρ_{p} with ρ_{ch} in Eq. (2.10), and then we correct the total binding energy (Eq. (1.12)) by adding the difference $\Delta E_{FS} = E_C(\rho_{\mathrm{ch}},\rho_{\mathrm{ch}}) - E_C(\rho_{\mathrm{p}},\rho_{\mathrm{ch}})$.

Table 2.1: The table shows how the binding energy of ^{40}Ca and ^{208}Pb changes applying the Finite Size correction. The results are obtained by subtituting the indicated densities in Eq. (2.10)

	$\rho_p\,\rho_p$	$\rho_p\,\rho_{ch}$	$\rho_{ch}\,\rho_{ch}$
^{40}Ca	-344.306	-345.188	-345.949
^{208}Pb	-1635.984	-1639.709	-1643.170

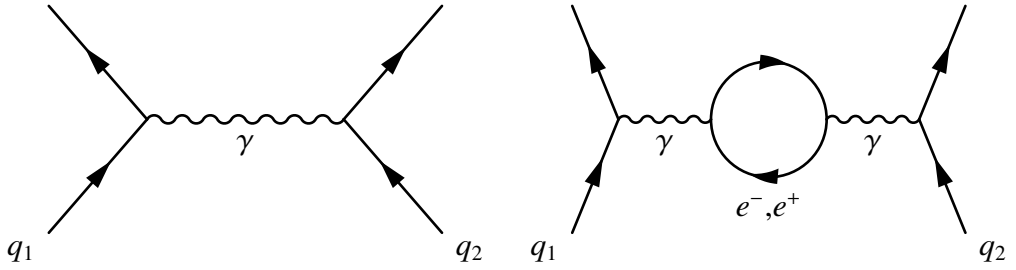

Figure 2.1: The direct electromagnetic interaction between protons is mediate by the exchange of a photon (left). But there is the possibility for a couple of electron-positron to be created and to contribute to the total interaction in second order of approximation (right).

Tab. 2.1 shows few examples of how binding energy (in MeV) changes with this correction, calculated by using Skyrme SLy4 [7] interaction between $\rho_p\,\rho_p$, $\rho_p\,\rho_{ch}$, $\rho_{ch}\,\rho_{ch}$ in Eq. (2.10).

2.4 Vacuum Polarization

Another correction to the electromagnetic interaction between protons is the vacuum polarization, that is the effect of quantum fluctuations in the vacuum.

The direct (or first order) interaction happens just through the exchange of a photon between the particles (see Fig. 2.1 on the left). But one should consider also the perturbation due to the creation of a couple of virtual particle-antiparticle which mediates the interaction (Fig. 2.1 on the right) and contributes in the second order in the fine structure constant. These virtual particles are usually electrons and positrons, since they are the lightest charged elementary particles, so the most probable to be created. This is a virtual process: energy is not conserved, but this is allowed if the particles live for a very short time, according to the uncertanty relation $\Delta t \Delta E \geq \hbar/2$.

Fullerton and Rinker [16] showed that the perturbation to the Coulomb potential in Eq. (1.10) due to the vacuum polarization is given by the potential [1]:

$$V_{\mathrm{VP}}(\vec{r}) = \frac{2\alpha e^2}{3\pi} \int \mathrm{d}^3 r' \frac{\rho_{\mathrm{ch}}(\vec{r}')}{|\vec{r} - \vec{r}'|} K_1\Big(\frac{2}{\lambda\!\!\!^{-}_e} |\vec{r} - \vec{r}'|\Big) \tag{2.11}$$

where

$$K_1(x) := \int_1^{+\infty} \mathrm{d}t\, e^{-xt} \Big(\frac{1}{t^2} + \frac{1}{2t^4}\Big) \sqrt{t^2 - 1} \tag{2.12}$$

[1] Actually they wrote it with opposite sign, since they considered electrons as interacting particles in their work, not protons.

and $\lambda\!\!\!^{-}_e = \hbar/m_e c$ is the reduced electron Compton wavelength, and α is the electromagnetic fine structure constant. As we see, the perturbation is always positive, so it gives a repulsive contribution to the interaction.

For a spherically symmetric system, the angular integral can be performed and the potential (2.11) becomes:

$$V_{\rm VP}(\vec{r}) = \frac{2\alpha e^2 \lambda\!\!\!^{-}_e}{r} \int_0^{+\infty} \mathrm{d}r' r' \rho_{\rm ch}(r') \Big[K_0\Big(\frac{2}{\lambda\!\!\!^{-}_e}|r - r'|\Big) - K_0\Big(\frac{2}{\lambda\!\!\!^{-}_e}|r + r'|\Big)\Big] \tag{2.13}$$

with

$$K_0(x) := \int \mathrm{d}x K_1(x) = \int_1^{+\infty} \mathrm{d}t\, e^{-xt}\Big(\frac{1}{t^3} + \frac{1}{2t^5}\Big)\sqrt{t^2 - 1} \tag{2.14}$$

We decide to neglet higher order terms (that are smaller, since they are proportional to higher powers of the fine-structure constant), and we add this correction to the Coulomb potential (Eq. (1.10)). Within our code, we stop the integration in Eq. (2.14) when $t \simeq 1.5/x$, as a compromise between accuracy and computational time [2].

2.5 Results

Binding Energy

Now we show in Tab. 2.2 the binding energy calculated with the sum of eigenvalues (Eq. (1.12)), for some nuclei. We choose a SLy4 interaction and doubly magic nuclei, as they are spherical.

Concerning the Isospin Symmetry Breaking terms in nuclear Hamiltonian, we used some values for the free parameters u_0, s_0, z_0, y_0 (see the caption of the table) not far from what we found in [17, 18]. We did not find any examples for the other parameters in literature, so we chose random values for them, just to verify the good implementation of the code. One may better use fitted values, as we will discuss later, in Chapter 3. We see that the binding energy become lower in modulus, so it has a repulsive effect, in general.

Instead, the finite size correction has an actractive effect, in fact considering finite size protons implies a lower electrostatic repulsion than point-like particles.

The vacuum polarization has a repulsive effect. It is a small perturbation which contributes about $\approx 0.4\%$ on the total Coulomb energy, even less than the finite size ($\approx 0.8\%$).

[2] We estimate that from $t \simeq 5/x$ to $t \simeq 1.5/x$ we make an error of about 1% on the contribution of the vacuum polarization to the total binding energy, but the computational time becomes 5 times smaller.

Table 2.2: Binding energy (in MeV) calculated for some nuclei, with SLy4 interaction, with each corrections discussed in this chapter, separately. The ISB parameters used are: $u_0 = 20,\ s_0 = -20,\ u_1 = u_2 = 5,\ s_1 = s_2 = -5,\ z_0 = z_1 = y_0 = y_1 = -1,\ z_2 = y_2 = 1$.

	no corrections	nuclear ISB	Finite Size	Vacuum Polarization	Exact Coulomb Exchange
^{16}O	−128.515	−126.240	−129.022	−128.426	−129.683
^{40}Ca	−344.306	−337.550	−345.948	−343.900	−347.188
^{48}Ca	−417.968	−413.706	−419.538	−417.569	−420.822
^{56}Ni	−483.432	−472.908	−485.994	−482.718	−487.537
^{132}Sn	−1103.728	−1097.039	−1107.888	−1102.048	−1110.655
^{208}Pb	−1635.984	−1622.755	−1643.164	−1632.333	−1647.242

A more significant correction is the exact treatment of Coulomb exchange (about $\approx$ 1.5% on the Coulomb energy), which makes nuclei more bound. We find that the new eigenvalues $\tilde{\epsilon}_i$ for ^{208}Pb are the same of those in Ref. [14], where *Roca-Maza et al.* did the same calculations.

Displacement Energy

We would like to estimate the contribution of each of the corrections discussed in this chapter to the Displacement Energy (DE). The DE is defined as the difference in energy between two adjacent states that belong to the same isospin multiplet.

We consider the nucleus ^{48}Ca, whose total experimental DE is 7.175 ± 0.015 MeV [1]. The Coulomb contribution to the DE can be calculated; the direct and the exchange part are [19]:

$$\begin{cases} DE_{direct} = \dfrac{e^2}{N-Z} \displaystyle\iint \mathrm{d}^3 r \mathrm{d}^3 r' \frac{\rho_p(\vec{r})(\rho_n(\vec{r'}) - \rho_p(\vec{r'}))}{|\vec{r} - \vec{r'}|} \\ DE_{exch} = -900 \dfrac{Z}{A}\,\mathrm{keV} \end{cases} \tag{2.15}$$

that, for ^{48}Ca, give respectively 7.272 MeV − 0.375 MeV = 6.897 MeV, which is about $\sim$ 96% of the experimental value. The remaining 4% should be given by the contribution of all the other ISB correction.

For a nucleus of atomic number Z, one can do a rough estimation of these contributions if one calculates the difference of the binding energies of the ground state of $Z+1$ and Z, using each of these corrections separetely. Then one subtructs the same difference of energy calculated without any corrections.

Table 2.3: Estimation ΔE of the contribution of different corrections to the Displacement Energy compared to the calculated DE.

	no corrections	nuclear ISB	Finite Size	Vacuum Polarization	Exact Coulomb Exchange
^{48}Ca	−417.968	−413.706	−419.538	−417.569	−420.822
^{48}Sc	−417.340	−412.098	−419.031	−416.905	−420.202
E_{Sc}-E_{Ca}	0.628	1.608	0.507	0.664	0.620
ΔE	0	0.980	−0.121	0.032	−0.008
DE		0.954	−0.100	0.047	

The estimated ΔE are shown in Tab. 2.3; they are compared to the calculated DE, and we see that they are compatible. The DE are obtained using approximated formulae described by *Auerbach et al.* [19] for the Vacuum Polarization and the Finite Proton Size corrections only ($DE_{VP} = 8.5\frac{Z}{A^{1/3}}$ keV and $DE_{FP} \simeq -100$ keV). The Exact Coulomb Exchange correction gives a contribution that seems it may be neglected, because much lower than the total Coulomb Exchange DE (2.15), or lower than the other corrections. Actually, in Ref. [17] *Roca-Maza et al.* show that it is not so negligible for the description of some observables, but it is still important. We calculated the contribution for the ISB interaction exactly, as described in detail in Appendix B. Its expression is:

$$
\begin{aligned}
DE_{CSB} = \int & -\frac{s_0}{8T_0}(1-y_0)(\rho_n^2-\rho_p^2) \\
& +\frac{3}{64T_0}\{s_1(1-y_1)-s_2(1+y_2)\}(\rho_n\nabla^2\rho_n-\rho_p\nabla^2\rho_p) \\
& -\frac{1}{16T_0}\{s_1(1-y_1)+3s_2(1+y_2)\}(\rho_n\tau_n-\rho_p\tau_p) \\
& -\frac{1}{32T_0}\{s_1(1-y_1)-s_2(1+y_2)\}(J_n^2-J_p^2) \\
DE_{CIB} = \int & -\frac{u_0}{4T_0}(1-z_0)(\rho_n-\rho_p)^2 \\
& +\frac{3}{32T_0}\{u_1(1-z_1)-u_2(1+z_2)\}(\rho_n\nabla^2\rho_n+\rho_p\nabla^2\rho_p-\rho_n\nabla^2\rho_p-\rho_p\nabla^2\rho_n) \\
& -\frac{1}{8T_0}\{u_1(1-z_1)+3u_2(1+z_2)\}(\rho_n\tau_n+\rho_p\tau_p-\rho_p\tau_n-\rho_n\tau_p) \\
& -\frac{1}{8T_0}\{u_1(1+2z_1)-u_2(1+2z_2)\}(J_n^2+J_p^2-\frac{1}{2}J^2)
\end{aligned}
$$

The sum of the different contributions to the DE is not equal to the experimen-

tal measure, since we used random values for the parameters of ISB interaction for checking purposes. One must fit the DE of some nuclei to find the best values for them. Actually, we prefer to fit the Mirror Displacement Energy, as explained in the next chapter.

In this work we neglected two small effects which depends on isospin too. The proton-neutron mass difference contributes with just ≈ 200 keV on the binding energy of ^{208}Pb (much less than the other effects discussed above) and with few tens of keV ($\approx 30 - 40$ keV) on the Displacement Energy [17, 2]. The electromagnetic spin-orbit contributes with about the 1% of the nuclear spin-orbit splitting [2], and its contribution on the Displacement Energy is about ≈ 10 keV only.

Chapter 3

Fitting the nuclear energies

In this chapter we discuss the procedure we follow to find the values for the free parameters of the ISB interaction proposed, which best reproduce both the nuclear binding energies BE and the Mirror Displacement Energies (MDE) of some selected nuclei.

In the previous chapter we explained that the difference in energy between the theoretical and experimental Isobaric Analogue States cannot be described without the introduction of some interactions which depend on the isospin. So we decide to fit the energy difference between mirror nuclei (they belong to the same isospin multiplet in their ground states) by varying the parameters of our interaction, previously discussed.

First of all we need to select the couples of mirror nuclei to fit. We look for them in *AME2016* [20] and in *National Nuclear Data Center* of *Brookhaven Laboratory* [21]. They necessarily have to be even-even and spherical, so that we can use our code, then we select only nuclei with deformation parameter $\beta < 0.1$. We also chose those with separation energies $S_n, S_p > 1$ MeV, so that their single-particle levels are far enough from the continuum. Eventually we find 12 couples of mirror nuclei (see next section). Most of them are open-shell nuclei, that means we need to add also a pairing interaction (see Sec. 1.3).

For the fit we use `minuit` [22], a program that minimizes a function by varying the free parameters with a *gradient* method. It means it needs to know a starting value for them and a small interval to calculate the derivative of that function, and then it searches for the minimum by following the direction of the gradient. This method may, in principle, find a relative minimum, but we suppose to find the absolute one with a good guess for the starting values.

The function we chose to minimize is the *reduced χ squared*:

$$\tilde{\chi}^2 := \frac{1}{N_{exp} - N_{par} - 1} \sum_{i=1}^{N_{exp}} \frac{(E^i_{exp} - E^i_{teo})^2}{\sigma^2} \tag{3.1}$$

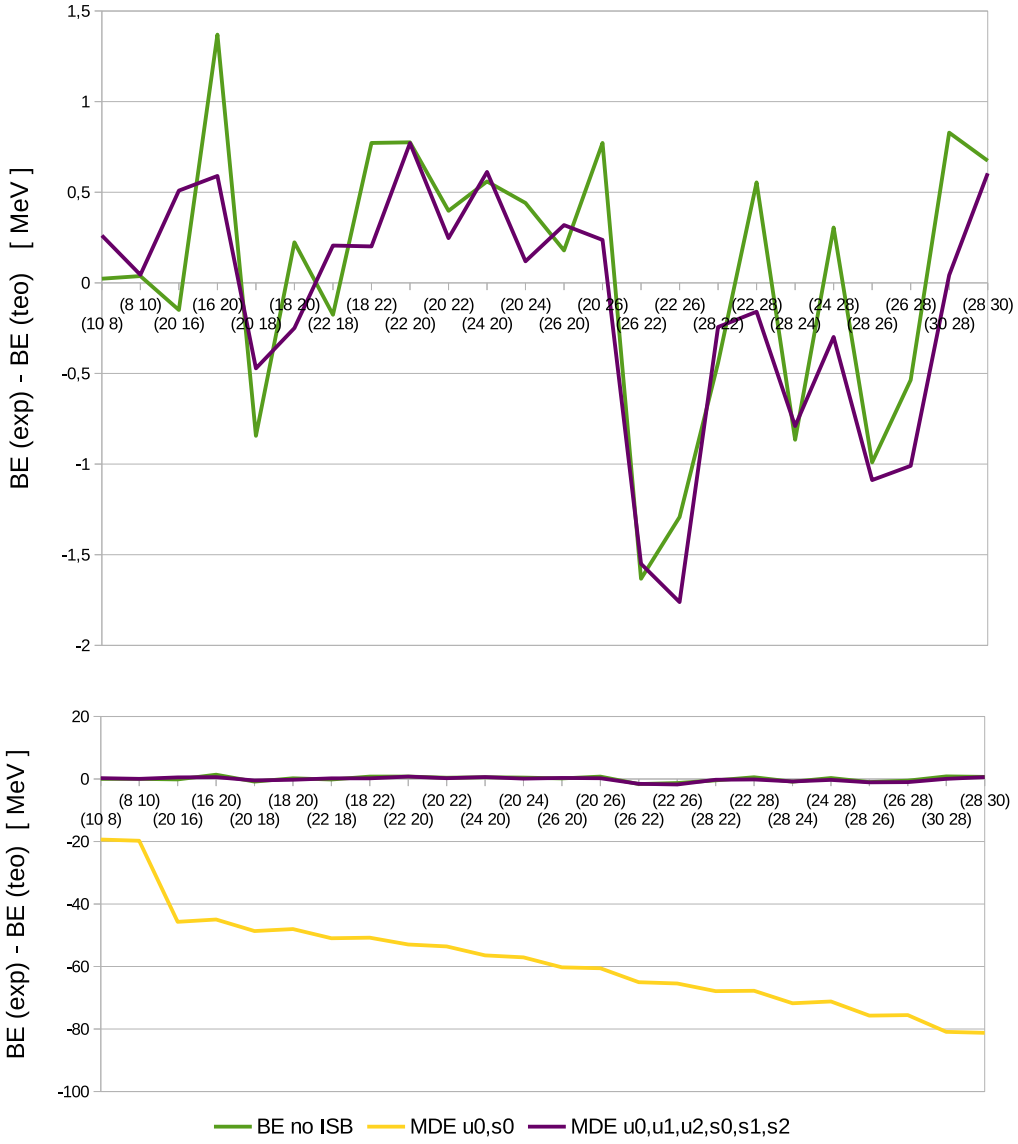

Figure 3.1: Difference between experimental and theoretical binding energies, using a set of interaction parameters fitted to the Binding Energies without nuclear ISB interactions (green line), a set fitted to the Mirror Displacement Energies including the first terms of nuclear ISB interactions, depending on u_0, s_0 only (yellow line), and at last including all ISB interactions (violet line). Nuclei are written as (N,Z) on the x-axis. In the upper figure we used a smaller scale, so that yellow line is not visible. See Tab. 3.2 for the parameters used.

where N_{exp} and N_{par} are the experimental data number and the free parameters number, E^i_{exp} and E^i_{teo} are the experimental measures and the theoretical results, and $\sigma^2 = \sigma^2_{exp} + \sigma^2_{teo}$ is the squared sum of experimental and theoretical uncertanties (we chose $\sigma_{teo} = 1$ MeV for the binding energies and $\sigma_{teo} = 2$ MeV for the MDE).

We proceed in this way: firstly, we fit all the binding energies by varying the parameters of the standard Skyrme interaction (Eq. (1.6)), while the ISB nuclear interactions are turned off (Eqs. (2.1)). Then we will turn these on, and, by varying their parameters, we will fit the MDE. This procedure is based upon the assumption that ISB interactions do not contribute significantly to the total binding energy. If we find not good enough total binding energies, then we repeat the fit with ISB turned on, until both binding energies end energy differences are substantially improved.

3.1 Results

First of all, we fit the binding energies BE of the selected nuclei, by varying the parameters of the interactions that conserve isospin symmetry, which are t_0, t_1, t_2, t_3, $x_0, x_1, x_2, x_3, W_0, W'_0, \alpha$ (see Eq. (1.6)), while the pairing constants $V_0 = 680\,\text{MeV fm}^3$ and $\gamma = 1$ are fixed to reasonable values. We turn on the electromagnetic corrections discussed in the previous chapter, but we keep the nuclear ISB interaction switched off. The BE obtained are shown in Fig. 3.1, while the MDE are shown in Fig. 3.2 (green lines).

Then, we fix the parameters found, we add the ISB interaction parameters u_0, s_0, z_0, y_0 only (see Eq. (2.1)), and we fit the MDE. We include only these parameters for now, to see if they alone fit the MDE well enough or not. In fact they improve the MDE, as shown in Fig. 3.2 (yellow line), but the BE becomes much worse now (Fig. 3.1). So, we add all the ISB parameters to fit the MDE and we obtain improvements both in MDE and BE (violet lines).

We summarise the values of the parameters obtained with the three fits in

Table 3.1: Root mean square errors of Binding Energy and Mirror Displacement Energy for the results of the fits, that are made with no Isospin Symmetry Breaking interactions, with u_0, s_0 ISB parameters only (related to central forces) and with the complete set of ISB parameters.

	fit BE (no ISB)	fit MDE (u_0, s_0)	fit MDE ($u_0, u_1, u_2, s_0, s_1, s_2$)
BE	0.760	61.389	0.695
MDE	0.829	0.490	0.336

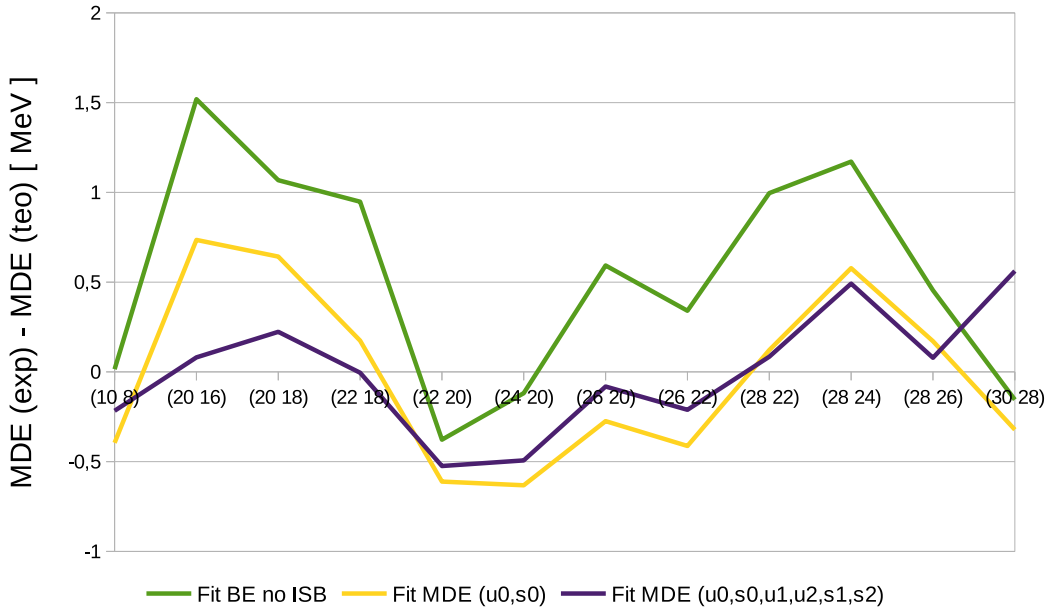

Figure 3.2: Difference between experimental and theoretical Mirror Displacement Energies, using three sets of interaction parameters (see Tab. 3.2)

Tab. 3.2, and the root mean square errors of BE and MDE (expressed in MeV) in Tab. 3.1. We conclude that the last fit is the best that reproduces both the Binding Energies and the Mirror Displacement Energies.

Pairing

In all these fits we kept the pairing intensity fixed to $V_0 = 680$ MeV fm^3 (see Eq. (1.17)). We wonder if there may be a better value for that. That means we look for a value which reproduces the pairing gap better. As explained in Chap. 1.3, the pairing gap Δ can be calculated self-consistently through the BCS equations (already implemented in our program), and it can be estimated experimentally with the three-point formula:

$$\Delta_q^{(3)}(N_0) := \frac{\pi_{N_0}}{2}\Big[E(N_0-1) - 2E(N_0) + E(N_0+1)\Big] \tag{3.2}$$

According to Ref. [23], for even nuclei it is better to calculate $\Delta(N+1)$, that means centering the three-point formula on the next odd nucleus. This because $\Delta(N)$ contains not only information about pairing gap, but also a contribution related to the splitting of single-particle levels.

We consider some isotopes and isotones chains, which our mirror nuclei belong to, and we shall see how the pairing gap changes with the pairing intensity

Table 3.2: Results of the fit of the binding energies and the fit of mirror displacement energies. For the MDE we fixed the parameters of the interactions which conserve isospin symmetry (found in the first fit). The pairing parameter is fixed to $V = 680$ MeV every times.

	fit BE	fit MDE 1	fit MDE 2
t_0 [MeV fm^3]	−2463	−2463	−2463
t_1 [MeV fm^5]	401	401	401
t_2 [MeV fm^5]	−615	−615	−615
t_3 [MeV fm$^{3\alpha+3}$]	13 700	13 700	13 700
x_0	1.483	1.483	1.483
x_1	−0.485	−0.485	−0.485
x_2	−0.999	−0.999	−0.999
x_3	2.336	2.336	2.336
α	0.154	0.154	0.154
W_0 [MeV fm^5]	95.5	95.5	95.5
W'_0 [MeV fm^5]	147.9	147.9	147.9
u_0 [MeV fm^3]	0	57.39	−6.74
s_0 [MeV fm^3]	0	−14.21	−32.98
z_0	0	−2.089	−0.826
y_0	0	−0.421	−0.994
u_1 [MeV fm^5]	0	0	3.83
u_2 [MeV fm^5]	0	0	2.37
s_1 [MeV fm^5]	0	0	3.65
s_2 [MeV fm^5]	0	0	16.31
z_1	0	0	−0.412
z_2	0	0	1.161
y_1	0	0	−1.164
y_2	0	0	1.010

within the shells (we fixed all the other interaction parameters found with the third fit). We realize that in general we should increase V_0, as shown in Figs. 3.3 3.4. We conclude that $V_0 = 680$ MeV fm^3 is good enough to describe light even-even nuclei paring gaps ($Z, N = 8$ chains), but we need $V_0 = 800$ MeV fm^3 for most of the other nuclei, and even $V_0 = 1000$ MeV fm^3 for $(Z, N) = (28, 30)$.

We expect that this increase (of about $\approx 15 - 30\%$) of the pairing intensity will not change the total binding energies too much, because pairing contributes with about $\approx 1 - 2$ MeV to the binding energy. Neither it should change significantly the Mirror Displacement Energies, because the MDE are differences between total binding energies. This is confirmed by Figs. 3.5. We see that BE and MDE become slightly worse only in nuclei in the middle ($A \approx 38 - 48$) in general. We give the root mean square errors (in MeV) in Tab. 3.3.

In conclusion, the third set of parameters is the best which can describe both

Table 3.3: Root mean square errors of Binding Energy and Mirror Displacement Energy for different values of pairing intensity.

	V_0 = 680 MeV fm^3	V_0 = 680 – 1000 MeV fm^3
BE	0.695	0.720
MDE	0.336	0.421

the masses and the difference of energy between mirror nuclei. And even if the pairing intensity varying between $V_0 = 680 - 1000$ MeV fm^3 gives slightly worse results for the nuclear energies than $V_0 = 680$ MeV fm^3, it is more correct, because it better reproduces the pairing gaps.

We can see now if this set of ISB parameters is good to predict the Displacement Energy of ^{48}Ca, which we discussed about at the end of the previous chapter. We show the contribution of each correction (in MeV) in Tab. 3.4.

The total DE is slightly improved from what we found with Coulomb contribution only in the previous chapter, since the discrepancy (0.250 MeV) is lower than before (0.278 MeV).

Table 3.4: Contribution of ISB corrections to the Displacement Energy for ^{48}Ca.

	Coulomb Direct	Coulomb Exchange	nuclear ISB	Finite Size	Vacuum Polarization	Total
DE	7.737	−0.375	0.116	−0.100	0.047	7.425

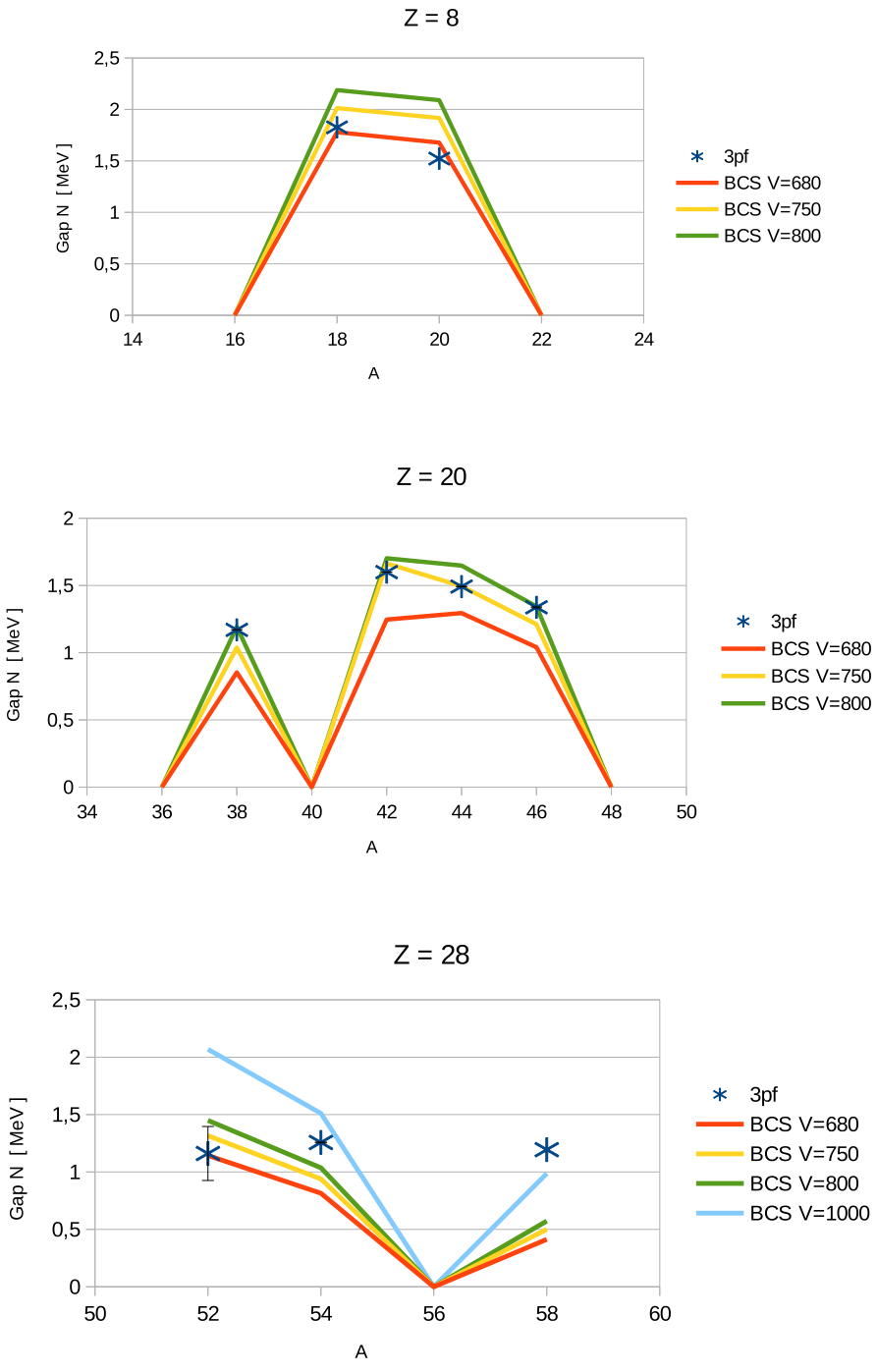

Figure 3.3: Neutronic pairing gaps for Z = 8, 20, 28 isotopic chains. We compare results obtained experimentally by the three-points formula with the BCS theoretical calculation, employing different values for pairing intensity.

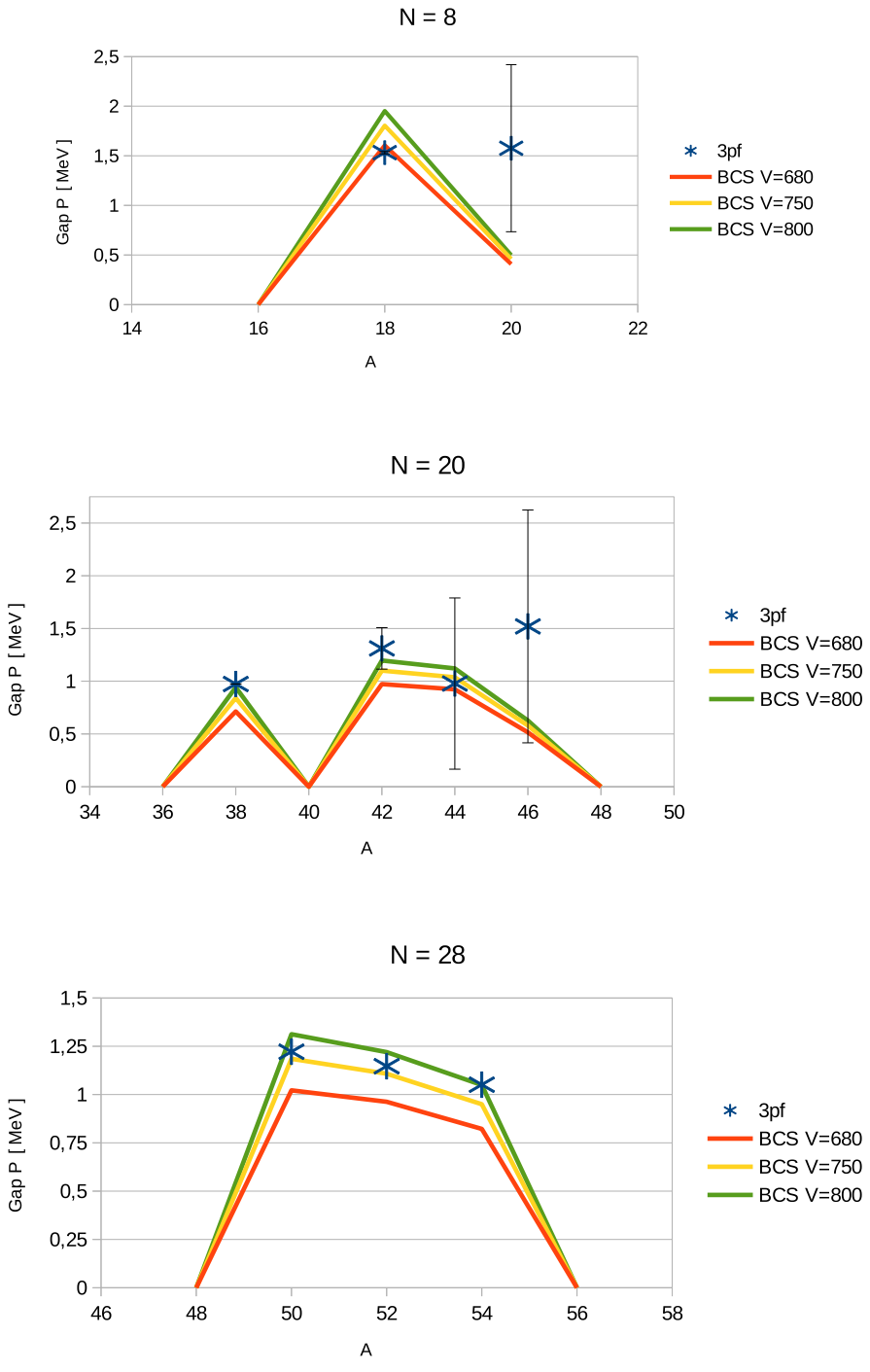

Figure 3.4: Neutronic pairing gaps for N = 8, 20, 28 isotonic chains. We compare results obtained experimentally by the three-points formula with the BCS theoretical calculation, employing different values for pairing intensity.

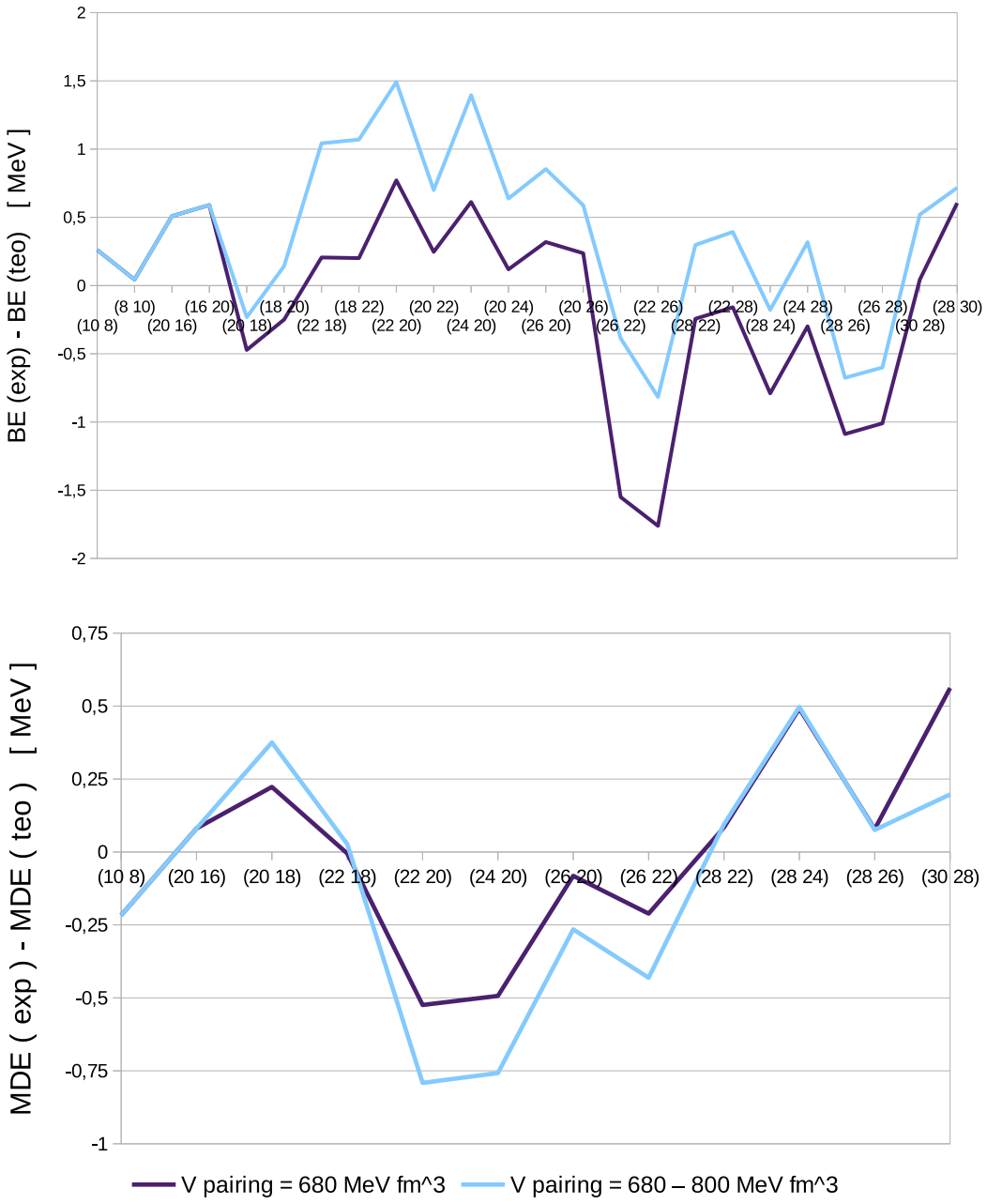

Figure 3.5: Comparison between difference of experimental and calculated Binding Energy (upper figure) and Mirror Displacement Energy (lower figure) with a pairing intensity V_0 = 680 MeV fm^3 fixed and V_0 varying between 680-1000 MeV fm^3. We fixed the interaction with all ISB parameters obtained in the last fit of Tab. 3.2.

Chapter 4

Application to the neutron stars

Neutron stars

Neutron stars are the last stage of the evolution of those stars who have a mass greater than 8 $M_\odot$ during their lifetime in main sequence, but they are not so heavy to evolve into a black hole [24]. They are the most compact stars in the universe and they are made of neutron rich matter.

When the star is in the main sequence, it produces energy through nuclear fusion reactions. While the inner temperature grows up, these reactions burn hydrogen first, then heavier and heavier elements up to produce iron, which is accumulated in the core. Iron is the most stable nucleus, since its energy per particle is the lowest; that means heavier elements can not be created by fusion reactions anymore. For a detailed description of stellar structure and evolution see Ref. [25]. The core of such a massive star, during the last stage in the main sequence, can be approximately viewed as made of an iron-group elements (Fe, Co, Ni) lattice surrounded by an electrons degenerate gas, in hydrostatic equilibrium between gravity and degeneracy pressure of electrons. When it stops burning fuel, it becomes unstable, and the hydrostatic equilibrium breaks. This happens when the core mass comes closer to the Chandrasekhar limit $M_{Ch} \simeq 1.4\, M_\odot$ [26] (that is the greatest mass which can be supported by electrons degeneracy pressure) and it has no pressure enough to balance its own weight. Then, it collapses and within seconds a powerful shock wave occurs from the core surface, which spreads though the whole star. This arises as an explosion called *supernova*, that releases the envelope of the star and a huge amount of energy (about $\approx 10^{52}$ erg) into the space. In the centre of the explosion remains the collapsed core, which is now a proto-neutron star that will cool down until the neutron star is finally formed.

During this collapse, matter reaches very high densities: in such conditions reactions of electronic capture start, while β-decay is prevented by electronic de-

generacy, so matter becomes *neutron rich*. Neutrons produce a pressure that stops the collapse of the core firstly, it produces the shock wave and then mantains the hydrostatic equilibrium within the neutron star.

Neutron stars have peculiar properties: typical values of mass ($\approx 1.4\, M_\odot$) and radius ($\approx$ 10 km) make them reach very high densities (even more than nuclear saturation density $\rho_0 \simeq 2 \cdot 10^{14}\,\mathrm{g/cm^3}$ in the centre of the star). They have extreme typical values of the rotation frequency (up to $\approx 10^3$ Hz), gravitational potential ($\phi := GM/Rc^2 \approx 0.1 - 0.2$) and magnetic field ($B \approx 10^{12} - 10^{15}\,\mathrm{G}$). At the final stage of their formation, neutron stars show temperatures $T \approx 10^8 - 10^9\,\mathrm{K} \approx 10 - 100\,\mathrm{keV}$, that can be approximated to zero because it is much less than the mean kinetic energy of the constituent neutrons (about tens of MeV); that is why neutron stars are considered cold stars.

We do not know much about the behaviour of matter in such extreme conditions, that are impossible to reproduce in a laboratory. That is why all we know about the inner structure of these stars depends on some models. Yet neutron stars are really interesting objects, because from the observations we are able, in some cases, to extract information about nuclear properties, and to test the validity of theoretical models up to some extent [27, 28].

Hydrostatic equilibrium

The inner structure of a neutron star is quite complex: there is a thin atmosphere ($\approx$ 10 cm thick), then an outer crust ($\approx$ 100 m) where density varies between almost 7 orders of magnitude ($10^4 - 10^{11}$ g/cm^3). In this region matter is constituted by a lattice of nuclei embedded in a relativistic electron gas. The lattice is made of iron ^{56}Fe near the atmosphere, then of heavier neutron rich elements going deeper, up to ^{118}Kr [27]. The inner crust begins where density reaches the so-called *neutron drip line* $\rho \approx 10^{11}\,\mathrm{g/cm^3}$: here nuclei coexist with a gas of free neutrons and electrons. Going deeper into the star, the density become higher and higher, so that nuclei are not spherical anymore, but they are deformed by the huge pressure. This state of matter is called *pasta phase*. The outer core begins at nuclear density ($\rho \approx 10^{14}\,\mathrm{g/cm^3}$) and it contains most of the mass of the star. There are no nuclei anymore, but a homogenious gas of neutrons (and a fraction of protons and electrons) strongly interacting, which is very similar to what we know as *infinite neutron matter*. Within the inner core of the star, at last, there must be some kind of unknown matter, in fact we do not know the properties of matter in such extreme conditions of density and pressure. Theoretical models predict the exsitence of hyperons and there exist also some works based on the hypothesis of the existence of meson condensates and deconfined quarks (named strange stars).

We then understand that a neutron star is made of layers with different states of matter, so a complete work would be considering all of these states. But here

we do not aim to describe neutron stars structure in an exhaustive way. We will try to see if a simple model that considers a star made of neutron gas only, obeying to one Equation of State, is able to describe the general properties of the star, like mass and radius [27, 28].

We consider a star as a mass of gas in *hydrostatic equilibrium*, that means equilibrium between gravity and pressure. An easy calculation of newtonian hydrostatic equilibrium equations can be done by equating the weight of a thin layer of gas in spherical symmetry with the pressure that supports it. One can find [29]:

$$\begin{cases} \dfrac{\mathrm{d}P}{\mathrm{d}r} = -G\dfrac{\rho(r)M(r)}{r^2} \\ \dfrac{\mathrm{d}M}{\mathrm{d}r} = 4\pi r^2\rho(r) \end{cases} \tag{4.1}$$

Actually, we need to add some general relativity corrections to these equations, since neutron stars are very compact objects, because of its strong gravitational potential . So we use the *Tolman-Oppenheimer-Volkoff* (TOV) equations [26]:

$$\begin{cases} \dfrac{\mathrm{d}P(r)}{\mathrm{d}r} = -G\dfrac{\mathcal{H}(r)M(r)}{c^2r^2}\left[1+\dfrac{P(r)}{\mathcal{H}(r)}\right]\left[1+\dfrac{4\pi r^3P(r)}{c^2M(r)}\right]\left[1-\dfrac{2GM(r)}{c^2r}\right]^{-1} \\ \dfrac{\mathrm{d}M(r)}{\mathrm{d}r} = 4\pi r^2\dfrac{\mathcal{H}(r)}{c^2} \end{cases} \tag{4.2}$$

These are differential equations for pressure and mass radial profile. They depends on the *Equation of State* (EoS), that is the relation between pressure p and energy density $\mathcal{H}$, which depends on the microscopic model for the interaction between the constituent neutrons. Note that $\mathcal{H}$ substitutes the mass density here, according to the relativistic equality between mass and energy. We shall integrate TOV equations numerically until pressure becomes zero, to find mass and radius of the star.

We want to solve these equations for many initial (central) values of density and draw a mass vs radius curve. This is very useful and interesting, because we can compare our results with observational data (neutron stars masses can be measured very accurately). Also, we want to see the effects of the introduction of Isospin Symmetry Breaking terms discussed in this work on the masses of neutron stars.

Nuclear equation of state

In order to solve TOV equations we need an Equation of State, which describes properties of infinite matter. It depends, of course, on the interaction between particles. From the definition of pressure, we can calculate the EoS:

$$P := -\frac{\partial E}{\partial V}\Big|_A = -\frac{\partial (E/A)}{\partial (V/A)}\Big|_A = -\frac{\partial e}{\partial (1/\rho)}\Big|_A = \rho^2 \frac{\partial (\mathcal{H}/\rho)}{\partial \rho} = \rho \frac{\partial \mathcal{H}}{\partial \rho} - \mathcal{H} \tag{4.3}$$

where $e(\rho) := E/A = \mathcal{H}/\rho$ is the energy per particle. As one can see, we just need an expression for the energy density $\mathcal{H}(\rho)$.

We consider a standard Skyrme effective interaction (Eq. (1.6)). Its energy density is $\mathcal{H} = \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_{eff} + \mathcal{H}_{fin} + \mathcal{H}_3 + \mathcal{H}_{so} + \mathcal{H}_{sg}$, each term is shown in details in Ref. [7]. For infinite matter (invariant for translations) $\vec{\nabla}\rho = 0$, so $\mathcal{H}_{fin}$, $\mathcal{H}_{so}$ and $\mathcal{H}_{sg}$ are equal to zero; also we consider *pure neutron matter*, so Coulomb field is zero too, and we neglect pairing. Then remains [30]:

$$\mathcal{H}(\rho) = \frac{\hbar^2}{2m}\tau + \frac{t_0}{4}(1-x_0)\rho^2 + \frac{3}{40}[t_1(1-x_1)+3t_2(1+x_2)](3\pi^2)^{2/3}\rho^{8/3} + \frac{t_3}{24}(1-x_3)\rho^{\alpha+2} \tag{4.4}$$

Skyrme model is non-relativistic, because it is fitted to ordinary nuclei, so the kinetic density is $\tau = \frac{3}{5}k_F^2\rho$, where $k_F = (3\pi^2\rho)^{1/3}$ is the Fermi momentum (in unit of $\hbar$). Using (4.3), we find that the Equation of State is the implicit relation between $\mathcal{H}$ and P given by the system:

$$\begin{cases} \mathcal{H}(\rho) = \frac{3}{5}\frac{\hbar^2}{2m}(3\pi^2)^{2/3}\rho^{5/3} + \rho mc^2 + \frac{t_0}{4}(1-x_0)\rho^2 \\ \qquad + \frac{3}{40}[t_1(1-x_1)+3t_2(1+x_2)](3\pi^2)^{2/3}\rho^{8/3} + \frac{t_3}{24}(1-x_3)\rho^{\alpha+2} \\ P(\rho) = \frac{2}{5}\frac{\hbar^2}{2m}(3\pi^2)^{2/3}\rho^{5/3} + \frac{t_0}{4}(1-x_0)\rho^2 \\ \qquad + \frac{1}{8}[t_1(1-x_1)+3t_2(1+x_2)](3\pi^2)^{2/3}\rho^{8/3} + \frac{\alpha+1}{24}t_3(1-x_3)\rho^{\alpha+2} \end{cases} \tag{4.5}$$

where we added the mass contribution to the energy density.

Now we calculate the contribution of Isospin Symmetry Breaking interactions in the same way, and we add it to the Equation of State (4.5):

$$\begin{cases} \mathcal{H}_{ISB}(\rho) = \frac{1}{8}[u_0(1-z_0)+s_0(1-y_0)]\rho^2 \\ \qquad + \frac{3}{80}[u_1(1-z_1)+3u_2(1+z_2)+s_1(1-y_1)+3s_2(1+y_2)](3\pi^2)^{2/3}\rho^{8/3} \\ P_{ISB}(\rho) = \frac{1}{8}[u_0(1-z_0)+s_0(1-y_0)]\rho^2 \\ \qquad + \frac{1}{16}[u_1(1-z_1)+3u_2(1+z_2)+s_1(1-y_1)+3s_2(1+y_2)](3\pi^2)^{2/3}\rho^{8/3} \end{cases} \tag{4.6}$$

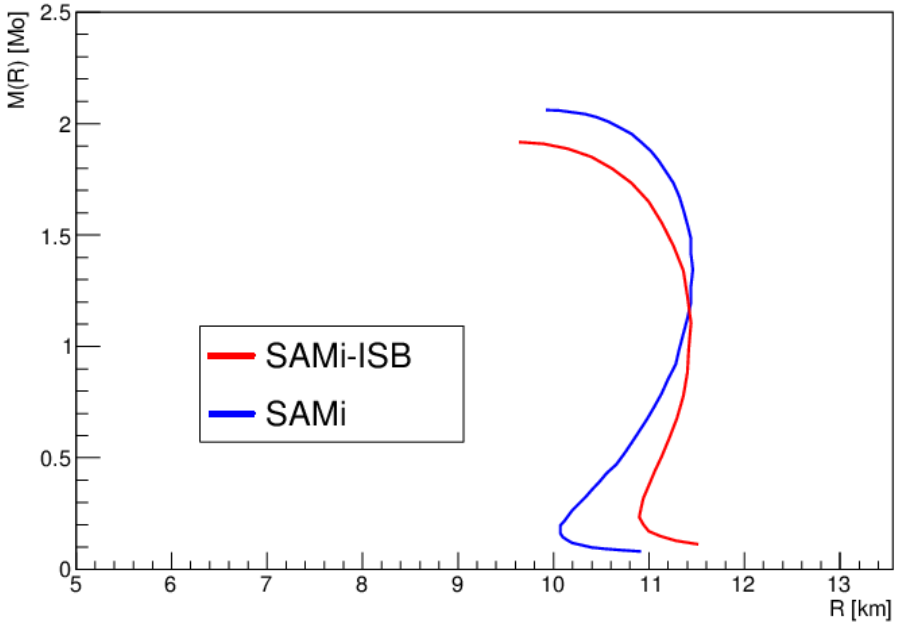

Figure 4.1: Neutron stars mass-radius curves obtained with pure neutron matter Equations of State SAMi and SAMi-ISB

There is no garancy that this EoS is good for every density, as explained in the previous paragraph. Also, Skyrme interaction is fitted to finite nuclei, at ordinary conditions. All we can do is to extrapolate this model and compare to observations when available.

Results

The interaction discussed in the previous chapter has been determined by fitting the Mirror Displacement Energy of even-even spherical nuclei with mass number $18 \leq A \leq 58$, that are not heavy nuclei, nor neutron rich nuclei. The EoS we obtain from that does not agree with all the theoretical and experimental results we have about neutron matter. So, we think that the solutions of the TOV equations for this EoS, that we omitted here, are not suitable for the study of neutron star matter. One could improve this model by fixing some constraints on the EoS of neutron matter, for example by studying the neutron skin of heavy nuclei, like ^{208}Pb.

We consider here the two interactions SAMi [31] and SAMI-ISB [17]. These have been fitted to reproduce the Isobaric Analogue State energy of ^{208}Pb, and they agree with our theoretical and empirical knowledge about the Equation of

State of neutron matter. SAMi-ISB includes ISB forces depending on u_0, s_0 only. We solved TOV equations with these EoS, as an example to show the effects of the Isospin Symmetry Breaking terms on the calculated mass and radius of neutron stars. We plot the results in Fig. 4.1. In spite of its great simplicity and its many approximations, this model reproduces the standard values of the masses ($M \simeq 1.4\, M_\odot$); also, it reaches the highest value ever measured (M=1.97±0.04 $M_\odot$ [32]) in the case of SAMi. Standard values for radii are reproduced as well ($R \simeq 10 - 12$ km). Masses can be measured very accurately when they are part of a binary system, through the measure of the revolution period. On the other hand, we still do not have direct measures of radii, but only estimations based on complicated observational analysis relying on some modelization of the star. We observe that for observed mass values (over 1 $M_\odot$), the ISB contribution in the EoS gives smaller radii.

Conclusion

In this thesis we studied forces that break isospin symmetry and their contribution to the Mirror Displacement Energy.

Aside the direct and the Slater exchange Coulomb terms, we discussed some electromagnetic corrections: the exact Coulomb exchange, the finite size correction and the vacuum polarization. Other smaller effects like the proton-neutron mass difference and the electromagnetic spin-orbit has been neglected. We also introduced some nuclear interactions that break Charge Symmetry and Charge Independence, based on Skyrme model. Recent works have already introduced ISB forces that depend on the difference of the spatial coordinates [17, 18]. We extended this model by adding momentum-dependent ISB forces. We calculated the mean potential associated to these interactions, and we added it to a standard Skyrme interaction. We then calculated the binding energies of nuclei in a Hartree-Fock scheme.

The ISB interactions depends on free parameters. We fitted them to find the best values that reproduce the Mirror Displacement Energy of even-even spherical nuclei (turning on the electromagnetic corrections discussed before). So we determined a new interaction, defined by the set of parameters shown in Tab. 3.2. The introduction of not just ISB central forces, but even momentum dependent ISB forces, seems necessary to describe both the binding energies and the MDE of the selected nuclei. We also found a good description of the pairing interaction: we found a value of the pairing strength adequate to fit the pairing gap, through comparison between the gap calculated with BCS equations and the experimental estimation with the 3-point formula. This model may be extended to odd (and odd-odd) and deformed nuclei, and generalized including corrections that have been neglected here. In this way one could have access to more experimental data, and could make a more systematic analysis.

In the last chapter we calculated the contribution of ISB interaction to the Equation of State for pure neutron infinite matter. Then we applied that to the calculation of mass and radius of neutron stars, by solving Tolman-Oppenheimer-Volkoff equations. We used interaction SAMi and SAMi-ISB, which are obtained in an analogous way [31, 17], and we observed that ISB effects are to make stars

more compact, in the region of interest (M$\approx 1.4 M_{\odot}$).

Appendix A

Isospin Symmetry Breaking energy density

We report here the calculation for the energy density and the contribution to the mean field of the CIB and CSB potentials, defined as in Sec. 2.1:

$$v_{\mathrm{CIB}}(i,j) := \frac{1}{2}\,\tau_z(i)\tau_z(j)\,\delta(\vec{r_i}-\vec{r_j})\cdot \tag{A.1a}$$
$$\left\{u_0(1+z_0P_\sigma^{ij}) + \frac{1}{2}u_1(1+z_1P_\sigma^{ij})(k^2+k'^2) + u_2(1+z_2P_\sigma^{ij})\vec{k'}\cdot\vec{k}\right\}$$

$$v_{\mathrm{CSB}}(i,j) := \frac{1}{4}\,[\tau_z(i)+\tau_z(j)]\,\delta(\vec{r_i}-\vec{r_j})\cdot \tag{A.1b}$$
$$\left\{s_0(1+y_0P_\sigma^{ij}) + \frac{1}{2}s_1(1+y_1P_\sigma^{ij})(k^2+k'^2) + s_2(1+y_2P_\sigma^{ij})\vec{k'}\cdot\vec{k}\right\}$$

We start from the first term in Eq. (A.1b).

$$\begin{aligned}
E^{(0)}_{\mathrm{CSB}} &= \frac{1}{2}\sum_{ij}\langle ij|v^{(0)}_{\mathrm{CSB}}(i,j)|ij\rangle_{\mathrm{AS}} \\
&= \frac{1}{8}\sum_{ij}\langle ij|\delta(\vec{r_i}-\vec{r_j})[\tau_z(i)+\tau_z(j)]s_0(1+y_0P_\sigma^{ij})(1-P_r^{ij}P_\tau^{ij}P_\sigma^{ij})|ij\rangle \\
&= \frac{s_0}{8}\sum_{ij}\langle ij|\delta(\vec{r_i}-\vec{r_j})[\tau_z(i)+\tau_z(j)](1+y_0P_\sigma^{ij}-P_\tau^{ij}P_\sigma^{ij}-y_0P_\tau^{ij})|ij\rangle
\end{aligned}$$

We antisymmetrized the interaction by multiplying it by a factor $(1-P_r^{ij}P_\tau^{ij}P_\sigma^{ij})$. P_r^{ij} is the operator exchanging the positions and it has no effect here, because of the delta force, while P_τ^{ij} and P_σ^{ij} are the isospin and spin exchange operators,

respectively, which are usually defined as $\frac{1+\vec{\sigma}_i\cdot\vec{\sigma}_j}{2}$. Here we can substitute P_σ^{ij} with a factor $1/2$, because Pauli matrices have zero trace ($\sum_i \langle i|\vec{\sigma}|i\rangle = 0$), and P_τ^{ij} becomes just δ_{q_i,q_j}. Also, for symmetry reason, $[\tau_z(i)+\tau_z(j)] = 2\tau_z(i)$.

We obtain:

$$\begin{aligned}
E^{(0)}_{\rm CSB} &= \frac{s_0}{8}\sum_{ij}\langle ij|\delta(\vec{r_i}-\vec{r_j})\tau_z(i)[2+y_0-(2y_0+1)\delta_{q_i,q_j}]|ij\rangle \\
&= \frac{s_0}{8}\int \mathrm{d}^3r\,[(2+y_0)\rho(\rho_n-\rho_p)-(2y_0+1)(\rho_n^2-\rho_p^2)] \\
&= \frac{s_0}{8}(1-y_0)\int \mathrm{d}^3r\,(\rho_n^2-\rho_p^2) \\
&\equiv \int \mathrm{d}^3r\,\mathcal{H}^{(0)}_{\rm CSB} \\
&\Rightarrow \mathcal{H}^{(0)}_{\rm CSB} = \frac{s_0(1-y_0)}{8}\,(\rho_n^2-\rho_p^2) \qquad \text{(A.2)}
\end{aligned}$$

We do the calculation for next terms in the same way. We use now the definition of the relative momentum $\vec{k} = \frac{1}{2i}(\vec{\nabla}_i - \vec{\nabla}_j)$, and the property $[\tau_z(i)+\tau_z(j)]P_\tau = \tau_z(i)+\tau_z(j) = 2\tau_z(i)$.

$$\begin{aligned}
E^{(1)}_{\rm CSB} &= \frac{1}{2}\sum_{ij}\langle ij|v^{(1)}_{\rm CSB}(i,j)|ij\rangle_{\rm AS} \\
&= \frac{1}{16}\sum_{ij}\langle ij|\delta(\vec{r_i}-\vec{r_j})[\tau_z(i)+\tau_z(j)]s_1(1+y_1P_\sigma)(k^2+k'^2)(1-P_rP_\tau P_\sigma)|ij\rangle \\
&= -\frac{s_1}{32}\sum_{ij}\langle ij|\,\delta(\vec{r_i}-\vec{r_j})[\tau_z(i)+\tau_z(j)](\nabla_i^2+\nabla_j^2-2\vec{\nabla}_i\cdot\vec{\nabla}_j) \\
&\qquad\qquad \cdot\Big[1+y_1(\tfrac{1+\vec{\sigma}_i\cdot\vec{\sigma}_j}{2})-(\tfrac{1+\vec{\sigma}_i\cdot\vec{\sigma}_j}{2})P_\tau - y_1P_\tau\Big]|ij\rangle \\
&= -\frac{s_1}{32}\sum_{ij}\langle ij|\,\delta(\vec{r_i}-\vec{r_j})[2\tau_z(i)] \\
&\qquad \cdot\left\{\frac{1-y_1}{2}(\nabla_i^2+\nabla_j^2-2\vec{\nabla}_i\cdot\vec{\nabla}_j)+\frac{y_1-1}{2}(\vec{\sigma}_i\cdot\vec{\sigma}_j)(-2)(\vec{\nabla}_i\cdot\vec{\nabla}_j)\right\}|ij\rangle
\end{aligned}$$

Now, the contribution of spin matrices is not zero, in fact, remembering the definition of the densities (1.8), we make use of the properties:

- $\nabla_i^2(\vec{\sigma}_i\cdot\vec{\sigma}_j) = 0$
- $\vec{\nabla}_i\cdot\vec{\nabla}_j(\vec{\sigma}_i\cdot\vec{\sigma}_j) = \frac{1}{2}(\vec{\nabla}_i\times\vec{\sigma}_i)(\vec{\nabla}_j\times\vec{\sigma}_j)$
- $\sum_i \phi_i^\star\vec{\nabla}_i\phi_i = \frac{1}{2}\vec{\nabla}\rho$

- $\sum_i \phi_i^\star \nabla_i^2 \phi_i = \frac{1}{2}\nabla^2\rho - \tau$

and we arrive to:

$$E^{(1)}_{\rm CSB} = -\frac{s_1(1-y_1)}{32}\int \mathrm{d}^3 r\Big[(\nabla^2\rho_{\rm ex} - 2\tau_{\rm ex})\rho + (\nabla^2\rho - 2\tau)\rho_{\rm ex} - \vec{\nabla}\rho_{\rm ex}\cdot\vec{\nabla}\rho + 2i\vec{J}_{\rm ex}\cdot i\vec{J}\Big]$$

where $\rho_{\rm ex} = \rho_n - \rho_p$ is the neutron excess densities, and $\tau_{\rm ex}, \vec{J}_{\rm ex}$ are analogously defined. Thus:

$$\Rightarrow \mathcal{H}^{(1)}_{\rm CSB} = \frac{s_1(1-y_1)}{32}\Big[-\frac{3}{2}(\rho_n\nabla^2\rho_n - \rho_p\nabla^2\rho_p) + 2(\rho_n\tau_n - \rho_p\tau_p) + (J_n^2 - J_p^2)\Big] \quad \text{(A.3)}$$

For the third term we use the following properties:

- $\vec{k'}\cdot\vec{k}$ is antisymmetric under the exchange of the spatial coordinates, so we substitute P_r with -1
- $(\vec{\nabla}'_i\cdot\vec{\nabla}_i - \vec{\nabla}'_j\cdot\vec{\nabla}_i)(\vec{\sigma}_i\cdot\vec{\sigma}_j) = -\nabla_i^2(\vec{\sigma}_i\cdot\vec{\sigma}_j) + (\vec{\nabla}_i\cdot\vec{\nabla}_j)(\vec{\sigma}_i\cdot\vec{\sigma}_j) = (\vec{\nabla}_i\cdot\vec{\nabla}_j)(\vec{\sigma}_i\cdot\vec{\sigma}_j)$
- $\int \vec{\nabla}\rho\cdot\vec{\nabla}\rho \mathrm{d}^3 r = \underbrace{\int \vec{\nabla}\cdot(\rho\vec{\nabla}\rho)\mathrm{d}^3 r}_{=\int \rho\vec{\nabla}\rho\cdot\mathrm{d}\vec{S}\ \underset{\rho\to 0}{\to}\ 0} - \int \rho\nabla^2\rho \mathrm{d}^3 r.$

So:

$$\begin{aligned}
E^{(2)}_{\rm CSB} &= \frac{1}{2}\sum_{ij}\langle ij|v^{(2)}_{\rm CSB}(i,j)|ij\rangle_{\rm AS} \\
&= \frac{s_2}{8}\sum_{ij}\langle ij|\delta(\vec{r_i}-\vec{r_j})[\tau_z(i)+\tau_z(j)](\vec{k'}\cdot\vec{k})(1+y_2P_\sigma)(1-P_rP_\tau P_\sigma)|ij\rangle \\
&= \frac{s_2}{32}\sum_{ij}\langle ij|\,\delta(\vec{r_i}-\vec{r_j})2\tau_z(i)\Big\{(1+y_2(\tfrac{1+\vec{\sigma}_i\cdot\vec{\sigma}_j}{2}) + (y_2+\tfrac{1+\vec{\sigma}_i\cdot\vec{\sigma}_j}{2})P_\tau\Big\} \\
&\qquad\qquad \cdot 2(\vec{\nabla}'_i\cdot\vec{\nabla}_i - \vec{\nabla}'_j\cdot\vec{\nabla}_i)\,|ij\rangle \\
&= \frac{s_2}{16}\int \mathrm{d}^3 r\Big\{\frac{3}{2}(1+y_2)(\tau_{\rm ex}\rho + \tau\rho_{\rm ex} - \frac{1}{2}\vec{\nabla}\rho\cdot\vec{\nabla}\rho_{\rm ex}) + \frac{1}{2}(1+y_2)i\vec{J}_{\rm ex}\cdot i\vec{J}\Big\} \\
&= \frac{s_2}{32}\int \mathrm{d}^3 r(1+y_2)\Big(3\tau_{\rm ex}\rho + 3\tau\rho_{\rm ex} + \frac{3}{2}\rho_n\nabla^2\rho_n - \frac{3}{2}\rho_p\nabla^2\rho_p - J_n^2 + J_p^2\Big)
\end{aligned}$$

$$\Rightarrow \mathcal{H}^{(2)}_{\rm CSB} = \frac{3}{32}s_2(1+y_2)\Big[\frac{1}{2}(\rho_n\nabla^2\rho_n - \rho_p\nabla^2\rho_p) + 2(\rho_n\tau_n - \rho_p\tau_p) - \frac{1}{3}(J_n^2 - J_p^2)\Big] \quad \text{(A.4)}$$

The total CSB energy density is the sum of Eqs. (A.2)(A.3)(A.4). We omit here the calculation for the CIB part, but it is very similar. The total ISB energy densities are finally:

$$\begin{aligned}\mathcal{H}_{\mathrm{CSB}} =& \frac{s_0}{8}(1-y_0)(\rho_n^2-\rho_p^2) \\ &+ \frac{3}{64}\{-s_1(1-y_1)+s_2(1+y_2)\}(\rho_n\nabla^2\rho_n-\rho_p\nabla^2\rho_p) \\ &+ \frac{1}{16}\{s_1(1-y_1)+3s_2(1+y_2)\}(\rho_n\tau_n-\rho_p\tau_p) \\ &+ \frac{1}{32}\{s_1(1-y_1)-s_2(1+y_2)\}(J_n^2-J_p^2) \end{aligned} \tag{A.5a}$$

$$\begin{aligned}\mathcal{H}_{\mathrm{CIB}} =& \frac{u_0}{8}[(1-z_0)(\rho_n^2+\rho_p^2)-2(2+z_0)\rho_n\rho_p] \\ &+ \frac{3}{64}\{-u_1(1-z_1)+u_2(1+z_2)\}(\rho_n\nabla^2\rho_n+\rho_p\nabla^2\rho_p) \\ &+ \frac{1}{64}\{3u_1(2+z_1)-u_2(2+z_2)\}(\rho_n\nabla^2\rho_p+\rho_p\nabla^2\rho_n) \\ &+ \frac{1}{16}\{u_1(1-z_1)+3u_2(1+z_2)\}(\rho_n\tau_n+\rho_p\tau_p) \\ &- \frac{1}{16}\{u_1(2+z_1)+u_2(2+z_2)\}(\rho_p\tau_n+\rho_n\tau_p) \\ &+ \frac{1}{32}\{u_1(1-2z_1)-u_2(1+2z_2)\}(J_n^2+J_p^2) \\ &+ \frac{1}{32}\{u_1z_1+u_2z_2\}J^2 \end{aligned} \tag{A.5b}$$

Appendix B

Displacement Energy

The Displacement Energy (DE) is defined as the difference in energy between two adjacent states that belong to the same isospin multiplet. We also give the definition, for convenience, of the isospin ladder operators $T^{\pm}$ and their following properties:

- $T^{\pm}\,|T\;T_z\rangle := \sqrt{T(T+1) - T_z(T_z \pm 1)}\,|T\;T_z \pm 1\rangle$
- $T^{-}\,|T_0 T_0\rangle = \sqrt{T_0(T_0+1) - T_0(T_0-1)}\,|T_0\;T_0 - 1\rangle = \sqrt{2T_0}\,|T_0\;T_0 - 1\rangle$
- $T^{+}T^{-}\,|T_0 T_0\rangle = \sqrt{2T_0}\,\sqrt{T_0(T_0+1) - (T_0-1)T_0}\,|T_0\;T_0\rangle = 2T_0\,|T_0 T_0\rangle$
- $T^{+}\,|T_0 T_0\rangle = 0$ (no isospin mixing)

where T_0 is the total isospin, $|T_0 T_0\rangle$ is the ground state (where $2T_0 = N - Z$), and $T^{+(-)}$ is the isospin raising (lowering) operator.

From the definition of the DE, we obtain:

$$\begin{aligned} DE :=& \langle T_0 T_0 - 1|\, H\, |T_0 T_0 - 1\rangle - \langle T_0 T_0|\, H\, |T_0 T_0\rangle \\ =& \frac{1}{2T_0}\,\langle T_0 T_0|\, T^{+} H T^{-}\, |T_0 T_0\rangle - \frac{1}{2T_0}\,\langle T_0 T_0|\, T^{+}T^{-} H\, |T_0 T_0\rangle \\ =& \frac{1}{2T_0}\,\langle T_0 T_0|\, T[H, T^{-}]\, |T_0 T_0\rangle \\ =& \frac{1}{2T_0}\,\langle T_0 T_0|\, [T, [H, T^{-}]]\, |T_0 T_0\rangle \end{aligned} \tag{B.1}$$

We see that the DE depends on the double commutator between H and the ladder operators. This is in agreement with the fact that only interactions depending on isospin contribute to the DE. Then the DE can be calculated; for example, the direct and the exchange parts of the Coulomb contribution are respectively [19]:

$$\begin{cases} DE_{direct} = \dfrac{e^2}{N-Z}\iint \mathrm{d}^3r\mathrm{d}^3r' \dfrac{\rho_p(\vec{r})(\rho_n(\vec{r'}) - \rho_p(\vec{r'}))}{|\vec{r} - \vec{r'}|} \\ DE_{exch} = -900\dfrac{Z}{A}\,\mathrm{keV} \end{cases} \tag{B.2}$$

where an approximated expression for the exchange term is given.

We concentrate now to demonstrate the contribution of the Isospin Symmetry Breaking nuclear interactions, defined as in Sec. 2.1:

$$v_{\mathrm{CIB}}(i,j) := \frac{1}{2}\,\tau_z^i\tau_z^j\,\delta(\vec{r_i} - \vec{r_j})\cdot \tag{B.3a}$$
$$\left\{u_0(1 + z_0P_\sigma^{ij}) + \frac{1}{2}u_1(1 + z_1P_\sigma^{ij})(k^2 + k'^2) + u_2(1 + z_2P_\sigma^{ij})\vec{k'}\cdot\vec{k}\right\}$$

$$v_{\mathrm{CSB}}(i,j) := \frac{1}{4}\,[\tau_z^i + \tau_z^j]\,\delta(\vec{r_i} - \vec{r_j})\cdot \tag{B.3b}$$
$$\left\{s_0(1 + y_0P_\sigma^{ij}) + \frac{1}{2}s_1(1 + y_1P_\sigma^{ij})(k^2 + k'^2) + s_2(1 + y_2P_\sigma^{ij})\vec{k'}\cdot\vec{k}\right\}$$

We start with considering the first term of CSB interaction (B.3b). We need first to calculate the double commutator in Eq. (B.1), making use of:

- $T^\pm = \sum_k t_k^\pm$
- $[\tau_z^i, t_k^\pm] = \pm 2\delta_{ik}t_k^\pm$
- $[\tau_k^+, t_i^-] = 2\delta_{ik}t_z^i$

$$\begin{aligned}[V_{\mathrm{CSB}}^{(0)}, T^-] &= \frac{1}{2}\sum_{ijk}\frac{s_0}{4}(1 + y_0P_\sigma)\delta(\vec{r_i} - \vec{r_j})[\tau_z^i + \tau_z^j, t_k^-] \\ &= \frac{s_0}{8}\sum_{ijk}(1 + y_0P_\sigma)\delta(\vec{r_i} - \vec{r_j})(-2\delta_{ik}t_k^- - 2\delta_{jk}t_k^-) \\ &= -\frac{s_0}{4}\sum_{ij}(1 + y_0P_\sigma)\delta(\vec{r_i} - \vec{r_j})(t_i^- + t_j^-)\end{aligned}$$

$$\begin{aligned}[T^+, [V_{\mathrm{CSB}}^{(0)}, T^-]] &= -\frac{s_0}{4}\sum_{ijk}(1 + y_0P_\sigma)\delta(\vec{r_i} - \vec{r_j})[t_k^+, t_i^- + t_j^-] \\ &= -\frac{s_0}{4}\sum_{ij}(1 + y_0P_\sigma)\delta(\vec{r_i} - \vec{r_j})(2t_z^i + 2t_z^j)\end{aligned}$$

We apply now the same rules used in Appendix A to calculate the energy density functional. Then the DE is:

$$\begin{aligned} DE^{(0)}_{\rm CSB} &= \frac{1}{2T_0}\sum_{ij}\langle ij|\,\frac{-s_0}{4}(1+y_0P_\sigma)\delta(\vec{r}_i-\vec{r}_j)2(t^i_z+t^j_z)(1-P_rP_\sigma P_\tau)\,|ij\rangle \\ &= -\frac{s_0}{4T_0}\sum_{ij}\langle ij|\,\delta(\vec{r}_i-\vec{r}_j)(t^i_z+t^j_z)(1+\frac{y_0}{2}-\frac{1}{2}P_\tau-y_0P_\tau)\,|ij\rangle \\ &= -\frac{s_0}{4T_0}\int \mathrm{d}^3r\,(1+\frac{y_0}{2})\rho_{ex}\rho-(\frac{1}{2}+y_0)\rho_{ex}\rho \\ &= -\frac{s_0}{8T_0}(1-y_0)\int \mathrm{d}^3r\,(\rho_n^2-\rho_p^2) \end{aligned} \tag{B.4}$$

In an analogous way, we find the expressions for the second and third terms.

$$[V^{(1)}_{\rm CSB},T^-] = \frac{1}{2}\sum_{ijk}\frac{s_1}{8}(1+y_1P_\sigma)\delta(\vec{r}_i-\vec{r}_j)\underbrace{[\tau^i_z+\tau^j_z,t^-_k]}_{-2t^-_i-2t^-_j}(P'^2+P^2)$$

$$[T^+,[V^{(1)}_{\rm CSB},T^-]] = -\frac{s_1}{8}\sum_{ijk}(1+y_1P_\sigma)\delta(\vec{r}_i-\vec{r}_j)\underbrace{[t^+_k,t^-_i+t^-_j]}_{2t^i_z+2t^j_z}(-\frac{1}{2})(\nabla^2_i+\nabla^2_j-2\vec{\nabla}_i\cdot\vec{\nabla}_j)$$

$$\begin{aligned} DE^{(1)}_{\rm CSB} &= \frac{s_1}{8}\frac{1}{2T_0}\sum_{ij}\langle ij|\,\delta(\vec{r}_i-\vec{r}_j)(t^i_z+t^j_z)(1+y_1P_\sigma-P_\sigma P_\tau-y_1P_\tau)(\nabla^2_i+\nabla^2_j-2\vec{\nabla}_i\cdot\vec{\nabla}_j)\,|ij\rangle \\ &= \frac{s_1}{16T_0}\sum_{ij}\langle ij|\,\delta(\vec{r}_i-\vec{r}_j)\Big\{(t^i_z+t^j_z)(1+\frac{y_1}{2}-\frac{1}{2}P_\tau-y_1P_\tau)(\nabla^2_i+\nabla^2_j-2\vec{\nabla}_i\cdot\vec{\nabla}_j) \\ &\qquad +\frac{1}{2}(t^i_z+t^j_z)(y_1-1)(\vec{\sigma}_i\cdot\vec{\sigma}_j)(-2\vec{\nabla}_i\cdot\vec{\nabla}_j)\Big\}\,|ij\rangle \\ &= \frac{s_1}{16T_0}\int \mathrm{d}^3r\,\frac{1}{2}(1-y_1)\Big[(\frac{1}{2}\nabla^2\rho_{ex}-\tau_{ex})\rho+(\frac{1}{2}\nabla^2\rho-\tau)\rho_{ex}\Big] \\ &\qquad -\frac{1}{4}(1-y_1)\vec{\nabla}\rho_{ex}\cdot\vec{\nabla}\rho+\frac{1}{2}(1-y_1)i\vec{J}_{ex}\cdot i\vec{J} \\ &= \frac{s_1}{32T_0}(1-y_1)\int \mathrm{d}^3r\,\frac{3}{2}[\rho_n\nabla^2\rho_n-\rho_p\nabla^2\rho_p]-2(\tau_n\rho_n-\tau_p\rho_p)-(J^2_n-J^2_p) \end{aligned} \tag{B.5}$$

$$[V^{(2)}_{\rm CSB},T^-] = \frac{1}{2}\sum_{ijk}\frac{s_2}{4}(1+y_2P_\sigma)\delta(\vec{r}_i-\vec{r}_j)\underbrace{[\tau^i_z+\tau^j_z,t^-_k]}_{-2t^-_i-2t^-_j}(\vec{P'}\cdot\vec{P})$$

$$[T^+,[V^{(2)}_{\rm CSB},T^-]] = -\frac{s_2}{4}\sum_{ijk}(1+y_2P_\sigma)\delta(\vec{r}_i-\vec{r}_j)\underbrace{[t^+_k,t^-_i+t^-_j]}_{2t^i_z+2t^j_z}\frac{1}{2}(\vec{\nabla}'_i\cdot\vec{\nabla}_i-\vec{\nabla}'_j\cdot\vec{\nabla}_i)$$

$$\begin{aligned}
DE^{(2)}_{\rm CSB} &= -\frac{s_2}{4}\frac{1}{2T_0}\sum_{ij}\langle ij|\,\delta(\vec{r}_i-\vec{r}_j)(t^i_z+t^j_z)(1+y_2P_\sigma+P_\sigma P_\tau+y_2P_\tau)(\vec{\nabla}'_i\cdot\vec{\nabla}_i-\vec{\nabla}'_j\cdot\vec{\nabla}_i)\,|ij\rangle \\
&= -\frac{s_2}{8T_0}\sum_{ij}\langle ij|\,\delta(\vec{r}_i-\vec{r}_j)\Big\{(t^i_z+t^j_z)(1+\frac{y_2}{2}+\frac{1}{2}P_\tau+y_2P_\tau)(\vec{\nabla}'_i\cdot\vec{\nabla}_i-\vec{\nabla}'_j\cdot\vec{\nabla}_i) \\
&\qquad\qquad +\frac{1}{2}(t^i_z+t^j_z)(y_2+1)(\vec{\sigma}_i\cdot\vec{\sigma}_j)(-\vec{\nabla}'_j\cdot\vec{\nabla}_i)\Big\}\,|ij\rangle \\
&= -\frac{s_2}{16T_0}\int {\rm d}^3r\,\frac{3}{2}(1+y_2)\Big[\tau_{ex}\rho+\tau\rho_{ex}-\frac{1}{2}\vec{\nabla}\rho\cdot\vec{\nabla}\rho_{ex}\Big]+\frac{1}{2}(1+y_2)i\vec{J}_{ex}\cdot i\vec{J} \\
&= -\frac{s_2}{32T_0}(1+y_2)\int {\rm d}^3r\,\frac{3}{2}[\rho_n\nabla^2\rho_n-\rho_p\nabla^2\rho_p]+6(\tau_n\rho_n-\tau_p\rho_p)-(J^2_n-J^2_p)
\end{aligned} \tag{B.6}$$

The sum Eqs. (B.4)(B.5)(B.6) gives the contribution of CSB interaction. We omit the calculation for the CIB part, but it is very similar. The DE due to the total ISB nuclear interactions is finally:

$$\begin{aligned}
DE_{CSB} = \int & -\frac{s_0}{8T_0}(1-y_0)(\rho^2_n-\rho^2_p) \\
& +\frac{3}{64T_0}\{s_1(1-y_1)-s_2(1+y_2)\}(\rho_n\nabla^2\rho_n-\rho_p\nabla^2\rho_p) \\
& -\frac{1}{16T_0}\{s_1(1-y_1)+3s_2(1+y_2)\}(\rho_n\tau_n-\rho_p\tau_p) \\
& -\frac{1}{32T_0}\{s_1(1-y_1)-s_2(1+y_2)\}(J^2_n-J^2_p) \\
\equiv & -\frac{1}{T_0}\int\mathcal{H}_{CSB} \qquad \text{(cft. Eq. (A.5a))} \\
DE_{CIB} = \int & -\frac{u_0}{4T_0}(1-z_0)(\rho_n-\rho_p)^2 \\
& +\frac{3}{32T_0}\{u_1(1-z_1)-u_2(1+z_2)\}(\rho_n\nabla^2\rho_n+\rho_p\nabla^2\rho_p-\rho_n\nabla^2\rho_p-\rho_p\nabla^2\rho_n) \\
& -\frac{1}{8T_0}\{u_1(1-z_1)+3u_2(1+z_2)\}(\rho_n\tau_n+\rho_p\tau_p-\rho_p\tau_n-\rho_n\tau_p) \\
& -\frac{1}{8T_0}\{u_1(1+2z_1)-u_2(1+2z_2)\}(J^2_n+J^2_p-\frac{1}{2}J^2)
\end{aligned}$$

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