### **Gianluca Salvioni**

# Model Nuclear Energy Density Functionals Derived from *Ab Initio* Calculations





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Cover picture: Conceptual picture of the atomic nucleus, by Gianluca Salvioni

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## Abstract

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This monograph focused on a method to link nuclear energy density functionals to the *ab initio* solution of the nuclear many-body problem. This method, proposed in Ref. [1], was here discussed in many aspects as well as applied to a state-of-art *ab initio* approach.

We introduced the basis of the density functional theory, paying attention to the concept of generators of the functional. In parallel, we explored the Self-Consistent Green's Function approach as *ab initio* framework to calculate ground-state energies. We derived the model functional based on the Levy-Lieb constrained variation, which exploited the response of the nucleus to an external perturbation.

Using the Green's function technique and the NNLOsat chiral interaction in the *ab initio* Hamiltonian, seven semi-magic nuclei were probed with perturbations induced by generators of two- and three-body contact interaction (Skyrme-like). We employed the same generators to built model functionals, whereupon the coupling constants were fitted to reproduce the perturbed ground-state energies. Several parametrizations of the functionals were obtained for given choices of generators, selection of data points, and assumed uncertainties. We analysed the derived parametrizations according to their statistical performances, magnitude of the propagated errors, and corresponding nuclear matter description. Two parametrizations emerged as the most promising, but the model functionals built from them did not produce meaningful results. As it turned out, zero-range generators provided a poor description of the chiral interaction. Moreover, the performed error analysis suggested that the actual precision of the *ab initio* approach may not be sufficient to improve the quality of the novel energy density functionals.

**Keywords:** energy density functionals, *ab initio* methods, chiral interaction, theoretical uncertainties.

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# Preface

The work presented in this thesis has been carried out during the years 2015-2019 at the University of Jyväskylä. In 2019, it has been supported by the Helsinki Institute of Physics.

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Jyväskylä, June 2019

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### 1. Introduction

The atomic nucleus is identified with the massive core at the center of the atom and it has the radial dimension of a few fm  $(10^{-15}\text{m})$ . It is formed by positively charged particles, protons (p) and neutral particles (n), that together are called nucleons. The different types of nuclei are distinguished by the proton number Zand the neutron number N, summing up to the mass number A = Z + N. Nuclei with the same Z (i.e. same chemical element) but different N are called isotopes. Nuclides are commonly presented within the nuclear chart as in Figure 1.1. Nuclei can contain between one and a couple of hundreds of nucleons, requiring a proper treatment as many-body systems.

A small part of them is stable, meaning that they have lifetimes larger than the age of the Universe. The majority are radioactive, i.e., they are produced naturally or in laboratory in certain unstable configurations, and then they decay until they reach stable structures.

Neutron and proton numbers are not enough to describe a nuclear system. There are other measurable quantities called experimental observables that define a particular nuclear state. These are, for example, binding energies (masses), spins, radii, electromagnetic moments as well as lifetimes, excitation energies, electromagnetic transitions, decays, particle emissions and so on. In fact, the nuclear chart presents only the lowest energy states (the ground states), on top of which a large variety of excited states exist.

The technical development of experimental facilities continuously increases the number of measured systems. With the help of theoretical models, boundaries have been identified to the existence of nuclear systems that do not spontaneously emit nucleons. These limits called "drip lines" predict that there are many more nuclei to be observed, especially on the neutron-rich side [2].

The nuclear mass M relates to the proton  $m_p$  and neutron  $m_n$  masses as

$$Mc^{2} = Z m_{p}c^{2} + N m_{n}c^{2} - BE, \qquad (1.1)$$



Figure 1.1: Section of the nuclear chart containing the lightest nuclei. The whole nuclear chart is shown in the inset. The known nuclei are plot according to the neutron number N (x-axis) and proton number Z (y-axis). Colors represent the primary decay mode for the ground state. Stable nuclei are in black. Neutron and proton magic numbers are indicated. Adapted from Ref. [3].

where BE represents the binding energy of the nucleus. In the simplest approximation, the nucleus can be described as a high-density and incompressible fluid of nucleonic matter, which organizes itself in a spherical drop. In this liquid-drop model the binding energy assumes the form [4]

$$BE = a_V A - a_s A^{2/3} - a_C \frac{Z(Z-1)}{A^{1/3}} - a_A \frac{(A-2Z)^2}{A} + \delta(A,Z).$$
(1.2)

Every term stands for a specific effect of the residual interaction that binds the system in a sphere of fermions. The first term is the volume energy, which accounts for the interaction of each nucleon with its neighbors. The second term, surface

energy, corrects the volume term for the nucleons on the surface of the drop. The third term is the Coulomb energy, which describes the electric repulsion among the protons. The fourth term is the symmetry energy accounting for the unbalance of N and Z. The last term is the pairing energy, which models the preference of the system to form pairs of like nucleons when A is even. The expression for the pairing energy is

$$\delta(A,Z) = \begin{cases} a_P A^{k_P} & \text{for } N, Z \text{ both even} \\ 0 & \text{for } A \text{ odd} \\ -a_P A^{k_P} & \text{for } N, Z \text{ both odd} \end{cases}$$
(1.3)

The parameters  $a_V$ ,  $a_S a_C$ ,  $a_A$ ,  $a_P$  and  $k_P$  are obtained by fitting experimental masses, reason why Eq.(1.2) is called the semi-empirical mass formula. This gives a simple estimation of the binding energy.

Similarly as in the atomic physics, where closed electronic configurations make the atom less susceptible to ionization, in nuclear physics one also finds experimental evidence of shell closure. We consider the separation energy, i.e., the energy to remove a nucleon from a nucleus, defined respectively for neutron and proton as

$$S_n(N,Z) = BE(N,Z) - BE(N-1,Z)$$
(1.4)

$$S_p(N,Z) = BE(N,Z) - BE(N,Z-1).$$
 (1.5)

Nuclei with a specific number N and/or Z, have much larger separation energy than the neighboring nuclei, indicating that the former systems are more bound. Such "magic numbers" (for spherical nuclei) equal 2, 8, 20, 28, 50, 82 (for protons and nucleons) and 126 (only nucleons). When a nucleus has N or Z equal to one of these numbers the nucleus is called "semi-magic", if both N and Z are magic numbers the nucleus is called "doubly magic". The effect of large binding in semi-magic and doubly-magic nuclei appears also in their stability against excitations. In these systems, collective  $2^+$  excitations are higher in energy than in the neighboring systems.

The evidence of closed shells can be simulated by an average potential that localizes the wave function of the nucleons inside the nuclear volume.

The shell configuration is fairly well described by the three-dimensional harmonic oscillator (HO) potential with the addition of a spin-orbit term (the Nilsson model [5]). The spin-orbit term, with tuned coupling constant, is able to separate harmonic oscillator eigenstates with same angular momentum l but different  $j = |\mathbf{l} + \mathbf{s}|$ , in the way that correct magic numbers are obtained. The resulting potential works fine to approximate the nuclear mean field.

The description of the average potential can be improved by the Woods-Saxon

potential [6], which provides more accurate single-particle wave functions of the nucleons at the price that these solutions are not analytical.

It is a common practice in the many-body nuclear physics to expand the nuclear wave function on a basis made of HO eigenstates. In fact, the analytical expression of the HO eigenstates helps to simplify the theoretical calculations and implementations of the relevant equations in numerical codes. Furthermore, in the HO system, analogously to the nuclear Hamiltonian, the center-of-mass motion can be decoupled from the relative motion.

For the large majority of nuclei, away from closed shell configurations, it is necessary to introduce a "residual" interaction to account for interplays among nucleons that go beyond the average potential.

Intending to study the structure of the nuclear system, we deal with phenomena at low-energy scale, it usually means of the order of MeV (compared to the rest mass of the nucleons  $\sim 1 \text{GeV}$ ). It is fundamental to characterize the residual interaction at the level of low-energy physics, highlighting the relevant degrees of freedom in the system. It is instructive to begin the discussion from the world of quarks, gluons, and QCD towards the domain of neutrons, protons, and effective Hamiltonians.

### 1.1 Fundamental particles and forces in nuclear physics

Nucleons are composite particles, their fundamental constituents are known to be quarks and gluons.

Quarks (q) are elementary particles with spin 1/2 and non-integer electric charge, that is, the charge is proportional to a fraction of the elementary charge e. They possess also color charge, which is responsible for their strong interaction. Quarks are divided in six flavors, each flavor has specific mass and mean lifetime. Antiquarks  $(\bar{q})$ , antiparticle of quarks, also exist, with the same flavor, mass, spin and lifetime than quarks, but opposite charges. Gluons are elementary particles with spin 1, mediators of the strong interactions of quarks, that also carry color charge, i.e., they participate in the interaction in addition to mediating it.

While separating two color charges, the phenomenon of color confinement shows that it is energetically more favorable a new quark-antiquark pair to appear rather than increasing the separation distance, due to the fact that gluons are color charged. It means that particles with singular color charge cannot be isolated, but only states with global neutral color can be observed, namely, quarks and antiquarks manifest in composite particle called hadrons. Hadrons are formed by valence quarks, from which they get their quantum numbers, plus an indefinite number of virtual sea quarks, antiquarks and gluons. Among the hadrons, there are mesons, formed by valence quark and antiquark  $(q\bar{q})$ , such as pions, and baryons, formed by three valence quarks (qqq), such as proton p and neutrons n. Recently have been investigated states of tetraquarks  $(qq\bar{q}\bar{q})$  and pentaquarks  $(qqqq\bar{q})$  [7].

Quarks and antiquarks interact with all the four fundamental forces: gravitational, weak, electromagnetic and strong interaction (see Table 1.1). Then the atomic nucleus, being composed by quarks, also experiences all the four forces, even if only the last three play an active role in shaping its structure and regulating its dynamics. The effects of the gravitational force are negligible, since its strength is much smaller than that of the other interactions.

**Table 1.1:** Fundamental interactions and their properties. The strong interaction is characterized as (fundamental) residual force. Adapted from Ref. [8], with values from Ref. [9].

				Strong
Interaction	Gravitational	Weak	Electromagnetic	(fundamental)
				residual
Particles	all	quarks loptons	charged particles	(quarks, gluons)
experiencing	an	quarks, leptons	charged particles	hadrons
Mediators	(graviton)	$W^+$ , $W^-$ and $Z^0$	photons $\gamma$	(gluons)
Mediators				mesons
Strength	10-36	10-7	1	20
p-p in nucleus	10	10	1	20
Range	$\infty$	$10^{-18}$ m	$\infty$	$10^{-15}$ m
Effects		Bota docar	Coulomb,	Binding,
in nucleus	-	Deta decay	EM transitions	N-N scattering

The strong force is the one which keeps the nucleons together to form a bound system and for this reason it is called "nuclear" force. At the fundamental level of quarks and gluons, it is described by the quantum chromodynamics (QCD). At the hadronic level, instead, the strong force emerges as residual interaction primarily mediated by mesons.

QCD is a non-abelian gauge field theory, that is, the QCD Lagrangian is an invariant of gauge transformations of the symmetry group SU(3) of color, and the symmetry group is non-commutative. Colored particles, quark and gluons,

interact weakly at short distances (corresponding to high-momentum transferred) and strongly at distances larger than 1 fm (low energy). As a consequence, the interaction can be treated perturbatively at high energy (asymptotic freedom) while it is non-perturbative in the low-energy regime we are interested.

We briefly recall the notation commonly used in relativistic quantum field theory with the spacetime index  $\mu$  of a four-vector  $x^{\mu} \equiv (ct, x, y, z)$ , in contrast with a space vector  $\mathbf{x} \equiv (x, y, z)$ , and the Einstein convention for the sum on repeated indices. The QCD Lagrangian density reads

$$\mathcal{L}_{QCD} = \bar{q} \left( i \gamma^{\mu} D_{\mu} - \mathcal{M} \right) q - \frac{1}{4} g_{\mu\nu,a} g_{a}^{\mu\nu}, \qquad (1.6)$$

where  $q \equiv q(\mathbf{x})$  are quark fields,  $\mathcal{M}$  is the quark mass matrix,  $\gamma^{\mu}$  are Dirac matrices. Gluon fields  $A_{\mu,a}(\mathbf{x})$  enter in the gauge-covariant derivatives  $D_{\mu}$  as

$$D_{\mu} = \partial_{\mu} - ig \frac{\lambda_a}{2} A_{\mu,a} \tag{1.7}$$

and in the gluon field strength tensors  $g_{\mu\nu,a}$ , defined as

$$g_{\mu\nu,a} = \partial_{\mu}A_{\nu,a} - \partial_{\nu}A_{\mu,a} + gf_{abc}A_{\mu,b}A_{\nu,c}, \qquad (1.8)$$

where g is the strong coupling constant while the Gell-Mann matrices  $\lambda_a$  [10] and the structure constants  $f_{abc}$  are elements of the  $SU(3)_{color}$  Lie algebra [11]. The last term on the right-hand side of Eq.(1.8) represents the peculiarity of the strong force, in which gluons interact also among themselves.

Up (u) and down (d) quarks are the lightest quarks with masses  $m_u \approx 2.5$  MeV and  $m_d \approx 5$  MeV. They are the valence quarks that form protons (uud), neutrons (udd) and pions ( $u\bar{d}$ ,  $u\bar{u}$ ,  $d\bar{d}$ ,  $\bar{u}d$ ). We limit our attention only to these two quark flavors.

In the limit of vanishing quark masses  $m_i = 0$ , we can rewrite Eq.(1.6) in the form

$$\mathcal{L}_{QCD}^{0} = \bar{q}_{R} \left( i \gamma^{\mu} D_{\mu} \right) q_{R} + \bar{q}_{L} \left( i \gamma^{\mu} D_{\mu} \right) q_{L} - \frac{1}{4} g_{\mu\nu,a} g_{a}^{\mu\nu}, \qquad (1.9)$$

emphasizing the projection of the quark fields on their right-handed,  $q_R = P_R q$ , and left-handed,  $q_L = P_L q$ , components.  $\mathcal{L}^0_{QCD}$  are invariant under a global unitary transformation induced by elements of the symmetry group  $SU(2)_R \times SU(2)_L$ . Namely, the right- and left-handed components of massless quarks do not mix under such transformation, and this property is known as chiral symmetry.

The chiral symmetry is broken explicitly by the mass matrix  $\mathcal{M} = m_i \delta_{ij}$  because  $m_u \neq m_d$ . Such breaking is small since quark masses are a couple of order of magnitude lower than pion and nucleon masses.

Furthermore, the hadronic phenomenology indicates that the chiral symmetry can

be spontaneously broken. It happens when the ground state of the system does not realize the symmetry of the Lagrangian. If the global symmetry is broken spontaneously, there exist bosons with the same quantum numbers of the broken generators, called massless Goldstone bosons [12]. In the case of the chiral symmetry, the Goldstone bosons correspond to the isospin triplet of pseudoscalar pions. Pions break the chiral symmetry spontaneously and explicitly. In fact, they are the lightest mesons but their mass is not zero due to  $m_u \neq m_d \neq 0$ .

The nuclear force can be described directly in terms of quark and gluons only in the framework of lattice QCD. It requires an enormous computing power, which makes this method feasible only to calculate observables of low-energy nucleon-nucleon scattering or other few-body observables [13].

A more manageable approach is the effective field theory (EFT) [14], with a separation of scales placed around the breakdown scale  $\Lambda_b$ . The contributions to the force are expanded in powers of  $Q/\Lambda_b$ , where Q is the soft scale. The physics at energies around Q is accounted explicitly, while the high-energy effects are integrated in the constants of the theory.

The separation of scales is fundamental to obtain an accurate representation of the phenomena. In order to describe the large n-p scattering lengths, the pion-less EFT is preferred, with the hard scale set at  $\Lambda_b \approx m_{\pi}c^2 = 139.6$  MeV. When the pion degrees of freedom are included, the pion-full EFT places  $\Lambda_b \approx 770$  MeV. To study heavy nuclei and nuclear matter the Fermi momentum  $k_F$  is the reference scale, with the value  $k_F \approx 2m_{\pi}c^2$  at nuclear matter saturation density [15]. Yukawa meson theory [16] and pion-exchange theory show that in nuclear structure and reactions, nucleons and pions emerge as proper degrees of freedom, instead of quarks and gluons.

The chiral perturbation theory (ChPT) is the EFT where the effective Lagrangian is built satisfying the broken symmetries of QCD and using the pions and nucleons as degree of freedom. Scattering matrix elements or Green's functions, calculated with the ChPT Lagrangian, admit an expansion of the form [17]

$$\mathfrak{M} = \sum_{\nu} \left(\frac{Q}{\Lambda_b}\right)^{\nu} \mathcal{F}\left(\frac{Q}{\mu}, g_i\right).$$
(1.10)

Q represents the momentum or pion mass, corresponding to derivatives and mass terms in the Lagrangian,  $\Lambda_b$  is around the mass of the  $\rho$  meson,  $M_{\rho} \approx 770$  MeV and the power  $\nu$  is bound from below. The function  $\mathcal{F}$  is of order 1 (naturalness), depending on the regularization scale  $\mu$  and the low-energy constants (LECs)  $g_i$ . LECs are usually obtained by fitting data, in the way that they mimic the unknown high-energy physics. In ChPT Eq.(1.10) is justified by the vanishing interaction in the limit of pion mass or momentum going to zero. The relativistic expression of the effective Lagrangian reads

$$\mathcal{L}_{eff} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \dots = \mathcal{L}_{\pi N}^{(1)} + \mathcal{L}_{\pi\pi}^{(2)} + \mathcal{L}_{\pi N}^{(2)} + \mathcal{L}_{\pi N}^{(3)} + \mathcal{L}_{\pi\pi}^{(4)} + \mathcal{L}_{\pi N}^{(4)} + \dots, \quad (1.11)$$

containing terms of increasing number of derivatives and pion mass insertions. Ellipsis points include higher order dimensions as well as interaction of pions with more nucleons.

The relativistic formulation is problematic because the mass of nucleons in  $\mathcal{L}_{\pi N}$  is of the same order of the breakdown scale  $\Lambda_b$ . An improvement consists in going to the non-relativistic limit through the heavy baryon chiral perturbation theory (HBChPT) [18], where the Lagrangian assumes the form

$$\mathcal{L}_{eff} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN} + \mathcal{L}_{NNN} + \dots, \qquad (1.12)$$

including many-nucleons contact interaction terms like  $\mathcal{L}_{NN}$ ,  $\mathcal{L}_{NNN}$ , ... [14].

Through the chiral perturbation theory, the nuclear force is represented by longintermediate range interaction, via pion(s) exchange, and short-range contact interaction.

The naturalness of  $\mathcal{F}$  makes the contribution to the next-to-leading order (NLO) smaller than the leading order (LO), namely  $\mathfrak{M}_{LO}(\Lambda_b) > \mathfrak{M}_{NLO}(\Lambda_b) > \mathfrak{M}_{NNLO}(\Lambda_b)$ , as shown in Figure 1.2.

Renormalized terms, derived from chiral effective field theory, are employed to describe the nuclear Hamiltonian in *ab initio* methods.

Ab initio approaches include all the theoretical techniques that solve the nonrelativistic Schrödinger equation, with a Hamiltonian in which all the nucleons are active and obey the Pauli exclusion principle. They are applied mostly to light nuclei, in fact, the exact solution is available only for system of few nucleons  $A \leq 4$ , while with certain controllable approximations heavier nuclei can be studied. State-of-art calculations can reach Ni (Z=28), Zr (Z=40) and Sn (Z=50) isotopic chains [19, 20]. In the interaction part of the Hamiltonian, the parameters are fitted to reproduce 2N and 3N experimental data.

In the literature, there are several available *ab initio* methods, distinguished by the technique adopted to calculate the many-body solution. The most developed approaches are:

- In-Medium Similarity Renormalization Group (IM-SRG) [20]
- No-Core Shell Model (NCSM) [21]
- Lattice EFT [22]
- Many-Body Perturbation Theory (MBPT) [23]
- Coupled-Cluster (CC) [24]



Figure 1.2: Schematic contributions to the potentials entering the Lagrangian density of chiral EFT. The expansion is limited to next-to-next-to-leading orderd (NNLO), for 2N (two-nucleons or two-body) and 3N forces. Continuous (dashed) lines represent nucleons (exchanged mesons). Adapted from Ref. [14]

- Self-Consistent Green's Function (SCGF) [25]
- Green's Function Monte Carlo (GFMC) [26]

When the number of nucleons is larger, due to the limits in computational resources, more severe approximations need to be introduced. This is the case of the **Configuration Interaction** (CI) theory (also known as nuclear shell model)[27]. The nucleus is divided in an inert core and valence nucleons, that is, the computing resources are reduced by truncating the model space. The Hamiltonian contains an average potential (usually harmonic oscillator or Woods-Saxon plus spin-orbit interaction), that determines the single-particle energies, and a residual two-body interaction, which accounts for interactions between nucleons in specific orbitals. The solution of the Hamiltonian is simplified by a linear combination of Slater determinants, made by single-particle wave functions. The Slater determinants form the basis in which the Hamiltonian matrix is diagonalized. This approach focuses particularly on medium-mass nuclei,  $16 \leq A \leq 132$ . The parameters of the interaction are fitted for the specific model space to observables available in the same model space (e.g. ground and excited states of nuclei, in which valence nucleons lie in a certain model space).

Recently this method was applied to the Hg isotopes  $(A \approx 190)$  [28], where the

valence nucleon space was extended with the Monte Carlo Shell Model technique [29]. This procedure is able to select the most relevant Slater determinants to describe a certain nuclear state by Monte Carlo sampling, and the reduced basis makes the diagonalization possible.

When the dimension of the CI matrices overshoots the computational resources, the nucleus can be modeled by the **nuclear Energy Density Functionals** (EDF) or self-consistent mean-field method [30]. The force is parametrized by an average mean-field potential, acting on each nucleon and originated by the interactions with all the others. The information on the system is reduced to its densities. This method requires to self-consistently calculate solutions of single-particles Schrödinger equations. This approach, on the one hand, allows us to describe heavy nuclei, on the other hand, is restricted mainly to study ground-state properties. Extensions to beyond mean-field theory and projection techniques help to broaden the applicability to excited configurations.

#### 1.2 "Effective" interactions

The term "effective" has assumed different meanings in the history of nuclear physics.

The modern connotation tells that such interaction describes the degrees of freedom at a certain energy scale, while the degrees of freedom relative to other scales are integrated out and included in the parameters of the effective theory. The chiral effective interaction is an example of this kind of force.

Conversely, the concept of microscopic effective interaction started in the context of the Brueckner-Hartree-Fock calculations. The hard core part of the nucleon-nucleon interaction, evaluated for a Slater determinant, will push the interaction energy to explode. To avoid such divergence, an effective interaction can be calculated by renormalization of bare nucleon-nucleon force. This can be achieved using the Brueckner G-matrix [31], i.e., treating the two nucleons as if they scatter in the nuclear medium. The independent particle picture still represents a good approximation because the healing distance is smaller than the mean distance between two nucleons inside the nucleus. That is, the two nucleons return to their single-particle behavior before the next collision takes place.

Due to the difficulties to work with the microscopic potential, since the 1950s, nuclear physics has seen a huge development of phenomenological effective forces to be applied directly in the Hartree-Fock method. The adjective "phenomenological"

indicates that the interaction is described by a certain number of parameters fitted to reproduce experimental data.

The nuclear wave functions should satisfy the invariance principles of the nuclear Hamiltonian, but in the case of phenomenological interaction, these invariance principles are not always fulfilled. Then, because of the phenomenon of spontaneous symmetry breaking, the obtained solutions need to be projected on good quantum numbers to be compared to experiments.

Since the range of the nuclear force is rather short, the simplest phenomenological effective force is zero-range, i.e., described by a  $\delta$ -function in the space coordinates. More realistic forces require momentum dependence, density dependence or finite-range.

Historically, the Skyrme-type force is an example of phenomenological effective interaction. There are many parametrizations available in the literature due to the different observables used to fit the parameters [30, 32].

In this work, we understand the components of the Skyrme potential as the "generators" of the energy density functionals. Namely, these components are operators that, when calculating their average values with a Slater determinant, generate the terms of the interaction part of the functionals, as shown in Section 2.5.

#### **1.3** Motivation

We aim to explore the link between chiral EFT interactions and mean-field forces. This may allow us to extend the description of nuclear interaction typical of the *ab initio* framework to the domain of the EDFs. On one side we have a fundamental description of the interaction among nucleons and on the other side we have a method to describe medium- and heavy-mass systems. The development of *ab initio* methods proceeds quickly, but the applicability to heavy systems is still far to be reached with the actual computing resources. The scientific community working with nuclear density functionals, instead, is looking towards new forms and parametrizations of functionals that can increase precision of their predictions. A successful extension could apply information from the chiral force to tackle a larger variety of phenomena. Improving in the theoretical models are beneficial in the comparison with experiments, especially when the theory is able to offer uncertainties to the estimated values. The effective interaction can redefine the driplines and it can increase the performance of the functionals on the whole nuclear chart.

The research for a connection between *ab initio* and density functionals has already started. In particular, possible ways to combine *ab initio* with EDFs are addressed in the review article [33].

A formal construction of EDF kernels grounded on *ab initio* methods is proposed in Ref. [34].

In this work, I proceed by fitting parameters that enter the energy functional, to *ab initio* calculations. Such derivation was suggested by Dobaczewski in [1], where also a proof-of-principle was provided. In this thesis, I explore the potentiality and limits of such a derivation, employing full-fledged *ab initio* calculations with chiral interaction.

The thesis is organized as follows: Chapter 2 reviews the foundation of Energy Density Functional theory in nuclear physics and Chapter 3 presents the current status of nuclear functionals. Chapter 4 introduces the Self-Consistent Green's Function method and the *ab initio* technique we adopt in the calculations of ground state energies. The methodology to derive the model functional is given in Chapter 5. In Chapter 6 the results obtained for the relevant case of NNLOsat with two-and three-body interaction are discussed. Conclusions are given in Chapter 7.

## 2. Energy Density Functionals

We present the principal aspects of the Density Functional Theory (DFT). The DFT method was introduced in the 1960s to describe the properties of electronic systems and very soon thereafter applied to atomic nuclei. We start from an overview of foundations of electronic DFT [35], which then becomes a baseline for the extension to the nuclear case.

#### 2.1 Hohenberg-Kohn theorems

A many-body system composed of N electrons, subject to Coulomb repulsion and immersed in an external potential  $v(\mathbf{r})$  is represented by the Hamiltonian operator

$$\hat{H} = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_e} \nabla_i^2 + \sum_{i$$

where the contributes from kinetic energy  $\hat{T}$ , Coulomb  $\hat{V}_{ee}$  and external  $\hat{U}_{ext}$  potential are separated. From the (assumed) non-degenerate ground-state wave function  $|\Psi(\mathbf{r}_1, ..., \mathbf{r}_N)\rangle$ , solution of the Schrödinger equation

$$\hat{H}|\Psi\rangle = E|\Psi\rangle,$$
 (2.2)

the electronic density  $\rho(\mathbf{r})$  of the system is obtained as

$$\rho(\mathbf{r}) = N \int \mathrm{d}\mathbf{r}_2 \cdots \mathrm{d}\mathbf{r}_N |\Psi(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N)|^2.$$
(2.3)

The density satisfies the N particle number constraint

$$\int d\mathbf{r} \ \rho(\mathbf{r}) = N. \tag{2.4}$$

The wave function  $|\Psi\rangle$  depends on the potential  $v(\mathbf{r})$  through Eq.(2.2), then the density, Eq.(2.3), is also a functional of  $v(\mathbf{r})$ . Density associated with the (anti-symmetric) ground state wave function of a Hamiltonian like Eq.(2.1) is called *v*-representable. Hohenberg and Kohn [36] pointed out interesting properties related with the *v*-representability.

**Theorem 1**: the external potential  $v(\mathbf{r})$  is a unique functional of the density  $\rho(\mathbf{r})$ , apart from a trivial additive constant.

The theorem establishes a one-to-one mapping between the v-representable density and the external potential  $v(\mathbf{r})$ . The ground state wave function is the mediator of this relation, in fact  $v(\mathbf{r})$  determines  $\hat{H}$ , which determines  $|\Psi\rangle$ , which defines  $\rho$  and the chain rules equivalently in the opposite direction.

All the information about the interacting system of fermions is included in the function  $\rho(\mathbf{r})$ . In fact, the density determines the ground-state properties, such as the number of electrons N, in Eq.(2.4), and the energy functional

$$E_{v}[\rho] = T[\rho] + V_{ee}[\rho] + U_{ext}[\rho] = F_{HK}[\rho] + \int d\mathbf{r} \ \rho(\mathbf{r})v(\mathbf{r}), \qquad (2.5)$$

where the universal functional,  $F_{HK}[\rho] \equiv \langle \Psi | \hat{T} + \hat{V}_{ee} | \Psi \rangle$ , is separated from the *v*-dependent part.  $F_{HK}[\rho]$  is defined "universal" because it is the same for all the systems with density  $\rho$ , independently from the details of the external potential. For the ground state density  $\rho_0$ , the energy functional  $E_v[\rho_0]$  is equal to the ground state energy  $E_0$ .

**Theorem 2**: for a trial density  $\tilde{\rho}(\mathbf{r})$ , such that  $\tilde{\rho}(\mathbf{r}) \ge 0$  and  $\int d\mathbf{r} \ \tilde{\rho}(\mathbf{r}) = N$ , it results  $E_v[\tilde{\rho}] \ge E_0$ , i.e., the functional  $E_v[\tilde{\rho}]$  assumes its minimum if  $\tilde{\rho} = \rho_0$ .

Alternatively it can be said that for all the *v*-representable densities  $\rho(\mathbf{r})$  constrained to  $\int d\mathbf{r} \ \rho(\mathbf{r}) = N$ , the ground-state density  $\rho_0$  is the one that minimize the total energy:

$$E_v[\rho] \geqslant E_v[\rho_0]. \tag{2.6}$$

#### 2.2 Levy-Lieb constrained-search

The v-representability is a strict condition that not all the density can satisfy. For example a density obtained from degenerate ground state wave functions is not v-representable. This condition can be relaxed by considering N-representable density, which means density obtained from antisymmetric wave function that satisfies  $\rho(\mathbf{r}) \ge 0$ ,  $\int d\mathbf{r} \ \rho(\mathbf{r}) = N$  and  $\int d\mathbf{r} |\nabla \rho^{1/2}(\mathbf{r})|^2 < \infty$ .

Furthermore, given the ground state density  $\rho_0$ , there can be found an infinite number of wave functions  $|\Psi\rangle$  that square integrated give  $\rho_0$  (we write  $\Psi \to \rho_0$ ), including the ground state wave function  $|\Psi_0\rangle$ . Determining  $|\Psi_0\rangle$  from  $\rho_0$  is not trivial and it requires to consider the minimum energy principle of the ground state. In fact, the ground state wave function is the one that minimizes the energy functional and therefore the functional  $F_{HK}[\rho]$  as

$$F_{HK}[\rho_0] = \langle \Psi_0 | \hat{T} + \hat{V}_{ee} | \Psi_0 \rangle = \min_{\Psi \to \rho_0} \langle \Psi | \hat{T} + \hat{V}_{ee} | \Psi \rangle.$$
(2.7)

Levy [37] and Lieb [38, 39, 40] suggested a solution that eliminates the restriction on the v-representability in the Hohenberg-Kohn variational principle (see Eq.(2.6)) and determines the ground-state wave function  $|\Psi_0\rangle$ . This procedure is called constrained-search. The Levy-Lieb functional  $F_{LL}$  is an extension of the  $F_{HK}$ functional, and it is defined as

$$F_{LL}[\rho] \equiv \min_{\Psi \to \rho} \langle \Psi | \hat{T} + \hat{V}_{ee} | \Psi \rangle, \qquad (2.8)$$

where  $\rho$  is a N-representable density. The minimization of the energy is carried out in two steps:

$$E_{0} = \min_{\Psi} \langle \Psi | \hat{T} + \hat{V}_{ee} + \sum_{i=1}^{N} v(\mathbf{r}_{i}) | \Psi \rangle$$

$$= \min_{\rho} \left\{ \min_{\Psi \to \rho} \langle \Psi | \hat{T} + \hat{V}_{ee} + \sum_{i=1}^{N} v(\mathbf{r}_{i}) | \Psi \rangle \right\}$$

$$= \min_{\rho} \left\{ \min_{\Psi \to \rho} \left[ \langle \Psi | \hat{T} + \hat{V}_{ee} | \Psi \rangle + \int d\mathbf{r} \ \rho(\mathbf{r}) v(\mathbf{r}) \right] \right\}$$

$$= \min_{\rho} \left\{ F_{LL}[\rho] + \int d\mathbf{r} \ \rho(\mathbf{r}) v(\mathbf{r}) \right\} \equiv \min_{\rho} E[\rho].$$
(2.9)

The inner minimization is restricted to the wave functions that give a certain density profile  $\rho$ , while the outer minimization runs over all N-representable  $\rho$ . In such a way, an universal functional  $F_{LL}[\rho]$  and an energy functional minimum principle are obtained for N-representable densities.

#### 2.3 Kohn-Sham method

The Hohenberg-Kohn theorems and the Levy-Lieb constrained-search indicate the existence and other properties of the ground-state density, without giving practical

recipe how to calculate it. Help in this direction comes from the Kohn-Sham method [41].

We consider a system of non-interacting electrons, with N-representable groundstate density  $\rho(\mathbf{r})$ . Kohn and Sham suggested to represent such density by specific single-particle orbitals  $|\phi_i\rangle$ . These Kohn-Sham orbitals are assumed to satisfy the one-particle Schrödinger equations

$$\hat{h}_{KS}|\phi_i(\mathbf{r})\rangle = \left[-\frac{\hbar^2}{2m_e}\nabla^2 + v_{KS}(\mathbf{r})\right]|\phi_i(\mathbf{r})\rangle = \epsilon_i|\phi_i(\mathbf{r})\rangle, \qquad (2.10)$$

with the one-body Hamiltonian  $\hat{h}_{KS}$ , the Kohn-Sham (external) potential  $v_{KS}(\mathbf{r})$ and the single-particle energies  $\epsilon_i$ . Due to the fact that the electrons do not interact among themselves in this system, we can rewrite the many-body Hamiltonian  $\hat{H}_{KS}$ by the sum of one-body Hamiltonians as

$$\hat{H}_{KS} = \sum_{i=1}^{N} \hat{h}_{KS}^{(i)} = \sum_{i=1}^{N} \left[ -\frac{\hbar^2}{2m_e} \nabla_i^2 \right] + \int d\mathbf{r} \ v_{KS}(\mathbf{r}) \hat{\rho}(\mathbf{r}).$$
(2.11)

The eigenstates of  $\hat{H}_{KS}$  are given by the Slater determinant  $|\Phi_{KS}\rangle$  built of the Kohn-Sham orbitals. The ground-state density results

$$\rho(\mathbf{r}) = \langle \Phi_{KS} | \hat{\rho}(\mathbf{r}) | \Phi_{KS} \rangle = \sum_{i=1}^{N} |\phi_i(\mathbf{r})|^2, \qquad (2.12)$$

namely, the density is determined by these specific orbitals. The ground-state of the system reads

$$E_{KS}[\rho] = \langle \Phi_{KS} | \hat{H}_{KS} | \Phi_{KS} \rangle = T_{KS}[\rho] + \int d\mathbf{r} \ v_{KS}(\mathbf{r})\rho(\mathbf{r}), \qquad (2.13)$$

where  $T_{KS}[\rho] \equiv \sum_{i=1}^{N} \langle \phi_i | - \frac{\hbar^2}{2m_e} \nabla^2 | \phi_i \rangle$  is the kinetic energy of a system of noninteracting electrons with density  $\rho$ . Applying the Hohenberg-Kohn theorems to the non-interacting system  $(V_{ee}=0)$ ,  $T_{KS}[\rho]$  appears as a universal functional, after defining it in the restricted domain of v-representable densities. The extension of the functional  $T_{KS}[\rho]$  to N-representability is a conjecture with open discussions about the methods to accomplish it [35].

When we are interested in characterizing the potential  $v_{KS}(\mathbf{r})$ , we look now at an interacting system described by Eq.(2.1) with the same ground-state density  $\rho(\mathbf{r})$  of the Kohn-Sham system. For the former, we rearrange the universal functional  $F_{HK}[\rho]$  introducing the exchange-correlation functional  $E_{xc}[\rho]$ , that is,

$$F_{HK}[\rho] \equiv T_{KS}[\rho] + E_H[\rho] + E_{xc}[\rho].$$
(2.14)

Here the Hartree functional  $E_H[\rho]$  represents the classical Coulomb interaction, i.e., the direct term of  $V_{ee}[\rho]$ ,

$$E_H[\rho] = \frac{1}{2} \int d\mathbf{r} \, d\mathbf{r}' \, \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}.$$
(2.15)

The exchange and correlation energies are included in the functional  $E_{xc}[\rho]$ , that we can rewrite as  $E_{xc}[\rho] = T[\rho] - T_{KS}[\rho] + V_{ee}[\rho] - E_H[\rho]$ , pointing out the difference between the true  $T[\rho]$  and the Kohn-Sham  $T_{KS}[\rho]$  kinetic energy functionals. The minimum condition, Eq.(2.6), is equivalent to require

$$\frac{\delta F_{HK}[\rho]}{\delta \rho(\mathbf{r})} = -v(\mathbf{r}). \tag{2.16}$$

Expressing  $F_{HK}[\rho]$  by Eq.(2.14), and using Eq.(2.13) for the Kohn-Sham kinetic functional, Eq.(2.16) provides the expression of the Kohn-Sham effective potential as

$$v_{KS}(\mathbf{r}) = v(\mathbf{r}) + v_H(\mathbf{r}) + v_{xc}(\mathbf{r}), \qquad (2.17)$$

where the Hartree potential is  $v_H(\mathbf{r}) \equiv \int d\mathbf{r}' \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$  and the exchange-correlation potential is  $v_{xc}(\mathbf{r}) \equiv \frac{\delta E_{xc}[\rho]}{\delta \rho(\mathbf{r})}$ .

The derivation of the Kohn-Sham potential is fundamental to link the noninteracting system with the interacting one. The Kohn-Sham method suggests that the ground-state energy of interacting electrons can be obtained as the ground-state energy of non-interacting electrons with the same ground-state density of the interacting ones and the effective Kohn-Sham potential  $v_{KS}(\mathbf{r})$ .

Looking at the components on the right-hand side of Eq.(2.17),  $v_{KS}(\mathbf{r})$  depends on the density  $\rho$ , then Eq.(2.10) needs to be solved self-consistently.

At this point the principal difficulties are located in finding a good approximation for the exchange-correlation functional  $E_{xc}[\rho]$ . The Linear Density Approximation (LDA) considers the system locally equivalent to the homogeneous electron gas of density  $\rho(\mathbf{r})$ , meaning that the exchange-correlation functional takes the form

$$E_{xc}^{LDA}[\rho] = \int d\mathbf{r} \left[ \epsilon_x(\rho(\mathbf{r})) + \epsilon_c(\rho(\mathbf{r})) \right].$$
 (2.18)

 $\epsilon_x(\rho)$  and  $\epsilon_c(\rho)$  represent respectively the exchange and correlation energy per volume unit for a homogeneous system of density  $\rho$ .

More accurate expressions are studied in the Generalized Gradient Approximation (GGA) [42], where

$$E_{xc}^{GGA}[\rho] = E_{xc}^{LDA}[\rho] + \int d\mathbf{r} f(\rho(\mathbf{r}), \nabla \rho(\mathbf{r})), \qquad (2.19)$$

i.e., the exchange-correlation functional is expanded in functionals of the density and its gradient. The LDA is the zero-order term of such expansion.

#### 2.4 Nuclear Density Functional Theory

Extending the density functional method to the nucleus faces new challenges. On the one hand, the electronic system is subject to the external potential, usually due to the interaction with the charged nuclei. This interaction has the effect of localizing the electronic density. On the other hands, the nucleus is a self-bound system, due to the attractive strong force among nucleons, which is responsible for the nuclear density localization.

Moreover, on the one hand, the electrons interact among themselves through the well-established Coulomb force, which is a two-body interaction. On the other hand, the nuclear interaction at the level of nucleons involves two-body and three-body terms at least. As discussed in Section 1.1, it is formed by a long-range part, the pion-exchange and Coulomb potentials, and by a short-range part, described by a contact interaction. In the vertex of the contact interaction all the high-energy contributions are integrated out.

Experimental evidence shows that the inner part of the nucleus has almost constant density  $\rho_{sat} \approx 0.16 \text{ fm}^{-3}$ , and the density sharply drops down at the surface, which has a thickness of around 0.6 fm. The Pauli exclusion principle and the range of nuclear interaction, around 1 fm, shorter than the average distance between two nucleons  $2r_0 \approx 2.5$  fm, suggest that the nucleons experience the mutual interaction not so often. In fact, inside the nucleus the nucleon mean free path is of the order of the nuclear radius [43].

The mean-field theory can be used to describe such system, namely the nucleons move in an average potential created by the mutual interaction with the other nucleons. This consideration leaded to formulation of several mean-fields, among them stands the famous empirical Woods-Saxon potential [6].

At the same time, the shell model picture proposed the idea of single-particle orbitals filled by the nucleons, interacting through a residual potential.

The Nuclear Energy Density Functional theory attempts to connect the mean-field approximation with the orbital representation characteristic to the Kohn-Sham method. This requires to construct a functional to be employed in the framework of a microscopic mean-field approach, in nuclear physics known as the Hartree-Fock method. The many-body Hamiltonian  $\hat{H}$  for a system of A nucleons can be written as

$$\hat{H} = -\sum_{i=1}^{A} \frac{\hbar^2}{2m_N} \nabla_i^2 + \frac{1}{2} \sum_{i \neq j=1}^{A} \hat{V}(i,j), \qquad (2.20)$$

where  $m_N$  is the average nucleon mass and  $\hat{V}(i, j)$  is a two-body potential (threebody and many-body terms are neglected at the moment for simplicity). We assume that the ground-state solution of Eq.(2.20) is described by a Slater determinant  $|\Phi\rangle$  of single-particle states  $\phi_i$ . With the orbital  $\phi_i$  we indicate the wave function  $\phi_i(\mathbf{r}, \sigma, \tau)$  in the space-spin-isospin coordinates, which is equivalent to the ket  $|i\rangle$ . In second-quantization formalism,  $|i\rangle = a_i^{\dagger}|-\rangle$ , where the fermionic creation operator  $a_i^{\dagger}$  acts on the particle vacuum  $|-\rangle^{-1}$ . It results

$$|\Phi\rangle = \prod_{i=1}^{A} a_i^{\dagger} |-\rangle.$$
(2.21)

We recall that the complete set  $\{a_i^{\dagger}\}$  can be expanded on another complete set of eigenstates, a basis  $\{c_k^{\dagger}\}$ , through an unitary transformation. In the many-body nuclear physics, it is common practice to use the harmonic oscillator wave functions as basis in which expand the solutions. In fact, in the harmonic oscillator problem the wave functions are localized, i.e., their values approach zero at large distance  $|\mathbf{r}|$ .

In second-quantization, we rewrite the Hamiltonian  $\hat{H}$  in Eq.(2.20) as

$$\hat{H} = \hat{T} + \hat{V} = \sum_{ij} \langle i | \hat{T} | j \rangle \, a_i^{\dagger} a_j + \frac{1}{4} \sum_{ijkl} \langle ij | \hat{V} | kl \rangle \, a_i^{\dagger} a_j^{\dagger} a_l a_k, \qquad (2.22)$$

where  $\langle i|\hat{T}|j\rangle$  and  $\langle ij|\hat{V}|kl\rangle$  are respectively the kinetic one-body and the (antisymmetrized) potential two-body matrix elements.

The expectation value of the Hartree-Fock energy defines the energy functional as [44]

$$E_{HF}[\rho] \equiv \langle \Phi | \hat{H} | \Phi \rangle$$
  
=  $\sum_{i=1}^{A} \langle i | \hat{T} | i \rangle + \frac{1}{2} \sum_{i,j=1}^{A} \langle i j | \hat{V} | i j \rangle,$  (2.23)

<sup>&</sup>lt;sup>1</sup> The hermitian conjugate of the creation operator is represented by the annihilation or destruction operator  $a_i$ .  $a_i^{\dagger}$  and  $a_i$  obey the anticommutation rules for fermionic operators  $\left\{a_i, a_j^{\dagger}\right\} = \delta_{ij}$ .

where in the last line we applied the Wick theorem [45], and, after defining the one-body density matrix  $\rho_{ji} \equiv \langle \Phi | a_i^{\dagger} a_j | \Phi \rangle$ , we used that  $\rho_{ji} = \delta_{ji}$ . The minimization of the functional  $E_{HF}[\rho]$  with respect to the constrained density  $\rho$  can be replaced by a constrained variation respect to the single-particle states  $\phi_i^*$  as

$$\frac{\delta}{\delta\phi_j^*} \left[ E_{HF}[\rho] - \sum_{j=1}^A \epsilon_j \int d\mathbf{r} |\phi_j(\mathbf{r})|^2 \right] = 0.$$
(2.24)

Eq.(2.24) gives the set of Hartree-Fock single-particle equations as

$$-\frac{\hbar^2}{2m_N}\nabla^2\phi_j(\mathbf{r}) + \int d\mathbf{r}' V(\mathbf{r},\mathbf{r}') \left[\rho(\mathbf{r}')\phi_j(\mathbf{r}) - \rho(\mathbf{r}',\mathbf{r})\phi_j(\mathbf{r}')\right] = \epsilon_j\phi_j(\mathbf{r}). \quad (2.25)$$

These coupled equations need to be solved self-consistently. In fact, each singleparticle state depends on the mean field generated by the total density as shown in the integrand. Schematically the procedure consists of the following steps:

- 1. starting with a reasonable guess for  $\phi_i$ ;
- 2. calculating  $\rho$  from  $\phi_i$ ;
- 3. calculating the integrand in Eq.(2.25) with  $\rho$ ;
- 4. solving the Hartree-Fock equations to obtain new  $\phi_i$ ;
- 5. repeating the loop of steps 2 to 4 until the convergence of the solution, i.e., when the difference between the new solution and the previous one is smaller than a fixed value. The difference in the value of  $E_{HF}$  is commonly used as index of convergence.

In term of single-particle energies the ground-state energy in Eq.(2.23) becomes

$$E_{HF} = \sum_{i=1}^{A} \epsilon_i - \frac{1}{2} \sum_{i,j=1}^{A} \langle ij | \hat{V} | ij \rangle.$$
(2.26)

The single-particle equations Eq.(2.25) are formally similar to the Kohn-Sham equations Eq.(2.10), but they are conceptually diverse. The Kohn-Sham method reformulates the interacting problem to solve it exactly, while the Hartree-Fock method replaces the initial many-body problem by a simpler one-body problem. Here, the Hartree-Fock technique has been presented as the procedure to obtain Kohn-Sham like equations in the context of nuclear interaction.

### 2.5 Interactions and Skyrme energy density functionals

The interaction  $\hat{V}$  needs to satisfy the symmetry properties relevant for the nuclear system. We recall that, once the symmetry operator can be written as  $\hat{P}$ , the

Hamiltonian  $\hat{H}$  is invariant under  $\hat{P}$  if  $\hat{H}$  commutes with  $\hat{P}$ , that is,  $[\hat{H}, \hat{P}] = 0$ . Important symmetries are:

- Hermiticity,  $\hat{V}^{\dagger} = \hat{V}$ , such that the Hamiltonian  $\hat{H}$  has real eigenvalues.
- Invariance under exchange of particles,  $\hat{V}(1,2) = \hat{V}(2,1)$ .
- Translational invariance, represented by  $\hat{P} = e^{(i\mathbf{a}\cdot\hat{\mathbf{K}})}$ , where **a** is the shift vector and  $\hat{\mathbf{K}}$  is the total linear momentum operator.
- Rotational invariance, represented by  $\hat{P} = e^{(i\alpha \cdot \hat{\mathbf{J}})}$ , where  $\alpha$  is the rotation angle and  $\hat{\mathbf{J}}$  is the total angular momentum operator.
- Isospin invariance, represented by  $\hat{P} = e^{(i\beta \cdot \hat{\mathbf{T}})}$ , where  $\beta$  is the iso-rotation angle and  $\hat{\mathbf{T}}$  is the total isospin operator.
- Galileian invariance, that is,  $\hat{V}$  does not change if the system moves at constant velocity (for non-relativistic systems).
- Particle-number invariance,  $\hat{P} = e^{(i\theta\hat{N})}$ , with gauge angle  $\theta$  and total particle number operator  $\hat{N}$ , standing that the number of particles is fixed to A.
- Space reflection,  $\hat{P} = \prod_{i=1}^{A} \hat{\pi}_i$ , where  $\hat{\pi}_i$  is the particle parity operator, setting that the total parity is conserved.
- Time-reversal, represented by  $\hat{P} = e^{(i\pi\hat{S}_y)\hat{C}}$ , where  $\hat{S}_y$  is the y-component of the total spin operator and  $\hat{C}$  is the complex conjugation operator.

Such symmetries put limits to the possible form of the interaction. The potential must be a scalar, containing functions of the relative coordinates  $\mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2$ , of the square of relative momentum  $\mathbf{k}^2$ , where  $\mathbf{k} \equiv -\frac{i}{2} (\nabla_1 - \nabla_2)$ , of the spin-orbit product  $\mathbf{L} \cdot \mathbf{S}$ .

Including the spin and isospin-exchange operators [46],

$$P^{\sigma} = \frac{1}{2}(1 + \sigma_1 \cdot \sigma_2), \qquad (2.27)$$

$$P^{\tau} = \frac{1}{2} (1 + \tau_1 \cdot \tau_2), \qquad (2.28)$$

in the central potential facilitates the saturation of the nuclear density, the condition when the kinetic energy and the repulsive part of the potential balance the strong attractive part.

Furthermore, in order to obtain a distribution of nuclear levels comparable to the experimental one, a density-dependent term needs to be added to the two-body interaction, as shown in Ref. [47].

Many phenomenological interactions have been developed to built energy functionals and among them three families gain large success in their application. They use finite-range, zero-range or relativistic interactions [48] to describe the nuclear structure. The latter kind is just mentioned here since we consider the non-relativistic approach to the nuclear many-body problem. The finite-range Gogny interaction [49, 50], written as  $^2$ 

$$\hat{V}_{Gogny}(\mathbf{r_1} - \mathbf{r_2}) = \sum_{j=1}^{2} e^{\frac{|\mathbf{r_1} - \mathbf{r_2}|^2}{\mu_j^2}} (W_j + B_j \hat{P}^{\sigma} - H_j \hat{P}^{\tau} - M_j \hat{P}^{\sigma} \hat{P}^{\tau}) + i W_{ls}(\hat{\sigma}_1 + \hat{\sigma}_2) \cdot \left[ \hat{\mathbf{k}}' \times \delta(\mathbf{r_1} - \mathbf{r_2}) \hat{\mathbf{k}} \right] + t_3 (1 + x_0 \hat{P}^{\sigma}) \delta(\mathbf{r_1} - \mathbf{r_2}) \rho^{\alpha} \left( \frac{\mathbf{r_1} + \mathbf{r_2}}{2} \right), \qquad (2.29)$$

is formed by two Gaussians to mimic the finite-range, by the spin-orbit and by the density dependent term.

The zero-range momentum-dependent Skyrme interaction [51, 52],

$$\hat{V}_{Skyrme}(\mathbf{r_1} - \mathbf{r_2}) = t_0(1 + x_0\hat{P}^{\sigma})\delta(\mathbf{r_1} - \mathbf{r_2}) 
+ \frac{1}{2}t_1(1 + x_1\hat{P}^{\sigma})\left[\hat{\mathbf{k}}^{\prime 2}\delta(\mathbf{r_1} - \mathbf{r_2}) + \delta(\mathbf{r_1} - \mathbf{r_2})\hat{\mathbf{k}}^2\right] 
+ t_2(1 + x_2\hat{P}^{\sigma})\hat{\mathbf{k}}^{\prime} \cdot \delta(\mathbf{r_1} - \mathbf{r_2})\hat{\mathbf{k}} 
+ iw_0(\hat{\sigma}_1 + \hat{\sigma}_2) \cdot \left[\hat{\mathbf{k}}^{\prime} \times \delta(\mathbf{r_1} - \mathbf{r_2})\hat{\mathbf{k}}\right] 
+ \frac{1}{6}t_3(1 + x_3\hat{P}^{\sigma})\delta(\mathbf{r_1} - \mathbf{r_2})\rho^{\alpha}\left(\frac{\mathbf{r_1} + \mathbf{r_2}}{2}\right),$$
(2.30)

presents the momentum-dependent, the spin-orbit and the density-dependent terms. These effective interactions are used to generate the energy functional as

$$E[\rho] = \langle \Phi | \hat{T} + \hat{V}[\rho] | \Phi \rangle.$$
(2.31)

For this reason, the terms in Eq.(2.29) or in Eq.(2.30) are considered the generators of the functional  $E[\rho]$ , which is commonly expressed by the energy density  $\mathcal{E}$  as

$$E[\rho] = \int d\mathbf{r} \, \mathcal{E}[\rho]. \tag{2.32}$$

The Gogny interaction generates functionals of non-local densities, like  $\rho(\mathbf{r}, \mathbf{r}')$ , while Skyrme functionals contain quasi-local ones, as  $\rho(\mathbf{r})$ .

Both include a certain number of parameters,  $(\mu_j, W_j, B_j, H_j, M_j, W_{ls}, t_3, x_0)$  in Gogny and  $(t_0, x_0, t_1, x_1, t_2, x_2, w_0, t_3, x_3)$  in Skyrme, that are fitted to reproduce

<sup>&</sup>lt;sup>2</sup>The notation  $\hat{\mathbf{k}}' \equiv \hat{\mathbf{k}}^{\dagger}$  indicates that the derivatives act on the  $\langle bra |$  side.

experimental data. In the literature, there are many parametrizations available, corresponding to different choices of experimental properties to be described. Varying the relative strength of the parameters corresponds to tune the singular terms of the interaction.

In this work we are interested in Skyrme-type energy density functionals.

The generators of the Skyrme interaction in Eq.(2.30), acting on the density matrix  $\rho(\mathbf{r}, \sigma, t; \mathbf{r}', \sigma', t') \equiv \sum_{i} \phi_i^*(\mathbf{r}, \sigma, t) \phi_i(\mathbf{r}', \sigma', t')$ , can produce the following densities:

• isoscalar one-body density

$$\rho_0(\mathbf{r}) = \rho_0(\mathbf{r}, \mathbf{r}') \big|_{\mathbf{r}=\mathbf{r}'} = \sum_{\sigma t} \rho(\mathbf{r}, \sigma, t; \mathbf{r}', \sigma, t) \big|_{\mathbf{r}=\mathbf{r}'}$$
(2.33)

• isovector one-body density

$$\rho_1(\mathbf{r}) = \rho_1(\mathbf{r}, \mathbf{r}') \big|_{\mathbf{r}=\mathbf{r}'} = \sum_{\sigma t} t \,\rho(\mathbf{r}, \sigma, t; \mathbf{r}', \sigma, t) \big|_{\mathbf{r}=\mathbf{r}'}$$
(2.34)

• kinetic energy density

$$\tau_T(\mathbf{r}) = \nabla \cdot \nabla' \rho_T(\mathbf{r}, \mathbf{r}') \big|_{\mathbf{r}=\mathbf{r}'}$$
(2.35)

• spin-density

$$\mathbf{s}_{T}(\mathbf{r}) = \sum_{\sigma \, \sigma' \, t} \rho_{T}(\mathbf{r}, \sigma, t; \mathbf{r}', \sigma', t) \langle \sigma' | \hat{\sigma} | \sigma \rangle \Big|_{\mathbf{r} = \mathbf{r}'}$$
(2.36)

• current density

$$\mathbf{j}_T(\mathbf{r}) = \mathbf{k} \,\rho_T(\mathbf{r}, \mathbf{r}') \big|_{\mathbf{r}=\mathbf{r}'} \tag{2.37}$$

• spin-current tensor

$$\mathbb{J}_T(\mathbf{r}) = \mathbf{k} \otimes \mathbf{s}_T(\mathbf{r}, \mathbf{r}') \big|_{\mathbf{r} = \mathbf{r}'}$$
(2.38)

often approximated by the spin-orbit current

$$\mathbf{J}_T(\mathbf{r}) = \sum_{ijk} \epsilon_{ijk} \, \hat{\boldsymbol{\imath}} \, [\mathbb{J}_T(\mathbf{r})]_{jk}$$
(2.39)

• kinetic spin-density

$$\mathbf{T}_T(\mathbf{r}) = \nabla \cdot \nabla' \mathbf{s}_T(\mathbf{r}, \mathbf{r}') \big|_{\mathbf{r}=\mathbf{r}'}.$$
 (2.40)

The index T = 0 distinguishes the isoscalar densities from the isovector (T = 1) ones. For example  $\rho_0 \equiv \rho_n + \rho_p$  and  $\rho_1 \equiv \rho_n - \rho_p$ .

The EDF is invariant under time-reversal, then it separately contains bilinear terms with time-even and time-odd densities as

$$\mathcal{E}_{Skyrme}(\mathbf{r}) = \sum_{T=0,1} (\mathcal{E}_T^{even} + \mathcal{E}_T^{odd}).$$
(2.41)

The time-even part results

$$\mathcal{E}_T^{even} = C_T^{\rho} \rho_T^2 + C_T^{\Delta \rho} \rho_T \Delta \rho_T + C_T^{\tau} \rho_T \tau_T + C_T^J \mathbb{J}_T^2 + C_T^{\nabla J} \rho_T \nabla \cdot \mathbf{J}_T.$$
(2.42)

The time-odd part, different from zero only in case of odd number of nucleons, is

$$\mathcal{E}_T^{odd} = C_T^s \mathbf{s}_T^2 + C_T^{\Delta s} \mathbf{s}_T \cdot \Delta \mathbf{s}_T + C_T^{sT} \mathbf{s}_T \cdot \mathbf{T}_T + C_T^{\nabla s} (\nabla \cdot \mathbf{s})^2 + C_T^j \mathbf{j}_T^2 + C_T^{\nabla j} \mathbf{s}_T \cdot \nabla \times \mathbf{j}_T.$$
(2.43)

The coefficients  $C_T^i$  are called coupling constants and are linear combinations of the Skyrme parameters. The density-dependent term is absorbed in the coupling constant  $C_T^{\rho} \equiv C_T^{\rho \ 0} + C_T^{\rho \ dd} \rho_0^{\alpha}$ .

We focus on studying even-even nuclei and for this reason the time-odd part of the functional will be neglected later.

Eq.(2.42) and Eq.(2.43) have been derived from the generators of the interaction in Eq.(2.30) [44].

The total energy of the Skyrme-type functional results

$$E[\rho] = \int d\mathbf{r} \left[ \mathcal{E}_{kin}(\mathbf{r}) + \mathcal{E}_{Skyrme}(\mathbf{r}) \right] + E_{Coul}, \qquad (2.44)$$

including the kinetic energy density

$$\mathcal{E}_{kin}(\mathbf{r}) \equiv -\frac{\hbar^2}{2m_N} \tau_0(\mathbf{r}), \qquad (2.45)$$

and the Coulomb energy

$$E_{Coul} = \frac{e^2}{4\pi\epsilon_0} \int d\mathbf{r} d\mathbf{r}' \, \left[ \frac{\rho_{ch}(\mathbf{r})\rho_{ch}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} - \frac{\rho_{ch}^2(\mathbf{r}, \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \right], \qquad (2.46)$$

with the charge density  $\rho_{ch}$ .

### 3. Development of EDFs

Phenomenological energy density functionals can be constructed without a connection to the underlying Hamiltonian, but building them from bilinear terms of local densities and their derivatives, that are invariant with respect to translational, rotational, isospin, parity and time-reversal transformations. The pairing sector (see Section 3.1) can be described by a potential other than the force used in the particle-hole channel. The exchange terms can be treated in simplified forms, as in the case of the Slater approximation of the Coulomb exchange term. The density-dependent part of the potential can contain a non-integer power of the density,  $\alpha$  in Eqs.(2.29) or (2.30), as in the functional SLy4 [53]. Functionals can be formed by terms coming from finite-range interactions and from realistic microscopic interactions, as in the functional BCPM [54]. This large freedom in the selection of the building terms lead to an extended phenomenology of EDFs, complementary to the functionals derived in Sections 2.4 and 2.5. The most general total energy assumes the form

$$E = E_{kin} + E_{int} + E_{Coul} + E_{pair} - E_{spur}, \qquad (3.1)$$

with the pairing energy  $E_{pair}$  and the correction for spurious motion  $E_{spur}$ . Spurious effects, like self-interaction terms, can appear when the functional is not derived from a Hamiltonian or when the theory is extended beyond the mean-field approximation. Such difficulties, discussed in the Section 3.2, recommend the use of energy density functionals derived from generators rather than functionals built without an underlying Hamiltonian.

#### 3.1 Pairing and Hartree-Fock-Bogoliubov equations

Pairing effects are relevant to describe the stability of nuclear systems [5]. In the EDF theory pairing can be included, for example, through an effective density-dependent interaction that gives

$$E_{pair} = \sum_{q=p,n} \frac{V_q}{4} \int d\mathbf{r} \left[ 1 - \left(\frac{\rho(\mathbf{r})}{\rho_c}\right)^{\beta} \right] \tilde{\rho}_q(\mathbf{r}) \tilde{\rho}_q^*(\mathbf{r}), \qquad (3.2)$$

where  $\rho_c$  is called "switching" density and  $\tilde{\rho}_q(\mathbf{r})$  is the pair density [55]. The choice of the parameter  $\rho_c$  selects the kind of pairing, namely  $\rho_c \to \infty$  represents volume pairing concentrated in the inner part of the nucleus, while  $\rho_c \approx \rho_{sat}$  is the surface pairing.

A formal way to introduce pairing in the mean-field approach is the Hartree-Fock-Bogoliubov (HFB) method. The Bogoliubov-de Gennes transformation,

$$\begin{pmatrix} b \\ b^{\dagger} \end{pmatrix} = \begin{pmatrix} U^{\dagger} & V^{\dagger} \\ V^T & U^T \end{pmatrix} \begin{pmatrix} a \\ a^{\dagger} \end{pmatrix} \equiv \mathcal{W}^{\dagger} \begin{pmatrix} a \\ a^{\dagger} \end{pmatrix}, \qquad (3.3)$$

defines the quasiparticle creation  $b^{\dagger}$  and annihilation b operators as linear combinations (matrices U and V) of particle operators a and  $a^{\dagger}$ . Such transformation  $\mathcal{W}$  is unitary ( $\mathcal{WW}^{\dagger} = \mathcal{W}^{\dagger}\mathcal{W} = \mathbb{1}$ ).

The quasiparticle vacuum of this theory is the product state

$$|\Phi_{HFB}\rangle = \prod_{i=1}^{A} b_i |-\rangle, \qquad (3.4)$$

that satisfies the condition  $b_i |\Phi_{HFB}\rangle = 0 \forall i$ . Quasiparticles represent excitations of the system: the ground state corresponds to the vacuum, a state without excitation, while excited states are produced adding quasiparticle creation operators to the vacuum.

The one-body density matrix is defined as [30]

$$\rho_{ij} = \langle \Phi_{HFB} | a_j^{\dagger} a_i | \Phi_{HFB} \rangle = \left( V^* V^T \right)_{ij} = \rho_{ji}^*, \tag{3.5}$$

and the pairing tensor (or abnormal density) as

$$\kappa_{ij} = \langle \Phi_{HFB} | a_j a_i | \Phi_{HFB} \rangle = \left( V^* U^T \right)_{ij} = -\kappa_{ji}.$$
(3.6)

They are the components of the generalized quasiparticle density

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix}. \tag{3.7}$$

In HFB theory there is a one-to-one mapping between the reference state  $|\Phi_{HFB}\rangle$ , the matrices (U, V) of the Bogoliubov transformation and the set of densities  $(\rho, \kappa)$ . The ground state is calculated by minimization of the Routhian

$$R(\lambda_p, \lambda_n) = E - \lambda_p \langle \Phi_{HFB} | \hat{N}_p | \Phi_{HFB} \rangle - \lambda_n \langle \Phi_{HFB} | \hat{N}_n | \Phi_{HFB} \rangle, \qquad (3.8)$$

with the Lagrange multipliers  $\lambda$  used to constrain the expectation value of the particle number operator  $\hat{N}$  for both protons and neutrons, since the particle number symmetry is broken.

The total energy E in the Routhian consists of a functional derived by an effective Hamiltonian  $\hat{H}$  as

$$E = \langle \Phi_{HFB} | \hat{H} | \Phi_{HFB} \rangle$$
  
=  $\sum_{ij} \langle i | \hat{T} | j \rangle \rho_{ji} + \frac{1}{2} \sum_{ijkl} \langle ij | \hat{V} | kl \rangle \rho_{ki} \rho_{lj} + \frac{1}{4} \sum_{ijkl} \langle ij | \hat{V} | kl \rangle \kappa_{ij}^* \kappa_{kl} = E[\rho, \kappa, \kappa^*],$   
(3.9)

or of a functional of the generalized density not fully linked to any underlying Hamiltonian as

$$E = E[\rho, \kappa, \kappa^*] = E[\mathcal{R}]. \tag{3.10}$$

Analogously to the Hartree-Fock equations, the minimization of Eq.(3.8) gives the HFB equations

$$\begin{pmatrix} h - \lambda_i & \Delta \\ -\Delta^* & -h^* + \lambda_i \end{pmatrix} \begin{pmatrix} U_i \\ V_i \end{pmatrix} = \epsilon_i \begin{pmatrix} U_i \\ V_i \end{pmatrix}, \qquad (3.11)$$

with  $h_{ij} \equiv \frac{\partial E}{\partial \rho_{ji}}$  and  $\Delta_{ij} \equiv \frac{\partial E}{\partial \kappa_{ij}^*}$ . In case of energy obtained from a two-body Hamiltonian, we obtain again the Hartree-Fock single-particle hamiltonian  $h_{ij} = \langle i | \hat{T} | j \rangle + \Gamma_{ij}$ , where the Hartree-Fock self-consistent field is

$$\Gamma_{ij} \equiv \sum_{kl} \langle ik | \hat{V} | jl \rangle \,\rho_{lk},\tag{3.12}$$

plus the pairing gap

$$\Delta_{ij} \equiv \frac{1}{2} \sum_{kl} \langle ij | \hat{V} | kl \rangle \, \kappa_{kl}. \tag{3.13}$$

The eigenvalues of the HFB equations appear in pairs  $\pm \epsilon_i$  and only one value for each pair is considered. By the Bloch-Messiah theorem [5], the solution can be expressed in the canonical basis (natural orbitals), in which the density matrix  $\rho_{ij}$ is diagonal and the pairing tensor appears in its canonical form.

#### **3.2** Beyond the mean-field approach

HFB, like HF, is a mean-field method constructed by single-reference energy density functionals (SR-EDF) because the ground state wave function  $|\Phi\rangle$  is represented by a single product state or Slater determinant. Such wave function describes
the nucleus on its intrinsic reference system, the center-of-mass frame, where the symmetries of the nuclear interaction are broken by the quasiparticle operators. As an example the ground state, linear combination of quasiparticle wave functions, mixes particle creation and annihilation operators, breaking the particle number, angular momentum and parity symmetries.

On the contrary, experimental observables are measured in the laboratory frame, where the symmetries are conserved. Transferring the mean-field wave function to the laboratory system requires the "beyond mean-field" approach. The broken symmetries are restored by projecting the wave function on good quantum numbers, conserved by the nuclear interaction. The operator  $\hat{S}$ , generator of the symmetry group, and  $\hat{H}$  commute. Nevertheless the solution  $|\Phi\rangle$  is obtained by symmetry breaking, and it makes necessary to project the product state on the eigenstate  $|s\rangle$ of  $\hat{S}$ , namely  $|s\rangle = \hat{P}^{S} |\Phi\rangle$ . The projection, performed by the operator  $\hat{P}^{S}$ , can be included at two stages: projection-after-variation (PAV) or variation-after-projection (VAP). In PAV procedure, the projection operator acts on the state, solution of the variational method. In VAP way, the variational equation is solved in the subset of projected state  $\hat{P}^{S}|\Phi\rangle$ . The domain of this subset is larger than the domain of  $|\Phi\rangle$  and, as a consequence, the VAP strategy can find a lower minimum than the PAV. These techniques demand the construction of a set of several product states (configuration mixing), usually performed by the generator coordinate methods (GCM). In this context, the functionals are named multi-reference energy density functionals (MR-EDF).

In GCM the many-fermion state is approximated by

$$|\Psi\rangle = \int \mathrm{d}q \ f(q)|\Phi(q)\rangle, \qquad (3.14)$$

where f(q) is the weight and  $|\Phi(q)\rangle$  indicates a family of product states (generator states) parametrized by the continuous generator coordinates q. Such family can be derived from the solution of the constrained variation

$$\delta R = \delta \left[ \frac{\langle \Phi(q) | \hat{H} | \Phi(q) \rangle}{\langle \Phi(q) | \Phi(q) \rangle} - \sum_{i} \lambda_i \langle \Phi(q) | \hat{O}_i | \Phi(q) \rangle \right] = 0, \qquad (3.15)$$

where the Lagrange multipliers  $\lambda_i$  are determined by the constraint  $\langle \Phi(q) | \hat{O}_i | \Phi(q) \rangle = q_i$  for the operators  $\hat{O}_i$ . These operators describe the relevant degrees of freedom for the system to be parametrized, like particle numbers, quadrupole moments, ... Introduced the energy kernel  $\mathcal{H}(q,q') \equiv \langle \Phi(q) | \hat{H} | \Phi(q') \rangle$  and the norm kernel  $\mathcal{I}(q,q') \equiv \langle \Phi(q) | \Phi(q') \rangle$ , we can rewrite the average energy as

$$E = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\int \mathrm{d}q \mathrm{d}q' \ f^*(q) \mathcal{H}(q, q') f(q')}{\int \mathrm{d}q \mathrm{d}q' \ f^*(q) \mathcal{I}(q, q') f(q')}.$$
(3.16)

The variation of E with respect to the weight gives the Hill-Wheeler equation [56]

$$\int \mathrm{d}q' \left[\mathcal{H}(q,q') - E\mathcal{I}(q,q')\right] f(q') = 0, \qquad (3.17)$$

from which the weight f(q) is determined.

The projected energy on a quantum number s reads

$$E^{s}(q) = \frac{\langle \Phi(q) | \hat{H} \hat{P}^{S} | \Phi(q) \rangle}{\langle \Phi(q) | \hat{P}^{S} | \Phi(q) \rangle}.$$
(3.18)

Projection techniques can experience spurious effects when the functional is not derived from a proper Hamiltonian. An irregular behavior of the energy projected on particle number was pointed out in Ref. [57], due to the presence of the density-dependent term. Successive works [58, 59, 60] proposed a regularization method to remove spurious states limited to the case of density-dependent functionals with integer power  $\alpha$ .

Inaccuracies can regard also the angular momentum projection, for which a simple regularization scheme is discussed in Ref. [61], to treat the situation when the norm kernel  $\mathcal{I}(q, q')$  is null in the denominator of E.

In the context of GCM, we can define the transition density matrix as

$$\bar{\rho}_{ij}(q,q') = \frac{\langle \Phi(q) | a_j^{\mathsf{T}} a_i | \Phi(q') \rangle}{\langle \Phi(q) | \Phi(q') \rangle}.$$
(3.19)

After applying the generalized Wick's theorem to the energy and norm kernel, the kernels appear to depend on transition densities, namely  $\mathcal{H}(q,q')[\tilde{\rho}]$  and  $\mathcal{I}(q,q')[\tilde{\rho}]$ . In this sense, the beyond mean-field approach manifests itself as an extended formulation of EDFs with transition densities.

#### **3.3** Current status of nuclear functionals

The state-of-art functionals provide ground state energies close to the experimental values along the whole nuclear chart (see Figure 3.1). The root-mean-square difference between the theoretical and experimental binding energies reached below 0.8 MeV in the optimization described in Ref. [62], using the Gogny D1M interaction with quadrupole corrections. The Skyrme-type functionals showed a root-mean-square of about 1.4 MeV within the UNEDEFO [63] parametrization. This level of accuracy, even if it appears small compared to total binding energies of few hundreds MeV, is not sufficient to provide valid theoretical estimates. Nuclear



Figure 3.1: Performance of energy density functionals. The difference between theoretical and experimental binding energies, y-axis, is plotted in function of the neutron number N, x-axis. Continuous lines represent isotopic chains. The arch structures are typical features when the parameters are fitted to magic nuclei: energies of closed-shell nuclei are more constrained than the extrapolated energies of mid-shell systems. (Left) Computationals D1S, D1N and D1M, Plot taken from Ref

(Left) Gogny-type functionals D1S, D1N and D1M. Plot taken from Ref. [62]. (Right) Skyrme-type functionals SLy4 [53] and UNEDEF0. Plot adapted from Ref. [63].

observables are measured with higher precision in laboratory, and models based on nuclear structure outputs are sensitive to small differences in the value of observables. Other properties of nuclei as radii, quadrupole deformations, and of infinite nuclear matter systems (see Appendix B) provide terms for comparison with the available data.

The choice of the observables, which enter as inputs in the optimization procedure of the functional parameters, influences the quality of the functional in reproducing the observables themselves. If the optimization is done properly, the fitted functional returns the correct values of observables for the nuclei included in the fit, and it provides model extrapolations for the other nuclei.

The comparison with experiment addresses the fundamental aspect of estimating uncertainties in theoretical results. In this direction the research have improved recently. The topic has been more and more discussed in the literature concerning theoretical methods in nuclear physics, particularly in the context of energy density functional with Skyrme-type interaction [64, 65, 66, 67, 68].

Error analysis not only makes a solid link between model estimates and data, but

also offers hints on the limits and weaknesses of the model itself. In Ref. [69], the study of uncertainties brought the authors to conclude that the optimization of EDFs based on standard Skyrme generators reached its best.

In order to improve the prediction power (the quality of the theoretical outputs) new terms need to be considered in the functionals. The form of the Skyrme interaction can be extended using new pseudopotentials with higher order derivatives [70, 71]. EDFs generated from regularized finite-range pseudopotential have been examined in Refs. [72, 73]. Other improvement can emerge by adding specific terms in the functional to study particular configurations, as done in the case of isopin-breaking generators [74].

More terms in the functionals entail more parameters to be optimized, then a larger database of experimental inputs needs to be considered, including deformed nuclei.

In this work I explore another direction, namely, we are interested in studying the information that *ab initio* interactions can transfer to EDFs, when the parameters of Skyrme-type functional are fitted to *ab initio* results.

The formal attempts to derive EDFs from first principle [33] deal with the density matrix expansion (DME) technique. In Refs. [75, 76] DME was used to relate mean-field calculations performed with realistic 2N interactions to results of the Skyrme-interaction. For a general purpose, building quasilocal functionals from an expansion of the non-local one-body density matrix is an useful method. The interaction energy for an arbitrary two-body potential  $\hat{V}(\mathbf{r}_1, \mathbf{r}_2)$  can be written in function of density matrices in coordinate space as

$$E_{int} = \frac{1}{2} \int \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2 \, \hat{V}(\mathbf{r}_1, \mathbf{r}_2) \left[ \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) - \rho(\mathbf{r}_2, \mathbf{r}_1) \rho(\mathbf{r}_1, \mathbf{r}_2) \right], \qquad (3.20)$$

where the exchange term, depending on the non-local density  $\rho(\mathbf{r}_1, \mathbf{r}_2)$ , makes the corresponding energy density nonlocal.

The non-locality issue is absent in the Skyrme interaction because it is zero-range and, due to the symmetry property of the  $\delta$ -interaction,  $\delta(\mathbf{r}_1 - \mathbf{r}_2)$ , the functional generated is quasilocal. Skyrme-EDFs are local (depending only on  $\mathbf{r}$ ) in the momentum-independent and density-dependent terms, while they are quasilocal (depending on the derivatives of local densities) in the momentum-dependent and spin-orbit parts.

DME, instead, produces quasilocal density functionals to approximate finite-range interactions. Following Ref. [77], introducing the coordinates  $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$ ,  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ , the derivatives  $\nabla \equiv \frac{\partial}{\partial \mathbf{R}}$ ,  $\partial \equiv \frac{\partial}{\partial \mathbf{r}}$ , the non-local density can be expanded

$$\rho(\mathbf{r}_1, \mathbf{r}_2) = \rho(\mathbf{R}, \mathbf{r}) 
= \nu_0(r)\rho(\mathbf{R}) + i\nu_1(r)r_a j_a(\mathbf{R}) 
+ \frac{1}{2}\nu_2(r)r_a r_b \left[\frac{1}{4}\nabla_a \nabla_b \rho(\mathbf{R}) - \tau_{ab}(\mathbf{R}) + \frac{1}{5}\delta_{ab}k_F^2 \rho(\mathbf{R})\right] + \dots, \quad (3.21)$$

where  $j_a(\mathbf{R}) \equiv -i\partial_a \rho(\mathbf{R}, \mathbf{r})_{r=0}$  and  $\tau_{ab}(\mathbf{R}) \equiv \nabla_a^{(1)} \nabla_b^{(2)} \rho(\mathbf{r}_1, \mathbf{r}_2)_{\mathbf{r}_1 = \mathbf{r}_2}$ .  $\nu_0(r), \nu_1(r)$  and  $\nu_2(r)$  are auxiliary functions that define the quasi-local approxima-

 $\nu_0(r)$ ,  $\nu_1(r)$  and  $\nu_2(r)$  are auxiliary functions that define the quasi-local approximation and correct the asymptotic behavior of the expansion. They depend on the Fermi momentum  $k_F$  and on the local density  $\rho(\mathbf{R})$ , through their derivation from infinite nuclear matter properties.

The direct and exchange parts of the energy become  $^{1}$  respectively

$$E_{int}^{dir} = \frac{1}{2} \int d\mathbf{R} \left[ V_0 \rho^2(\mathbf{R}) + \frac{1}{6} V_2 \rho(\mathbf{R}) \Delta \rho(\mathbf{R}) \right], \qquad (3.22)$$

$$E_{int}^{exc} = -\frac{1}{2} \int d\mathbf{R} \left[ V_{\nu 0}^{00} \rho^2(\mathbf{R}) + \frac{1}{3} V_{\nu 2}^{02} \left( \frac{1}{4} \rho(\mathbf{R}) \Delta \rho(\mathbf{R}) - \left( \rho(\mathbf{R}) \tau(\mathbf{R}) - \mathbf{j}^2 \right) + \frac{3}{5} k_F^2 \rho^2(\mathbf{R}) \right) + \dots \right], \qquad (3.23)$$

where in the square brackets we can recognize quasilocal energy density functionals  $\mathcal{E}_{int}(\mathbf{R})$ . The moments of the interaction,

$$V_n = \int \mathrm{d}\mathbf{r} \ r^n V(r), \qquad (3.24)$$

$$V_{\nu n}^{ij} = \int \mathrm{d}\mathbf{r} \ r^n \nu_i(r) \nu_j(r) V(r), \qquad (3.25)$$

are running coupling constant, dependent on  $k_F$  or  $\rho(\mathbf{R})$ , and they contain all the information of the short-range interaction relevant to study low-energy nuclear physics.

as

<sup>&</sup>lt;sup>1</sup>The two-body interaction is assumed to depend only on the distance between the coordinates,  $\hat{V}(\mathbf{r}_1, \mathbf{r}_2) = \hat{V}(r)$ .

# 4. Self-Consistent Green's Function method

Several methods are available to perform *ab initio* low-energy nuclear physics calculations, and in Section 1.1 the principal ones are listed. They employ different approaches and controlled approximations to solve the many-body Schrödinger equation. We choose to apply the Self-Consistent Green's Function method (SCGF) in this work. SCGF has an affinity with DFT, in fact, both can be included in the family of Green's function methods, that study the ground state through its response to external probes [33]. A specific analogy between SCGF and quasiparticle-DFT for the electron case was discussed in Ref. [78].

The Green's function method was firstly introduced in the literature to extend the knowledge of quantum field theory to the Schrödinger field.

The many-body problem is studied in terms of fundamental excitations of the system. These excitations, rather than all the particles, are used as degrees of freedom. In fact, the method does not attempt to calculate the full many-body wave function, but, it determines the propagation of single-particles excitations and the correlated density matrix  $\rho_{\alpha\beta}$  of the system.

In the coming Chapter, we present the corner stone of this method, the propagator, starting from the trivial case of non-interacting particles, moving to the general case of an interacting one. We linger on the Hartree-Fock approximation and finally we consider the beyond mean-field truncation schemes that are used in this work. The exposure follows Ref. [79], which contains further details.

# 4.1 The non-interacting propagator as starting point

We describe the non-interacting system of A fermions by a Hamiltonian  $\hat{H}_0 = \hat{T} + \hat{U}$ , where an auxiliary one-body potential  $\hat{U}$  is accounted for.

The ground state  $|\Phi_0^A\rangle$ , solution of  $\hat{H}_0|\Phi_0^A\rangle = E_0^{(0)}|\Phi_0^A\rangle$ , is represented by a Slater determinant  $|\Phi_0^A\rangle = \prod_{\alpha < F} a_{\alpha}^{\dagger}|0\rangle$  and the ground-state energy reads  $E_0^{(0)} = \sum_{\alpha < F} \epsilon_{\alpha}$ . *F* represents the Fermi energy, then all the single particle states  $|\alpha\rangle$  below *F* are occupied.

The unperturbed single-particle propagator (also called one-body Green's function) is defined as

$$G^{(0)}_{\alpha\beta}(t,t') = -\frac{i}{\hbar} \langle \Phi_0^A | \mathcal{T}[a_{\alpha_I}(t)a^{\dagger}_{\beta_I}(t')] | \Phi_0^A \rangle, \qquad (4.1)$$

with the time ordering operator for fermions  $\mathcal{T}[a_{\alpha_I}(t)a_{\beta_I}^{\dagger}(t')] \equiv \theta(t-t')a_{\alpha_I}(t)a_{\beta_I}^{\dagger}(t') - \theta(t'-t)a_{\beta_I}^{\dagger}(t')a_{\alpha_I}(t)$ <sup>1</sup>. The subscript  $_I$  stands for interaction picture, that is, the operators carry a time dependence of the form  $a_{\alpha_I}(t) \equiv e^{\frac{i}{\hbar}\hat{H}_0 t}a_{\alpha}e^{-\frac{i}{\hbar}\hat{H}_0 t}$ . The time-independent Hamiltonian  $\hat{H}_0$ , due to the time translation invariance of the system, makes the one-body Green's function dependent only on the time difference t - t'. Eq.(4.1) can be interpreted as the probability amplitude for adding a particle in a state  $\beta$  and removing it from a state  $\alpha$  after a time t - t', or generating a hole in a state  $\alpha$  and annihilating it from a state  $\beta$  after a time t' - t, on top of the ground state.

Using the single-particle eigenstates and writing explicitly the time factors, Eq.(4.1) becomes

$$G^{(0)}_{\alpha\beta}(t-t') = -\frac{i}{\hbar} \delta_{\alpha\beta} \left[ \theta(t-t') \,\theta(\alpha-F) e^{-\frac{i}{\hbar}\epsilon_{\alpha}(t-t')} - \theta(t'-t) \,\theta(F-\alpha) e^{\frac{i}{\hbar}\epsilon_{\alpha}(t'-t)} \right]. \tag{4.3}$$

Note that, for the unperturbed propagator, it can only be  $\alpha = \beta$  since these single-particle states are eigenstates of  $\hat{H}_0$ .

$$\theta(x) = \begin{cases} 1 & \text{for } x \ge 0\\ 0 & \text{for } x < 0 \end{cases}$$

It satisfies the relation

$$\theta(\pm x) = \mp \lim_{\eta \to 0^+} \frac{1}{2\pi i} \int \mathrm{d}E \frac{e^{-\frac{i}{\hbar}Ex}}{E \pm i\eta},\tag{4.2}$$

where the term  $\pm i\eta$  in the denominator stands for the proper boundary conditions imposed by causality.

<sup>&</sup>lt;sup>1</sup>  $\theta(x)$  is the step function, defined as

The Fourier transform of Eq.(4.3), with the help of Eq.(4.2), gives

$$G_{\alpha\beta}^{(0)}(E) = \delta_{\alpha\beta} \left[ \frac{\theta(\alpha - F)}{E - \epsilon_{\alpha} + i\eta} + \frac{\theta(F - \alpha)}{E - \epsilon_{\alpha} - i\eta} \right], \tag{4.4}$$

showing that, in the complex plan, the poles of  $G_{\alpha\beta}^{(0)}(E)$  appear at value of the energy E corresponding to the single-particle energies  $\epsilon_{\alpha}$ . The one-body density matrix for the non-interacting system reads <sup>2</sup>

$$\rho_{\alpha\beta}^{(0)} \equiv \langle \Phi_0^A | a_\beta^\dagger a_\alpha | \Phi_0^A \rangle = \int_{-\infty}^{\epsilon_F} \mathrm{d}E \, \frac{1}{\pi} \mathrm{Im} \, G_{\alpha\beta}^{(0)}(E) = \delta_{\alpha\beta} \, \theta(F - \alpha), \qquad (4.6)$$

namely the density is diagonal with value 1 corresponding to the single-particle states with energy smaller or equal than the hole Fermi energy  $\epsilon_F^-$ .

### 4.2 The interacting case

We consider now the general case of a nuclear system described by a Hamiltonian  $\hat{H} = \hat{H}_0 + \hat{H}_1$ , where the interaction part  $\hat{H}_1 = -\hat{U} + \hat{V}$  includes the residual interaction operator  $\hat{V}$  (only two-body terms for the moment).

The ground state is indicated by  $|\Psi_0^A\rangle$ , to be distinguished from the non-interacting solution  $|\Phi_0^A\rangle$ . The single-particle propagator associated with  $|\Psi_0^A\rangle$  is defined as

$$G_{\alpha\beta}(t-t') = -\frac{i}{\hbar} \langle \Psi_0^A | \mathcal{T}[a_{\alpha_H}(t)a_{\beta_H}^{\dagger}(t')] | \Psi_0^A \rangle, \qquad (4.7)$$

where the annihilation and creation operators appear in the Heisenberg picture  $_H$ , that is, the operators carry a time dependence as  $a_{\alpha_H}(t) \equiv e^{\frac{i}{\hbar}\hat{H}t}a_{\alpha}e^{-\frac{i}{\hbar}\hat{H}t}$ . Notice the exponentials with arguments  $\hat{H}$ , in contrast to the interaction picture with  $\hat{H}_0$ .  $\{|\alpha\rangle\}$  is any single-particle basis defined by the model space, chosen for (computational) convenience. The propagator in Eq.(4.7) is "dressed" by the many-body correlations included in the solution  $|\Psi_0^A\rangle$ . The Fourier transform and Eq.(4.2) hold

$$G_{\alpha\beta}(E) = \langle \Psi_0^A | a_\alpha \frac{1}{E - (\hat{H} - E_0^A) + i\eta} a_\beta^\dagger | \Psi_0^A \rangle + \langle \Psi_0^A | a_\beta^\dagger \frac{1}{E - (E_0^A - \hat{H}) - i\eta} a_\alpha | \Psi_0^A \rangle,$$
(4.8)

$$\frac{1}{x \pm i\eta} = \mathcal{P}\frac{1}{x} \mp i\,\pi\,\delta(x),\tag{4.5}$$

which uses the concept of principal value  $\mathcal{P}$ .

 $<sup>^{2}</sup>$ We can separate the real and imaginary part of the propagator through the equality

where  $E_0^A$  is the ground state energy,  $\hat{H}|\Psi_0^A\rangle = E_0^A|\Psi_0^A\rangle$ . The intermediate  $(A \pm 1)$ body system is introduced through the complete set of eigenstates  $|\Psi_n^{A+1}\rangle$ ,  $|\Psi_k^{A-1}\rangle$ with eigenvalues  $E_n^{A+1}$ ,  $E_k^{A-1}$ , leading to the spectral representation (called also Lehmann representation [80]) of the one-body Green's function

$$G_{\alpha\beta}(E) = \sum_{n} \frac{\langle \Psi_{0}^{A} | a_{\alpha} | \Psi_{n}^{A+1} \rangle \langle \Psi_{n}^{A+1} | a_{\beta}^{\dagger} | \Psi_{0}^{A} \rangle}{E - (E_{n}^{A+1} - E_{0}^{A}) + i\eta}$$
  
+ 
$$\sum_{k} \frac{\langle \Psi_{0}^{A} | a_{\beta}^{\dagger} | \Psi_{k}^{A-1} \rangle \langle \Psi_{k}^{A-1} | a_{\alpha} | \Psi_{0}^{A} \rangle}{E - (E_{0}^{A} - E_{k}^{A-1}) - i\eta}$$
  
$$\equiv G_{\alpha\beta}^{p}(E) + G_{\alpha\beta}^{h}(E).$$
(4.9)

In Eq.(4.9), n and k are indices for propagating quasi-particle (p) and quasi-hole (h) states, with excitation energies  $\epsilon_n^+ \equiv E_n^{A+1} - E_0^A$  and  $\epsilon_k^- \equiv E_0^A - E_k^{A-1}$ . The Fermi energy is usually taken as  $E_F = \frac{1}{2}(\epsilon_0^+ + \epsilon_0^-)$ , with  $\epsilon_0^+$  the lowest of particle states and  $\epsilon_0^-$  the highest of hole states.

The one-body spectral function  $S_{\alpha\beta}(E) = S^p_{\alpha\beta}(E) + S^h_{\alpha\beta}(E)$  can be extracted from Eq.(4.9). Its components are defined for the particle case  $(E \ge \epsilon_0^+)$  as

$$S^{p}_{\alpha\beta}(E) \equiv -\frac{1}{\pi} \operatorname{Im} G_{\alpha\beta}(E)$$
  
=  $\sum_{n} \langle \Psi^{A}_{0} | a_{\alpha} | \Psi^{A+1}_{n} \rangle \langle \Psi^{A+1}_{n} | a^{\dagger}_{\beta} | \Psi^{A}_{0} \rangle \, \delta(E - \epsilon^{+}_{n}), \qquad (4.10)$ 

and for the hole case  $(E \leq \epsilon_0^-)$  as

$$S^{h}_{\alpha\beta}(E) \equiv \frac{1}{\pi} \operatorname{Im} G_{\alpha\beta}(E)$$
  
= 
$$\sum_{k} \langle \Psi^{A}_{0} | a^{\dagger}_{\beta} | \Psi^{A-1}_{k} \rangle \langle \Psi^{A-1}_{k} | a_{\alpha} | \Psi^{A}_{0} \rangle \, \delta(E - \epsilon^{-}_{k}).$$
(4.11)

The diagonal part of the spectral function has the interesting physical interpretation of the probability of adding  $(S^p_{\alpha\alpha}(E))$  or removing  $(S^h_{\alpha\alpha}(E))$  one particle in the single-particle state  $|\alpha\rangle$ , leaving the (A + 1)-body system in a state with energy  $E^A_0 + E$  or the (A - 1)-body system with energy  $E^A_0 - E$ . To shorten the notation, we define the removal (addition) spectroscopic amplitude as

$$\mathcal{Y}_{\alpha}^{k} \equiv \langle \Psi_{k}^{A-1} | a_{\alpha} | \Psi_{0}^{A} \rangle \qquad \left( \mathcal{X}_{\alpha}^{n} \equiv \langle \Psi_{n}^{A+1} | a_{\alpha}^{\dagger} | \Psi_{0}^{A} \rangle \right).$$
(4.12)

The one-body density matrix  $\rho_{\alpha\beta}$  is obtained directly from the hole spectral function

$$\rho_{\alpha\beta} \equiv \langle \Psi_0^A | a_\beta^\dagger a_\alpha | \Psi_0^A \rangle = \int_{-\infty}^{\epsilon_0^-} \mathrm{d}E \, S^h_{\alpha\beta}(E) = \sum_k (\mathcal{Y}_\beta^k)^* \mathcal{Y}_\alpha^k. \tag{4.13}$$

After introducing the supplemental quantity  $d_{\alpha\beta} \equiv \langle \Psi_0^A | a_\alpha a_\beta^\dagger | \Psi_0^A \rangle = \int_{\epsilon_0^+}^{\infty} dE S^p_{\alpha\beta}(E)$ , the anti-commutation relation gives the sum rule for the spectroscopic function as

$$\int dE S_{\alpha\beta}(E) = \rho_{\alpha\beta} + d_{\alpha\beta} = \langle \Psi_0^A | a_\beta^{\dagger} a_\alpha + a_\alpha a_\beta^{\dagger} | \Psi_0^A \rangle = \delta_{\alpha\beta}.$$
(4.14)

The spectroscopic amplitudes define the theoretical spectroscopic factors (for removal or addition of one particle)

$$\mathcal{Z}_k \equiv \sum_{\alpha} |\langle \Psi_k^{A-1} | a_{\alpha} | \Psi_0^A \rangle|^2 = \sum_{\alpha} |\mathcal{Y}_{\alpha}^k|^2$$
(4.15)

$$\mathcal{Z}_n \equiv \sum_{\alpha} |\langle \Psi_n^{A+1} | a_{\alpha}^{\dagger} | \Psi_0^A \rangle|^2 \equiv \sum_{\alpha} |\mathcal{X}_{\alpha}^n|^2.$$
(4.16)

Spectroscopic factors carry information on how strongly the single-particle levels are occupied.

In experiment of knockout reactions <sup>3</sup> as [81], the comparison between theoretical and experimental cross sections shows a non trivial reduction of the spectroscopic strength of dominant quasiparticle states (see Eq.(4.48) below) with respect to predictions from independent-particle models. This constitutes an experimental evidence that the single-particle levels are only partially filled in a correlated system.

Any one-body operator  $\hat{O}^{1B}$  in the ground state can be calculated as function of the spectroscopic amplitudes as

$$\langle \Psi_0^A | \hat{O}^{1B} | \Psi_0^A \rangle = \sum_{\alpha\beta} O^{1B}_{\alpha\beta} \rho_{\beta\alpha} = \sum_k \sum_{\alpha\beta} (\mathcal{Y}_\alpha^k)^* O^{1B}_{\alpha\beta} \mathcal{Y}_\beta^k.$$
(4.18)

If the Hamiltonian contains only up to two-body interactions,  $\hat{H} = \hat{T} + \hat{V}$ , the ground state energy depends only on the knowledge of the one-particle propagator. In fact, the Migdal-Galitski-Koltun (MGK) sum rule [82, 83] establishes that

$$E_0^A = \langle \Psi_0^A | \hat{H} | \Psi_0^A \rangle = \sum_{\alpha\beta} \frac{1}{2} \int_{-\infty}^{\epsilon_0^-} \mathrm{d}E \left[ \langle \alpha | \hat{T} | \beta \rangle + E \,\delta_{\alpha\beta} \right] S_{\beta\alpha}^h(E). \tag{4.19}$$

<sup>3</sup>Knockout reactions are phenomena of peripheral scattering, in which one nucleon (or more nucleons) is removed from the projectile nucleus, due to the interaction between target and projectile nuclei. The valence nucleon, occupying the most weakly bound states of the projectile system, is ejected and the surviving core is measured. In the Plane Wave Impulse Approximation, the Fermi's golden rule estimates the differential knockout cross section as being proportional to the hole spectral function  $S^h$ :

$$d\sigma = K \,\sigma_{sp} \,S^h(\mathbf{p}, E),\tag{4.17}$$

where K is a kinematic factor,  $\sigma_{sp}$  is the single-particle cross section for the reaction under study, and  $S^h$  depends on the momentum and energy of the removed particle. The comparison between theoretical and experimental cross sections, the observables of the reaction, allows us to estimate spectroscopic factors.

### 4.3 Irreducible self-energy and Dyson equation

In order to account for the time evolution of the propagator in Eq.(4.7), it is convenient to consider its perturbative expansion in powers of the interacting Hamiltonian  $\hat{H}_1$  [79, 84]. The propagator results

$$G_{\alpha\beta}(t-t') = -\frac{i}{\hbar} \sum_{n=0}^{\infty} \left(\frac{i}{\hbar}\right)^n \frac{1}{n!} \int dt_1 \dots \int dt_n$$
$$\times \langle \Phi_0^A | \mathcal{T} \left[ \hat{H}_{1_I}(t_1) \cdots \hat{H}_{1_I}(t_n) a_{\alpha_I}(t) a_{\beta_I}^{\dagger}(t') \right] | \Phi_0^A \rangle_{conn}, \tag{4.20}$$

where  $\hat{H}_1$ ,  $a_{\alpha}$  and  $a_{\beta}^{\dagger}$  appear in the interaction picture with respect to  $\hat{H}_0$ , and the time ordering operator acts on the non-interacting solution  $|\Phi_0^A\rangle$ .  $\hat{H}_1$  (see Eq.(4.40)) can contain terms of one-, two- (or three-) body interactions, with their creation and annihilation operators. When performing the Wick contractions [45] of the time-ordered product of these operators, a large number of contributions

[45] of the time-ordered product of these operators, a large number of contributions appears. These contributions can be organized in schematic diagrams, Feynman diagrams, that keep track of the terms and symmetries arising from the contractions. Presenting the rules to construct the Feynman diagrams is out of the scope of this thesis, since we present Green's function formulas already derived in the literature. However, we discuss some of the properties of the diagrams with examples and intuitive arguments. Each Wick contraction produces an unperturbed propagator  $G^{(0)}$  (solid single lines) that can be attached to vertices (dots) of the interaction (dashed lines). To calculate the propagator in Eq.(4.20) only the connected diagrams are relevant, as indicated by the subscript <sub>conn</sub>. The concepts of connected, oneparticle reducible or irreducible diagrams are illustrated with examples in Figure 4.1(a-c). Contributions to the propagator can come from one-particle reducible or irreducible diagrams, and for all of them the irreducible parts can be grouped inside the irreducible self-energy  $\Sigma^*$  insertions (see Figure 4.1(d-e)). After Fourier transforming to energy and introducing  $\Sigma^*$ , the expansion in Eq.(4.20)) becomes

$$G_{\alpha\beta}(E) = G_{\alpha\beta}^{(0)}(E) + \sum_{\gamma\delta} G_{\alpha\gamma}^{(0)}(E) \Sigma_{\gamma\delta}^{\star}(E) G_{\delta\beta}^{(0)}(E) + \sum_{\gamma\delta\epsilon\phi} G_{\alpha\gamma}^{(0)}(E) \Sigma_{\gamma\delta}^{\star}(E) G_{\delta\epsilon}^{(0)}(E) \Sigma_{\epsilon\phi}^{\star}(E) G_{\phi\beta}^{(0)}(E) + \dots$$
(4.21)

All the terms of this infinite sum are included in the Dyson equation [85] as

$$G_{\alpha\beta}(E) = G^{(0)}_{\alpha\beta}(E) + \sum_{\gamma\delta} G^{(0)}_{\alpha\gamma}(E) \Sigma^{\star}_{\gamma\delta}(E) G_{\delta\beta}(E).$$
(4.22a)



Figure 4.1: Example of Feynman diagrams. Solid single (double) lines indicate the undressed propagators  $G^{(0)}$  (dressed propagators G) for fermionic states, with the direction of propagation shown by the arrows, dashed lines are used for interactions. Gray filled circles stand for irreducible self-energy  $\Sigma^{\star}$  insertions. Dots correspond to labels of single-particle states, as the indices in the definition of propagators, self-energies or in the matrix elements of the interactions. (a) Disconnected diagram, that does not contribute to Eq.(4.20). (b) Connected and one-particle irreducible diagram, that is, if one of the propagator lines is cut, the diagram will not result disconnected. (c) Connected and one-particle reducible digram, that is, it can be reduced to a disconnected diagram by cutting one solid line. In fact, opening the fermionic line, where indicated by the scissors mark, creates two disconnected diagrams. (d) Irreducible self-energy insertion, that include all connected diagrams that are one-particle irreducible, as the one in panel (b). (e) One-particle reducible diagram made with irreducible self-energy insertions. The diagram in panel (c), contributes to this diagram, since the irreducible parts of the diagram (c) can be included in the corresponding self-energy insertions. (f) Representation of the Dyson equation, Eq.(4.22).

The irreducible self-energy  $\Sigma_{\gamma\delta}^{\star}(E)$  represents the nonlocal and energy-dependent potential to which each nucleons is subject when interacting with the nuclear medium. Through the self-energy the unperturbed propagator  $G_{\alpha\beta}^{(0)}$  is dressed by the many-body correlations.

The diagrammatic expression of the self-energy arises through the Feynman expansion in Eq.(4.20) or equivalently when the Dyson equation is derived from the equation of motion for the propagator. We consider here the latter method.

The time derivative of the single-particle propagator reads

$$i\hbar\frac{\partial}{\partial t}G_{\alpha\beta}(t-t') = \frac{\partial}{\partial t}\langle\Psi_0^A|\mathcal{T}[a_{\alpha_H}(t)a_{\beta_H}^{\dagger}(t')]|\Psi_0^A\rangle = \cdots$$
$$= \delta(t-t')\delta_{\alpha\beta} + \epsilon_{\alpha}G_{\alpha\beta}(t-t') - \sum_{\gamma}\langle\alpha|U|\gamma\rangle G_{\gamma\beta}(t-t')$$
$$- \frac{i}{2\hbar}\sum_{\gamma\zeta\theta}\langle\alpha\gamma|V|\theta\zeta\rangle\langle\Psi_0^A|\mathcal{T}\left[a_{\gamma_H}^{\dagger}(t)a_{\zeta_H}(t)a_{\theta_H}(t)a_{\beta_H}^{\dagger}(t')\right]|\Psi_0^A\rangle.$$
(4.23)

In the last line,  $\langle \Psi_0^A | \mathcal{T} \left[ a_{\gamma_H}^{\dagger}(t) a_{\zeta_H}(t) a_{\theta_H}(t) a_{\beta_H}^{\dagger}(t') \right] | \Psi_0^A \rangle$  mimics the propagation of two quasiparticles and introduces a hierarchy between the (n + 1)- and the *n*-particle propagators.

The two-particle propagator, formally defined as

$$G^{II}_{\alpha\beta\gamma\delta}(t_{\alpha}, t_{\beta}, t_{\gamma}, t_{\delta}) = -\frac{i}{\hbar} \langle \Psi_{0}^{A} | \mathcal{T} \left[ a_{\beta_{H}}(t_{\beta}) a_{\alpha_{H}}(t_{\alpha}) a^{\dagger}_{\gamma_{H}}(t_{\gamma}) a^{\dagger}_{\delta_{H}}(t_{\delta}) \right] | \Psi_{0}^{A} \rangle, \quad (4.24)$$

can be expanded in power of the interaction  $\hat{H}_{1_I}$  as

$$G^{II}_{\alpha\beta\gamma\delta}(t_{\alpha}, t_{\beta}, t_{\gamma}, t_{\delta}) = -\frac{i}{\hbar} \sum_{n=0}^{\infty} \left(\frac{i}{\hbar}\right)^{n} \frac{1}{n!} \int \mathrm{d}t_{1} \dots \int \mathrm{d}t_{n} \\ \times \langle \Phi^{A}_{0} | \mathcal{T} \left[ \hat{H}_{1_{I}}(t_{1}) \cdots \hat{H}_{1_{I}}(t_{n}) a_{\beta_{I}}(t_{\beta}) a_{\alpha_{I}}(t_{\alpha}) a^{\dagger}_{\gamma_{I}}(t_{\gamma}) a^{\dagger}_{\delta_{I}}(t_{\delta}) \right] | \Phi^{A}_{0} \rangle_{conn}$$

$$(4.25)$$

where only the connected diagrams are counted. The infinite expansion can be simplified as shown in Ref. [86] with

$$G^{II}_{\alpha\beta\gamma\delta}(t_{\alpha}, t_{\beta}, t_{\gamma}, t_{\delta}) = i\hbar \left[G_{\alpha\gamma}(t_{\alpha} - t_{\gamma})G_{\beta\delta}(t_{\beta} - t_{\delta}) - G_{\alpha\delta}(t_{\alpha} - t_{\delta})G_{\beta\gamma}(t_{\beta} - t_{\gamma})\right] + (i\hbar)^{2} \int dt_{\epsilon} \int dt_{\zeta} \int dt_{\eta} \int dt_{\theta} \sum_{\epsilon\zeta\eta\theta} G_{\alpha\epsilon}(t_{\alpha} - t_{\epsilon})G_{\beta\zeta}(t_{\beta} - t_{\zeta}) \times \langle\epsilon\zeta|\Gamma(t_{\epsilon}, t_{\zeta}, t_{\eta}, t_{\theta})|\eta\theta\rangle G_{\eta\gamma}(t_{\eta} - t_{\gamma})G_{\theta\delta}(t_{\theta} - t_{\delta}),$$
(4.26)

where  $\Gamma$  is the four-points vertex function, representing an effective interaction between the particles in the medium.

The Dyson equation, Eq.(4.22), can be extracted from the equation of motion, Eq.(4.23), with the help of Eq.(4.26), some algebra and Fourier transforms. The

comparison gives the expression for the irreducible self-energy

$$\Sigma_{\gamma\delta}^{\star}(E) = -\langle \gamma | U | \delta \rangle - i \int_{C\uparrow} \frac{\mathrm{d}E'}{2\pi} \sum_{\mu\nu} \langle \gamma \mu | V | \delta\nu \rangle G_{\nu\mu}(E') + \frac{1}{2} \int \frac{\mathrm{d}E_1}{2\pi} \int \frac{\mathrm{d}E_2}{2\pi} \sum_{\epsilon\mu\nu\zeta\rho\sigma} \langle \gamma\mu | V | \epsilon\nu \rangle G_{\epsilon\zeta}(E_1) G_{\nu\rho}(E_2) \times G_{\sigma\mu}(E_1 + E_2 - E) \langle \zeta\rho | \Gamma(E_1, E_2, E, E_1 + E_2 - E) | \delta\sigma \rangle, \qquad (4.27)$$

where  $C \uparrow$  means that the integration is performed on the positive imaginary part of the complex plane.

We can summarize that the irreducible self-energy is composed by three parts as

$$\Sigma^{\star}_{\gamma\delta}(E) = -\langle \gamma | U | \delta \rangle + \Sigma^{(\infty)}_{\gamma\delta} + \tilde{\Sigma}_{\gamma\delta}(E), \qquad (4.28)$$

respectively the auxiliary potential, the static mean-field and the energy-dependent component. These parts corresponds to the three terms in the right-hand side of Eq.(4.27) and their Feynman diagrams are presented in Figure 4.2.



Figure 4.2: Diagrammatic picture of the irreducible self-energy. In the right-hand side the auxiliary potential, the static mean-field and the energy-dependent contributions are shown. Adapted from Ref. [25].

To account for all the contributions,  $\Sigma^*(E)$  can be expanded in terms of skeleton [87, 79] diagrams constructed with dressed propagators, as explained in Figure 4.3. The advantages are that calculations are non-perturbative and independent from the choice of the reference state (the auxiliary potential U cancels out in the Dyson equation), the many-body correlations are expanded in terms of single-particle excitations of the true propagator, the conservation laws are satisfied at the level of the truncation of the self-energy, the number of one-particle irreducible diagrams is reduced. The disadvantage is that the dressed propagator contains a very large number of poles and it is, therefore, extremely difficult to handle beyond mean field.

The use of dressed propagators in  $\Sigma^{\star}(E)$  makes Eq.(4.22) to be nonlinear in  $G_{\alpha\beta}(E)$ .

Figure 4.3: Example of skeleton (a) and non skeleton (b) Feynman diagrams. Skeleton diagram means one-particle irreducible diagram that does not contain any portion that can be disconnected by cutting any two fermionic lines at different points. In panel (b), the scissors mark cuts the two fermionic lines, that make the diagram disconnected. This disconnected portion is contained by definition in the dressed fermionic loop of diagram (a).

The final unique solution of the Dyson equation is obtained by iterative calculations of self-energy and dressed propagator, until convergence is reached. This method is called Self-Consistent Green's Function theory.

### 4.4 Hartree-Fock approximation

It is interesting to compare the mean-field description of the SCGF formalism with the EDF one.

The mean-field or Hartree-Fock approximation is obtained imposing  $\Gamma = 0$  in Eq.(4.27). The corresponding Hartree-Fock self-energy becomes

$$\Sigma_{\gamma\delta}^{HF} = -\langle \gamma | \hat{U} | \delta \rangle - i \sum_{\mu\nu} \int_{C\uparrow} \frac{\mathrm{d}E'}{2\pi} \langle \gamma \mu | \hat{V} | \delta\nu \rangle G_{\nu\mu}^{HF}(E').$$
(4.29)

 $G^{HF}$  is different from the non-interacting propagator  $G^{(0)}$ , in fact, it is the solution of the Dyson equation when the self-energy is calculated at the lowest order (first order) in power of  $\hat{H}_{1_I}$ , namely

$$G_{\alpha\beta}^{HF}(E) = G_{\alpha\beta}^{(0)}(E) + \sum_{\gamma\delta} G_{\alpha\gamma}^{(0)}(E) \Sigma_{\gamma\delta}^{HF} G_{\delta\beta}^{HF}(E).$$
(4.30)

We expect that the Lehmann representation of  $G^{HF}$  has a simple-poles structure, allowing to write the propagator as

$$G_{\alpha\beta}^{HF}(E) = \sum_{n} \frac{z_{\alpha}^{n+}(z_{\beta}^{n+})^{*}}{E - \epsilon_{n}^{+} + i\eta} + \sum_{k} \frac{z_{\alpha}^{k-}(z_{\beta}^{k-})^{*}}{E - \epsilon_{k}^{-} - i\eta},$$
(4.31)

with energies  $\epsilon_n^+ = E_n^{A+1} - E_0^A$ ,  $\epsilon_k^- = E_0^A - E_k^{A-1}$  and amplitudes

$$z_{\alpha}^{n-} = \langle \Psi_n^{A-1} | a_{\alpha} | \Psi_0^A \rangle, \qquad (4.32)$$

$$z_{\alpha}^{n+} = \langle \Psi_0^A | a_{\alpha} | \Psi_n^{A+1} \rangle.$$
(4.33)

Recalling the expression for the one-body density matrix  $\rho_{\mu\nu}^{HF} = \sum_k z_{\nu}^{k-} (z_{\mu}^{k-})^*$ , Eq.(4.29) gives

$$\Sigma_{\gamma\delta}^{HF} = -\langle \gamma | \hat{U} | \delta \rangle + \sum_{\mu\nu} \langle \gamma \mu | \hat{V} | \delta \nu \rangle \rho_{\mu\nu}^{HF}.$$
(4.34)

 $\Sigma_{\gamma\delta}^{HF}$  emerges as an energy-independent potential that simulates the effects of the potential  $\hat{V}$  mediated over the one-body density of the nucleons (plus the auxiliary potential).

Solving the limit

$$\lim_{E \to \epsilon_k^-} (E - \epsilon_k^-) \left[ G_{\alpha\beta}^{HF}(E) - G_{\alpha\beta}^{(0)}(E) - \sum_{\gamma\delta} G_{\alpha\gamma}^{(0)}(E) \Sigma_{\gamma\delta}^{HF} G_{\delta\beta}^{HF}(E) \right] = 0, \quad (4.35)$$

we obtain the Hartree-Fock equations for hole states

$$\sum_{\delta} \left\{ \langle \alpha | \hat{T} | \delta \rangle + \sum_{\mu\nu} \langle \alpha \mu | \hat{V} | \delta \nu \rangle \rho_{\mu\nu}^{HF} \right\} z_{\delta}^{k-} = \epsilon_k^- z_{\alpha}^{k-}.$$
(4.36)

They need to be calculated self-consistently since the density depends on the removal amplitudes. The equations for the particle states read

$$\sum_{\delta} \left\{ \langle \alpha | \hat{T} | \delta \rangle + \sum_{\mu\nu} \langle \alpha \mu | \hat{V} | \delta \nu \rangle \rho_{\mu\nu}^{HF} \right\} z_{\delta}^{n+} = \epsilon_n^+ z_{\alpha}^{n+}, \tag{4.37}$$

which represent a linear eigenvalue problem because  $\rho_{\mu\nu}^{HF}$  depends only on the hole amplitudes  $z_{\alpha}^{k-}$ . The ground state energy of the system results (cfr. Eq.(2.26))

$$E_0^A = \sum_{k=1}^A \epsilon_k^- - \frac{1}{2} \sum_{\alpha\beta\mu\nu} \langle \alpha\mu | \hat{V} | \beta\nu \rangle \rho_{\mu\nu}^{HF} \rho_{\alpha\beta}^{HF}.$$
(4.38)

Eqs.(4.36) and (4.37) are analogous to Eq.(2.25) and they can be derived also from the constrained variational equation

$$\frac{\partial}{\partial z_{\alpha}^{i*}} \left[ E - \sum_{i=1}^{A} \epsilon_i z_{\alpha}^{i*} z_{\alpha}^i \right] = 0, \qquad (4.39)$$

consistent with Eq.(2.24) for the EDF case.

At the mean-field level, the equivalence of the SCGF approach with the variational theorem, fundament of the EDF method, establishes a point of contact between the two techniques. On one side the Green's function method studies the response of the ground state to adding or removing particles, on the other side the EDFs consider the perturbation induced by a source of interaction coupled to the density. At the first order in the perturbative expansion of the self-energy, the perturbation by the source is represented by a local shift in the density [33] that is exactly how the DFT faces the many-body problem.

### 4.5 ADC(3) approximation

After the illustrative case of the mean-field approximation, we are interested to study the self-energy for a more realistic bound state. In the nucleus, when the number of nucleons is larger than two, the correlations due to the three-body interaction become important to determine the ground state energy. We include the three-body potential  $\hat{V}^{3B}$  in the many body Hamiltonian  $\hat{H} = \hat{H}_0 + \hat{H}_1$ , written in the second quantization as

$$\hat{H} = \sum_{\alpha} \epsilon_{\alpha}^{0} a_{\alpha}^{\dagger} a_{\alpha} - \sum_{\alpha\beta} \langle \alpha | \hat{U} | \beta \rangle a_{\alpha}^{\dagger} a_{\beta} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{V}^{2B} | \gamma\delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} + \frac{1}{36} \sum_{\alpha\beta\mu\gamma\delta\nu} \langle \alpha\beta\mu | \hat{V}^{3B} | \gamma\delta\nu \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\mu}^{\dagger} a_{\nu} a_{\delta} a_{\gamma}, \qquad (4.40)$$

where  $\epsilon_{\alpha}^{0}$  are the single-particle energies of the unperturbed Hamiltonian  $\hat{H}_{0}$ . To further reorganize the contributions to the irreducible self-energy, we restrict the one-particle irreducible and skeleton diagrams to be also interaction-irreducible, as shown in Figure 4.4. In addition, we replace the bare interactions in these diagrams with effective interactions, which represent irreducible and system-dependent effective forces. The corresponding effective Hamiltonian [88] reads

$$\tilde{H}_1 = \tilde{U} + \tilde{V}^{2B} + \hat{V}^{3B}.$$
(4.41)



Figure 4.4: Examples of interaction-irreducible (a) and interaction-reducible (b) contributions to the irreducible self-energy. A diagram is considered interaction reducible if cutting an interaction vertex the whole diagram becomes disconnected. In panel (b), the scissors mark indicates the vertex that, when cut, makes the diagram disconnected. (c) Interaction-irreducible contribution to  $\Sigma^*$  with effective interactions represented by sinusoidal lines. Effective interactions appear in the effective Hamiltonian, Eq.(4.41) and they are illustrated in Figure 4.5. The diagrams (a) and (b) are included in (c) through the effective interactions.

 $\hat{V}^{3B}$  is the bare three-body force, while the effective one-body  $\tilde{U}$  and two-body  $\tilde{V}^{2B}$  forces are respectively

$$\tilde{U} = \sum_{\alpha\beta} \left[ -\langle \alpha | \hat{U} | \beta \rangle + \sum_{\gamma\delta} \langle \alpha\gamma | \hat{V}^{2B} | \beta\delta \rangle \rho_{\delta\gamma} + \frac{1}{4} \sum_{\mu\nu\gamma\delta} \langle \alpha\mu\nu | \hat{V}^{3B} | \beta\gamma\delta \rangle \Gamma_{\gamma\delta,\mu\nu} \right] a^{\dagger}_{\alpha}a_{\beta},$$
(4.42)

$$\tilde{V}^{2B} = \sum_{\alpha\beta\gamma\delta} \left[ \langle \alpha\beta | \hat{V}^{2B} | \gamma\delta \rangle + \sum_{\mu\nu} \langle \alpha\beta\mu | \hat{V}^{3B} | \gamma\delta\nu \rangle \rho_{\nu\mu} \right] a^{\dagger}_{\alpha} a^{\dagger}_{\beta} a_{\delta} a_{\gamma}.$$
(4.43)

The reduced two-body density matrix  $\Gamma_{\gamma\delta,\mu\nu}$  is obtained from the two-body Green's function  $G^{II}_{\gamma\delta,\mu\nu}(\tau)$  as

$$\Gamma_{\gamma\delta,\mu\nu} = \lim_{\tau\to 0^-} (-i) G^{II}_{\gamma\delta,\mu\nu}(\tau) = \langle \Psi_0^A | a^{\dagger}_{\nu} a^{\dagger}_{\mu} a_{\gamma} a_{\delta} | \Psi_0^A \rangle.$$
(4.44)

In Eq.(4.42), the static self-energy appears in the right-hand side as

$$\Sigma_{\alpha\beta}^{(\infty)} = \sum_{\gamma\delta} \langle \alpha\gamma | \hat{V}^{2B} | \beta\delta \rangle \rho_{\delta\gamma} + \frac{1}{4} \sum_{\mu\nu\gamma\delta} \langle \alpha\mu\nu | \hat{V}^{3B} | \beta\gamma\delta \rangle \Gamma_{\gamma\delta,\mu\nu}.$$
(4.45)

Staticity means that no intermediate excitations propagate in the system, and the Feynman diagrams of  $\Sigma_{\alpha\beta}^{(\infty)}$  have the form of one-body effective interaction, as shown in Figure 4.5. The static self-energy represents an extension of the Hartree-Fock potential (cfr. Eq.(4.34)), since, if calculated with dressed G and



Figure 4.5: One-body (a) and two-body (b) effective interactions, described respectively in Eq.(4.42) and Eq.(4.43). Sinusoidal lines represent effective interactions, short (long) dashed lines are two-body (three-body) bare interactions, where the dots show the interaction vertices. One-body interactions are presented with short dashed lines and a cross symbol in place of the second interaction vertex. Double solid fermionic lines indicate dressed propagators. Adapted from Ref. [89].

 $G^{II}$ , it includes more correlations then the Hartree-Fock case.

The energy dependent part of the self-energy,  $\tilde{\Sigma}(E)$ , propagates intermediate state configurations such as 2p1h (two particle one hole), 2h1p, 3p2h, etc. It appears starting from the second order in power of interaction because it is necessary to have at least one interaction to create and one to annihilate the intermediate states. We employ the Algebraic Diagrammatic Construction method [90, 91] up to the third order, ADC(3), to perform the calculations in this work. A pedagogical treatment of the method is presented in Ref. [89] in the context of nuclear physics. ADC(3) approach is based upon expressing  $\tilde{\Sigma}(E)$  in its Lehmann representation of the form

$$\tilde{\Sigma}_{\alpha\beta}(E) = \sum_{rr'} M_{\alpha,r}^{\dagger} \left[ \frac{1}{E - (E^{>} + C) + i\eta} \right]_{r,r'} M_{r',\beta} + \sum_{ss'} N_{\alpha,s} \left[ \frac{1}{E - (E^{<} + D) - i\eta} \right]_{s,s'} N_{s',\beta}^{\dagger}.$$
(4.46)

We specify with index n and k respectively the particle and hole single-particle states. In the forward part, the indices r stand for intermediate state configurations, as for example  $r = \{n_1 < n_2, k_3\}$  defines 2p1h configuration. M are coupling matrices, containing combinations of the spectroscopic amplitudes  $\mathcal{X}$ and  $\mathcal{Y}$ , defined in Eq.(4.12), two- and three-body matrix elements, unperturbed energies.  $E + i\eta$  is a diagonal matrix (proportional to  $\delta_{r,r'}$ ).  $E^>$  represents the unperturbed energies for the configuration, i.e.,  $E_{r,r'}^> = diag(\epsilon_{n_1}^+ + \epsilon_{n_2}^+ - \epsilon_{k_3}^-)$ . C is an interaction matrix, containing combinations of spectroscopic amplitudes and interaction matrix elements.

In the backward part, similarly we notice the configuration indices s, the coupling matrices N, the backward energies  $E^{<}$  and the interaction matrix D.

All the Feynman diagrams up to the order n = 3 are included by construction, which would make the expansion to be perturbative. The diagrams necessary to achieve the analytical form of Eq.(4.46) are added as well as infinite summations. ADC(3) method accounts for all these diagrams, resulting in a non-perturbative approximation. The precision of ADC(3) calculation is estimated as  $\mathcal{O}(\hat{H}_{1_I}^4)$ , giving an error of 1% on the total binding energy [89].

We identify with  $\epsilon_i$  and  $\mathcal{Z}^i_{\alpha}$  the energy and spectroscopic amplitudes for every state (without distinction if above or below the Fermi surface, because the following derivation is equivalent). Using the limit of residues

 $\lim_{E \to \epsilon_i} (E - \epsilon_i) \left[ G_{\alpha\beta}(E) - G_{\alpha\beta}^{(0)}(E) - \sum_{\gamma\delta} G_{\alpha\gamma}^{(0)}(E) \Sigma_{\gamma\delta}^{\star}(E) G_{\delta\beta}(E) \right] = 0, \text{ the eigen-value equation results}$ 

$$\epsilon_{i} \mathcal{Z}_{\alpha}^{i} = \sum_{\beta} \left[ \hat{T} + \hat{U} + \Sigma^{\star}(E) \right]_{\alpha\beta} \mathcal{Z}_{\beta}^{i} \Big|_{E=\epsilon_{i}}$$

$$= \sum_{\beta} \left[ \hat{T} + \Sigma^{(\infty)} + M^{\dagger} \frac{1}{E - (E^{>} + C) + i\eta} M + N \frac{1}{E - (E^{<} + D) - i\eta} N^{\dagger} \right]_{\alpha\beta} \mathcal{Z}_{\beta}^{i} \Big|_{E=\epsilon_{i}}.$$
(4.47)

The spectroscopic amplitudes provide the spectroscopic factor for the state i as

$$SF_{i} \equiv \sum_{\alpha} |\mathcal{Z}_{\alpha}^{i}|^{2} = \frac{1}{1 - \sum_{\beta\gamma} \left[ \left( \frac{\mathcal{Z}_{\beta}^{i}}{SF_{i}} \right)^{*} \frac{d\Sigma_{\beta\gamma}^{\star}(E)}{dE} \Big|_{E=\epsilon_{i}} \frac{\mathcal{Z}_{\gamma}^{i}}{SF_{i}} \right]}.$$
(4.48)

Eq.(4.47) should be solved by finding all the solutions that match the eigenvalues  $\epsilon_i$  with the arguments of  $\Sigma^*(\epsilon_i)$ , which is extremely time consuming. Instead, defining the intermediate configurations vectors  $\mathcal{W}^i$  and  $\mathcal{V}^i$  as

$$[E - E^{>} - C]_{r,r'} \mathcal{W}_{r'}^{i} \equiv M_{r,\beta} \mathcal{Z}_{\beta}^{i}$$

$$(4.49)$$

$$[E - E^{<} - D]_{s,s'} \mathcal{V}_{s'}^{i} \equiv N_{s,\beta}^{\dagger} \mathcal{Z}_{\beta}^{i}, \qquad (4.50)$$

we can rewrite Eq.(4.47) as

$$\begin{pmatrix} \hat{T} + \Sigma^{(\infty)} & M^{\dagger} & N \\ M & E^{>} + C & 0 \\ N^{\dagger} & 0 & E^{<} + D \end{pmatrix} \begin{pmatrix} \mathcal{Z}^{i} \\ \mathcal{W}^{i} \\ \mathcal{V}^{i} \end{pmatrix} = \epsilon_{i} \begin{pmatrix} \mathcal{Z}^{i} \\ \mathcal{W}^{i} \\ \mathcal{V}^{i} \end{pmatrix}, \quad (4.51)$$

where the normalization  $\sum_{\alpha} |\mathcal{Z}_{\alpha}^{i}|^{2} + \sum_{r} |\mathcal{W}_{r}^{i}|^{2} + \sum_{s} |\mathcal{V}_{s}^{i}|^{2} = 1$  holds and it is equivalent to Eq.(4.48).

Eq.(4.51) linearizes Eq.(4.47) in a matrix form. The matrix elements are energy independent, such that all the solutions can be obtained in one diagonalization. To deal with the large dimension of the Dyson matrix,  $E^{>} + C$  and  $E^{<} + D$  can be calculated in small Lanczos subspaces, reducing the number of poles of the propagator away from the Fermi surface, while keeping the overall strength to describe the ground state.

Accounting for the presence of the three-body interaction  $\hat{V}^{3B}$ , the ground state energy is approximated by the modified Migdal-Galitski-Koltun (MGK) sum rule in Ref. [92] as

$$E_{0}^{A} = \langle \Psi_{0}^{A} | \hat{H} | \Psi_{0}^{A} \rangle = \sum_{\alpha\beta} \frac{1}{2} \int_{-\infty}^{\epsilon_{0}^{-}} \mathrm{d}E \left[ T_{\alpha\beta} + E \,\delta_{\alpha\beta} \right] S_{\beta\alpha}^{h}(E) - \frac{1}{2} \langle \hat{V}^{3B} \rangle.$$
(4.52)

The expectation value of the three-body interaction  $\langle \hat{V}^{3B} \rangle$  requires to calculate many-body propagators (at least the two-body propagators). Using the fact that such interaction gives a smaller contribution to the total energy compared to the other terms of the Hamiltonian, we choose the lowest order approximation that gives

$$\langle \hat{V}^{3B} \rangle \approx \frac{1}{6} \sum_{\alpha \beta \mu \gamma \delta \nu} \langle \alpha \beta \mu | \hat{V}^{3B} | \gamma \delta \nu \rangle \rho_{\gamma \alpha} \rho_{\delta \beta} \rho_{\nu \mu}.$$
(4.53)

The implementation of the self-consistency in the ADC(3) approximation is done in the following steps:

- We start from a guess for the dressed propagator, called reference propagator, with its spectral amplitudes and single-particle energies.
- Using the reference propagator, the three-body interaction is contracted to give a contribution to the two-body effective interaction.
- We employ the reference propagator and the effective interactions to calculate the components of the energy dependent part of the self-energy in Eq.(4.46), namely the coupling matrices M and N, the interaction matrices C and D.
- The Dyson equation, or more precisely Eq.(4.51) is solved with the reference propagator and the irreducible self-energy, with its static and energy-dependent parts. The solution provides the dressed propagator, with the corresponding energy poles and spectral amplitudes.
- The large information, contained in the dressed propagator, is reduced to an optimized reference state propagator (defined in Section 4.6).

• The optimized propagator is used to restart the procedure from the contraction of the three-body force. The scheme is iterated until the solution converges, specifically, when the ground state energy differs less than 50 eV from the value of the previous iteration.

### 4.6 Expectation value of two-body operator

We are interested to estimate the expectation value of a two-body operator  $\hat{O}^{2B}$ . The exact value  $\langle \hat{O}^{2B} \rangle$  is given as infinite expansion in terms of the effective interaction and dressed propagators as pictured in Figure 4.6 (first line). From the



Figure 4.6: Diagrammatic representation of the expectation value of the two-body operator  $\hat{O}^{2B}$ , indicated with blue zigzag lines. Double straight lines are used for dressed propagators, single lines for OpRS propagators and sinusoidal lines for two-body effective interactions. These are Feynman diagrams in the energy formulation, i.e., they include forward and backward propagation. In the second line, from left to right we can recognize the leading order term LO, the next-to-leading order NLO (first order in the effective interaction), the NNLO ring and NNLO ladder (second order of  $\tilde{H}_1$ ). In the last line, we use the ph-RPA and pp/hh-RPA insertions to estimate the contributions from NNLO and higher order terms.

practical point of view, such summation becomes computationally difficult since the dressed propagators contain many poles, that multiplicate the matrix elements of every interaction line. We approximate the single-particle propagator  $G_{\alpha\beta}(E)$  with an optimized reference state (OpRS) propagator [93, 94] of the form

$$G^{OpRS}_{\alpha\beta}(E) = \sum_{n \notin F} \frac{(\phi^n_{\alpha})^* \phi^n_{\beta}}{E - \epsilon^{OpRS}_n + i\eta} + \sum_{k \in F} \frac{\phi^k_{\alpha}(\phi^k_{\beta})^*}{E - \epsilon^{OpRS}_k - i\eta}.$$
 (4.54)

This is a model propagator for independent-particle states with energy  $\epsilon^{OpRS}$  and wave function  $\phi$ . Such propagator contains a reduced number of poles compared to the dressed one. The lowest moments of spectral distribution with respect to energy poles can be defined as

$$M^{0}_{\alpha\beta} = \sum_{n} (\mathcal{X}^{n}_{\alpha})^{*} \mathcal{X}^{n}_{\beta} + \sum_{k} \mathcal{Y}^{k}_{\alpha} (\mathcal{Y}^{k}_{\beta})^{*}, \qquad (4.55)$$

$$M^{1}_{\alpha\beta} = \sum_{n} \frac{(\mathcal{X}^{n}_{\alpha})^{*} \mathcal{X}^{n}_{\beta}}{E_{F} - \epsilon^{+}_{n}} + \sum_{k} \frac{\mathcal{Y}^{k}_{\alpha} (\mathcal{Y}^{k}_{\beta})^{*}}{E_{F} - \epsilon^{-}_{k}}, \qquad (4.56)$$

and these quantities constrain the density distributions and the Koltun energy sum rule. The energies and wave functions of the OpRS propagator are selected in order that the OpRS momenta reproduce those of the dressed propagators, namely  $M^{0\ OpRS}_{\alpha\beta} = M^0_{\alpha\beta}$  and  $M^{1\ OpRS}_{\alpha\beta} = M^1_{\alpha\beta}$ .

We estimate  $\langle \hat{O}^{2B} \rangle$  using the dressed propagators in the leading order (LO) and the OpRS propagators in the next-to-leading order (NLO) and NNLO (see Figure 4.6). We account for higher order with the *ph*-, *pp*- and *hh*-RPA (Random Phase Approximation) insertions respectively in the NNLO-ring and NNLO-ladder diagrams.

The LO contribution, known also as Hartree-Fock average value, results

$$\langle \hat{O}^{2B} \rangle_{LO} = \langle \hat{O}^{2B} \rangle_{HF} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{O}^{2B} | \gamma\delta \rangle \rho_{\gamma\alpha} \rho_{\delta\beta}.$$
(4.57)

## 5. Model EDF linked to *ab initio*

Dobaczewski [1] proposed a method to employ *ab initio* calculations in the fit of EDF coupling constants for finite nuclear systems. The goal of this technique is to construct a model energy density functional of the form

$$\tilde{E}[\rho] = T[\rho] + V^{Coul}[\rho] + \sum_{j} C_j V_j^{gen}[\rho], \qquad (5.1)$$

as approximation to the *ab initio* ground state energy. The functional is built from a Slater determinant  $|\Phi\rangle$ , with the Hartree-Fock average value of the kinetic part  $T[\rho] \equiv \langle \Phi | \hat{T} | \Phi \rangle_{HF}$ , of the Coulomb potential  $V^{Coul}[\rho] \equiv \langle \Phi | \hat{V}^{Coul} | \Phi \rangle_{HF}$  and of the interaction components  $V_j^{gen}[\rho] \equiv \langle \Phi | \hat{V}_j^{gen} | \Phi \rangle_{HF}$ . The operators  $\hat{V}_j^{gen}$  represent our choice of the generators for the model EDF, when the functional is built from an underlying model Hamiltonian with potential  $\hat{V}^{mod} = \hat{V}^{Coul} + \sum_j C_j \hat{V}_j^{gen}$ . The coupling constants  $C_j$  are fitted to the *ab initio* energies, linking the model functional to the *ab initio* interaction.

#### 5.1 Derivation

In the spirit of the Levy-Lieb constrained-variation (see Section 2.2), a density functional can be built from a two-stage variation.

In the following discussion, we consider only one density, the particle density, and we neglect the spin and isospin dependency, namely our system is described by  $\rho(\mathbf{r})$ . Such assumption is made at this point to present the derivation in a simpler way, and, for the same reason, we consider only the direct contribution of the generators. Nevertheless the results presented in Chapter 6 include several densities, with their spin and isospin dependency, as well as direct and exchange terms of the generators.

In the standard Levy-Lieb construction, the first stage of the variation consists of

the minimization of the Routhian  $\hat{R}$  as

$$\delta_{\Psi} \langle \Psi | \hat{R} | \Psi \rangle = \delta_{\Psi} \left[ \langle \Psi | \hat{H}^{ab} | \Psi \rangle + \int d\mathbf{r} \ U(\mathbf{r}) \rho(\mathbf{r}) \right] = 0, \tag{5.2}$$

where  $\hat{H}^{ab}$  is the Hamiltonian of the system. We use the superscript  $^{ab}$  to indicate that it comes from the *ab initio* theory, distinguishing it from the Hamiltonian used to built the model functional.

The auxiliary potential  $U(\mathbf{r})$  is the Lagrange multiplier of the density operator, which average value is  $\langle \Psi | \hat{\rho}(\mathbf{r}) | \Psi \rangle \equiv \langle \Psi | a^{\dagger}(\mathbf{r}) a(\mathbf{r}) | \Psi \rangle = \rho(\mathbf{r}).$ 

The Routhian simulates a variation in which the one-body density is constrained to a given density profile. The minimization produces the solution  $|\Psi(U)\rangle$ . If we were able to probe the system with all the possible potential  $U(\mathbf{r})$ , we would obtain the functional  $E^{ab}[U] \equiv \langle \Psi(U) | \hat{H}^{ab} | \Psi(U) \rangle$ , that describes how the energy of the system changes with varying the auxiliary potential. The integrand on the right hand side of Eq.(5.2) introduces a perturbation to the system at rest. The response of the system to the perturbation causes a change in the density  $\rho$ . Inverting the relation  $\rho[U]$  in  $U[\rho]$ , we get the energy functional  $E^{ab}[\rho]$ .

In the second step, the functional  $E^{ab}[\rho]$  is minimized respect to  $\rho$ . This gives the ground state energy  $E^{ab}_{q.s.}$  and the ground state density  $\rho_{g.s.}$ .

Being unable to perturb the system with an infinite number of auxiliary potentials, we discretize the perturbation to a finite number of Lagrange multipliers  $\lambda$  and to the operators  $\hat{V}^{gen}$ .  $\lambda$  represents the strength of the perturbation and it can assume values around zero. With the choice of  $\hat{V}^{gen}$  we select the relevant terms for the model functional.

Let us assume that we are interested to built a model functional only of the local density  $\rho(\mathbf{r})$ . We can employ the  $\delta$ -interaction as generator, that is, in the configuration space it results  $\hat{V}^{gen}(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')(1 - P_r P_\sigma P_\tau) a^{\dagger}(\mathbf{r}) a^{\dagger}(\mathbf{r}') a(\mathbf{r}') a(\mathbf{r})$ . Eq.(5.1) in the specific case reads

$$\tilde{E}[\rho] = T[\rho] + V^{Coul}[\rho] + C \langle \Phi | \delta(\mathbf{r} - \mathbf{r}')(1 - P_r P_\sigma P_\tau) a^{\dagger}(\mathbf{r}) a^{\dagger}(\mathbf{r}') a(\mathbf{r}') a(\mathbf{r}') | \Phi \rangle$$

$$= T[\rho] + V^{Coul}[\rho] + C \int d\mathbf{r} d\mathbf{r}' \rho(\mathbf{r}) \rho(\mathbf{r}') \delta(\mathbf{r} - \mathbf{r}') - C \int d\mathbf{r} d\mathbf{r}' \rho^2(\mathbf{r}, \mathbf{r}') \delta(\mathbf{r} - \mathbf{r}')$$

$$\approx T[\rho] + V^{Coul}[\rho] + C \int d\mathbf{r} \rho^2(\mathbf{r}),$$
(5.3)

where we applied the Wick's theorem to the Slater determinant  $|\Phi\rangle$ , and used the definition  $\rho(\mathbf{r}, \mathbf{r}') \equiv \langle \Phi | a^{\dagger}(\mathbf{r}') a(\mathbf{r}) | \Phi \rangle$ . In the last line, the exchange term has been neglected for simplicity.

In the framework of the *ab initio* method, we minimize the Routhian as

$$\delta_{\Psi} \langle \Psi | \hat{R} | \Psi \rangle = \delta_{\Psi} \left[ \langle \Psi | \hat{H}^{ab} | \Psi \rangle + \lambda \langle \Psi | \hat{V}^{gen} | \Psi \rangle \right].$$
(5.4)

Dealing with the exact wave function  $|\Psi\rangle$ , the action of the creation and annihilation operators in the Wick's theorem produce the two-particle density  $\rho^{(2)}(\mathbf{r}, \mathbf{r}'; \mathbf{r}, \mathbf{r}') \equiv \langle \Psi | a^{\dagger}(\mathbf{r}) a^{\dagger}(\mathbf{r}') a(\mathbf{r}') a(\mathbf{r}) | \Psi \rangle$ . This can be replaced by

$$\rho^{(2)}(\mathbf{r}, \mathbf{r}'; \mathbf{r}, \mathbf{r}') = \rho(\mathbf{r})\rho(\mathbf{r}') - \rho^2(\mathbf{r}, \mathbf{r}') + \Lambda(\mathbf{r}, \mathbf{r}'; \mathbf{r}, \mathbf{r}'), \qquad (5.5)$$

where  $\Lambda$  is the two-particle density cumulant, that accounts for the correlations of the two-particle density not included in the products of one-particle densities. With the choice of  $\delta$ -interaction as generator, Eq.(5.4) becomes

$$\delta_{\Psi} \langle \Psi | \hat{R} | \Psi \rangle = \delta_{\Psi} \left[ \langle \Psi | \hat{H}^{ab} | \Psi \rangle + \lambda \int d\mathbf{r} \, \rho^{2}(\mathbf{r}) + \lambda \int d\mathbf{r} \, d\mathbf{r}' \, \rho^{2}(\mathbf{r}, \mathbf{r}') \delta(\mathbf{r} - \mathbf{r}') \right. \\ \left. + \lambda \int d\mathbf{r} \, d\mathbf{r}' \, \delta(\mathbf{r} - \mathbf{r}') \Lambda(\mathbf{r}, \mathbf{r}'; \mathbf{r}, \mathbf{r}') \right] \\ \approx \delta_{\Psi} \left[ \langle \Psi | \hat{H}^{ab} | \Psi \rangle + \lambda \int d\mathbf{r} \, \rho^{2}(\mathbf{r}) \right] = 0,$$
(5.6)

where in the last line we have neglected the exchange term and the cumulant for simplicity. Comparing Eq.(5.6) with Eq.(5.2), it appears that using  $\lambda$  and  $\hat{V}^{gen}$  is equivalent to an auxiliary potential of the form  $U(\mathbf{r}) = \lambda \rho(\mathbf{r})$ . In particular, due to the choice of the  $\delta$ -force, the main contribution from the perturbation part in Eq.(5.6) depends on the correlated local density  $\rho(\mathbf{r})$ . According to the Kohn-Sham method (Section 2.3), it exists an uncorrelated local density, Kohn-Sham local density, that can represent any local density. Such Kohn-Sham density will enter the model functional.

From Eq.(5.6) we obtain the solution  $|\Psi(\lambda)\rangle$  as function of the Lagrange multiplier. The *ab initio* energy of the perturbed state results

$$E^{ab}(\lambda) = \langle \Psi(\lambda) | \hat{T} | \Psi(\lambda) \rangle + \langle \Psi(\lambda) | \hat{V}^{ab} | \Psi(\lambda) \rangle$$
  
=  $\langle \Psi(\lambda) | \hat{T} | \Psi(\lambda) \rangle + \langle \Psi(\lambda) | \hat{V}^{ab}_{n} + \hat{V}^{Coul} | \Psi(\lambda) \rangle,$  (5.7)

where the *ab initio* potential is described by its nuclear  $\hat{V}_n^{ab}$  and Coulomb  $\hat{V}^{Coul}$  components. With the correlated  $\Psi(\lambda)$ , we calculate the Hartree-Fock average value of the generator as

$$\langle \Psi(\lambda) | \hat{V}^{gen} | \Psi(\lambda) \rangle_{HF} = \int \mathrm{d}\mathbf{r} \, \rho_{\lambda}^2(\mathbf{r}),$$
(5.8)

where  $\rho_{\lambda}(\mathbf{r})$  indicates that the local density is a function of  $\lambda$ . With "Hartree-Fock average value" we intend that the expectation value of the operator is calculated at the leading order of the expansion in effective interactions, as shown in Eq.(4.57).

We want to describe the *ab initio* energy with a functional of the form of Eq.(5.3) including the Coulomb term, that is

$$E^{ab}(\lambda) = T[\rho_{\lambda}] + C \int d\mathbf{r} \,\rho_{\lambda}^{2}(\mathbf{r}) + V^{Coul}[\rho].$$
(5.9)

Considering that the Kohn-Sham kinetic energy represents a good approximation to the total kinetic energy, we assume that

$$\langle \Psi(\lambda) | \hat{T} | \Psi(\lambda) \rangle \approx T[\rho_{\lambda}].$$
 (5.10)

Analogously we suppose that the Coulomb contribution in the *ab initio* Hamiltonian is close to the Hartree-Fock average in the functional, namely

$$\langle \Psi(\lambda) | \hat{V}^{Coul} | \Psi(\lambda) \rangle \approx V^{Coul}[\rho_{\lambda}].$$
 (5.11)

Then, we can subtract the kinetic energy and the Coulomb energy in the left-hand and in the right-hand sides of Eq.(5.9), rewriting it as

$$\langle \Psi(\lambda) | \hat{V}_n^{ab} | \Psi(\lambda) \rangle = C \int \mathrm{d}\mathbf{r} \, \rho_\lambda^2(\mathbf{r}).$$
 (5.12)

The coupling constant C is now fitted, knowing  $\langle \Psi(\lambda) | \hat{V}_n^{ab} | \Psi(\lambda) \rangle$  and  $\int d\mathbf{r} \rho_{\lambda}^2(\mathbf{r})$ , both calculated with the *ab initio* technique.

We can repeat the same machinery for different value of  $\lambda$  in order to fit the value of C to a larger dataset. The coupling constant is not dependent on  $\lambda$  but it is defined on the manifold generated by the Lagrange multiplier  $\lambda$ .

The obtained C is then inserted in Eq.(5.3) and the model functional is minimized in the space of local densities  $\rho(\mathbf{r})$ .

The ground state energy  $\tilde{E}_{g.s.}$  should be close to the *ab initio* energy  $E_{g.s.}^{ab}$  if the generator is adequate to reproduce the *ab initio* description of the system. Lack of accuracy in determining the coupling constant requires to modify or to extend the number of model EDF generators.

The ground state (local) density  $\rho_{g.s.}$  in the functional should be similar to the *ab initio* local density  $\rho_0(\mathbf{r})$ , for the unperturbed case  $\lambda = 0$ .

Our research aims is to study the validity of the assumption discussed above.

The earlier construction can be extended to a model functional of different densities  $\tilde{E}[\rho, \tau, \rho \Delta \rho, \mathbf{J}]$ , using perturbations by the generators that in the Hartree-Fock approximation induce such densities. The minimization of the Routhian is generalized as

$$\delta_{\Psi} \langle \Psi | \hat{R} | \Psi \rangle = \delta_{\Psi} \left[ \langle \Psi | \hat{H}^{ab} | \Psi \rangle + \lambda_i \langle \Psi | \hat{V}_i^{gen} | \Psi \rangle \right] = 0.$$
 (5.13)

The index *i* indicates the possible choices of values of  $\lambda$  as well as the choices of different generators. The perturbation technique not only tests the changes in the nucleus due to external probes, but also it enlarges the number of *ab initio* computable solutions, otherwise limited to experimental energies or unperturbed *ab initio* results. In this way, as many data points as the values of  $\lambda_i$  are made available for fitting. We obtain a number of coupling constants  $C_j$  equal to the number of generators of the model functional. We can calculate perturbations of several nuclei and fit the coupling constants simultaneously, in order to derive a model functional that can be applicable over the nuclear chart.

In the SCGF approach, we recall that not the wave function but the propagator is used to describe the ground state, solution of the Routhian minimization. From the propagator  $G_{\alpha\beta}$  we obtain the correlated one-body density matrix  $\rho_{\alpha\beta}$ , Eq.(4.13), used to extract the Hartree-Fock expectation value of any operator  $\langle O(\lambda_i) \rangle_{HF} \equiv \langle \Psi(\lambda_i) | \hat{O} | \Psi(\lambda_i) \rangle_{HF}$ . The kinetic energy as one-body operator reads

$$T(\lambda_i) \equiv \sum_{\alpha\beta} \langle \alpha | \hat{T} | \beta \rangle \, \rho_{\beta\alpha}(\lambda_i) = \langle T(\lambda_i) \rangle_{HF}.$$
(5.14)

Regarding the Hartree-Fock average value of the generators  $\langle V_j^{gen}(\lambda_i) \rangle_{HF}$ , we distinguish two- and three-body cases. The expectation value of the two-body potential, according to Eq.(4.57), reads

$$\langle \hat{V}^{2B}(\lambda_i) \rangle_{HF} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{V}^{2B} | \gamma\delta \rangle \rho_{\gamma\alpha}(\lambda_i) \rho_{\delta\beta}(\lambda_i), \qquad (5.15)$$

where  $\langle \alpha \beta | \hat{V}^{2B} | \gamma \delta \rangle$  are antisymmetric two-body matrix elements. In the case of three-body interaction, from Eq.(4.53), it follows that

$$\langle \hat{V}^{3B}(\lambda_i) \rangle_{HF} = \frac{1}{6} \sum_{\alpha\beta\mu\gamma\delta\nu} \langle \alpha\beta\mu | \hat{V}^{3B} | \gamma\delta\nu \rangle \ \rho_{\gamma\alpha}(\lambda_i)\rho_{\delta\beta}(\lambda_i)\rho_{\nu\mu}(\lambda_i), \tag{5.16}$$

where  $\langle \alpha \beta \mu | \hat{V}^{3B} | \gamma \delta \nu \rangle$  are antisymmetric three-body matrix elements. We extract the nuclear interaction energy as

$$V_n^{ab}(\lambda_i) = \langle \Psi(\lambda_i) | \hat{H}^{ab} - \hat{T} - \hat{V}^{Coul} | \Psi(\lambda_i) \rangle, \qquad (5.17)$$

rewriting Eq.(5.12) in the general form

$$V_n^{ab}(\lambda_i) = \sum_j C_j \langle V_j^{gen}(\lambda_i) \rangle_{HF}, \qquad (5.18)$$

where  $\langle V_j^{gen}(\lambda_i) \rangle_{HF}$  are specified in Eqs.(5.15) and (5.16).

Eq.(5.18) represents the cornerstone of the derivation. In fact, the coupling constants  $C_j$  are fitted by regression analysis (see Section 5.2) to carry the information of the *ab initio* interaction. Eq.(5.18), if validated through our analysis, suggests that the correlations of the ground state solution can be absorbed by the  $C_j$ .

We use the SCGF solver "BoccaDorata" [95], in which the contributions  $V_n^{ab}(\lambda_i)$ ,  $V^{Coul}(\lambda_i)$  and  $\lambda_i V^{pert}(\lambda_i) = \lambda_i \langle \Psi(\lambda_i) | \hat{V}_i^{gen} | \Psi(\lambda_i) \rangle$  to the interaction energy are not separated when solving Eq.(5.13). In the Routhian, the total interaction energy then becomes

$$V^{tot}(\lambda_i) = \langle \Psi(\lambda_i) | \hat{V}_n^{ab} + \hat{V}^{Coul} + \lambda_i \hat{V}_i^{gen} | \Psi(\lambda_i) \rangle, \qquad (5.19)$$

from which we approximate the *ab initio* contribution as

$$V_n^{ab}(\lambda_i) \approx V^{tot}(\lambda_i) - \langle V^{Coul}(\lambda_i) \rangle_{RL} - \langle \lambda_i V^{pert}(\lambda_i) \rangle_{RL}.$$
(5.20)

The subscript  $_{RL}$  indicates the inclusion of ring and ladder RPA contributions in  $\langle V^{2B}(\lambda_i) \rangle_{RL}$ , as shown in the Feynman diagrams in Fig. 4.6. We will discuss the uncertainties associated with Eq.(5.20) in Section 6.3.2.

### 5.2 Linear regression analysis

We perform the fit of the coupling constants  $C_j$  through the linear regression method.

From the perturbation method, we obtain d interaction energies  $V_n^{ab}(\lambda_i)$ , that represent the regression data  $y_i$ . We intend to describe the data in function of pregression parameters  $C_j$ , corresponding to the coupling constants.

The comparison with EDF methods (cfr. Eqs.(5.1) and (5.18)) and the idea that the *ab initio* correlations are absorbed in the coupling constants suggest a relation of the form

$$y_i = \sum_{j=0}^n C_j \langle \Psi(\lambda_i) | \hat{V}_j^{gen} | \Psi(\lambda_i) \rangle_{HF}.$$
(5.21)

Namely the Jacobian matrix is identified with the Hartree-Fock average of the generator  $\hat{V}_i^{gen}$ , for the wave function relative to the Lagrange multiplier  $\lambda_i$ , as

$$\mathcal{J}_{ij} \equiv \langle \Psi(\lambda_i) | \hat{V}_j^{gen} | \Psi(\lambda_i) \rangle_{HF}.$$
(5.22)

Ab initio data  $y_i$  and the Jacobian  $\mathcal{J}_{ij}$  are the inputs in the regression equation that reads (in vector notation)

$$\mathbf{y} = \mathcal{J}\mathbf{C}.\tag{5.23}$$

When fitting data, it is common procedure to rank different data according to the importance we want to attribute to them. In this way, the value of the parameters is constrained to specific data more strongly than to the others. The practice consists in introducing an artificial weight  $w_i$  for each data, then the larger the weight, the more importance is assigned to the corresponding data. In the present case, all the observables are of the same type (interaction energy) and there are not a priori reason to prefer some datapoints to others. The weight is then assigned by the inverse of the estimated error on each datapoint as

$$w_i = \frac{1}{(\Delta y_i)^2}.\tag{5.24}$$

The error  $\Delta y_i$  contains different contributions [65], that can be sintesized as

$$(\Delta y_i)^2 = (\Delta y_i^{ab})^2 + (\Delta y^{num})^2 + (\Delta y^{mod})^2.$$
 (5.25)

 $\Delta y_i^{ab}$  is the error attributed to the *ab initio* calculation and it will be presented in Chapter 6.  $\Delta y^{num}$  is the numerical precision. It can be taken from the convergence condition of the total energy in the SCGF calculations, where the convergence is reached if the difference between two consecutive iterations is smaller that  $5 \times 10^{-5}$  MeV. The numerical precision has the same value for all the data.

 $\Delta y^{mod}$  represents the error associated to the model and it can be tuned to normalize the penalty function  $\chi^2$ . In fact, starting from an arbitrary value  $\epsilon > 0$ ,  $\Delta y^{mod}$  can be increased iteratively up to the value at which the  $\chi^2$  approaches the value of 1. We build the penalty function by ordinary-least-squares (OLS) method as

$$\chi^{2}(\mathbf{C}) = \frac{1}{d-p} \sum_{i=1}^{d} w_{i} \left[ \sum_{j=1}^{p} \mathcal{J}_{ij}C_{j} - y_{i} \right]^{2}$$

$$= \frac{1}{d-p} \left( \mathcal{J}\mathbf{C} - \mathbf{y} \right)^{T} W \left( \mathcal{J}\mathbf{C} - \mathbf{y} \right),$$
(5.26)

where the weight matrix W is a diagonal matrix with elements  $W_{ii} = w_i$ . This penalty function satisfies the normalization property  $\chi^2(\mathbf{C}) \to 1$  at the minimum, typical of statistical analysis.

The optimal set of variables  $\mathbf{C}_{min}$  is obtained from the minimum of Eq.(5.26), i.e., we require that  $\forall j = 1, ..., n$ 

$$\left. \frac{\partial \chi^2(\mathbf{C})}{\partial C_j} \right|_{\mathbf{C}=\mathbf{C}_{min}} = 0.$$
(5.27)

The solution of Eq.(5.27) reads

$$\mathbf{C}_{min} = (\mathcal{J}^T W \mathcal{J})^{-1} \mathcal{J}^T W \mathbf{y}.$$
 (5.28)

It is important to underline that some parameters cannot be determined from the fit, as the parameters lying in the kernel of  $\mathcal{J}^T W \mathcal{J}$ , if this product is singular, or that some parameters can poorly describe the chosen dataset. In Appendix A the Singular Value Decomposition method is presented as solution to the ill-posed problem when  $\mathcal{J}^T W \mathcal{J}$  is singular.

The regression analysis can return the statistical error associated to the parameter  $C_i^{min}$ , namely

$$\Delta C_j^{min} = \sqrt{\mathcal{K}_{jj}}.\tag{5.29}$$

where the covariance matrix  $\mathcal{K}$ , between the parameters  $C_a$  and  $C_b$ , is defined as

$$\mathcal{K}_{ab} \equiv \langle (C_a - \langle C_a \rangle) (C_b - \langle C_b \rangle) \rangle = \chi^2(\mathbf{C}) \left( \mathcal{J}^T W \mathcal{J} \right)_{ab}^{-1}.$$
 (5.30)

For a general observable  $\mathcal{A}$ , that varies almost linearly with the variation of **C** around  $\mathbf{C}_{min}$ , the propagated error due to the uncertainties on the parameters is

$$\Delta \mathcal{A} = \sqrt{\sum_{il} G_i^A \, \mathcal{K}_{il} \, G_l^A},\tag{5.31}$$

where  $G_i^A \equiv \frac{\partial \mathcal{A}}{\partial C_i} \Big|_{\mathbf{C} = \mathbf{C}_{min}}$  is the Jacobian relative to the observable  $\mathcal{A}$ . In the specific case of the interaction energy, the observable used in the fit, we obtain

$$y_i^{th} = \sum_{j=1}^n \mathcal{J}_{ij} C_j^{min} \tag{5.32}$$

and the associated error becomes

$$\Delta y_i^{th} = \sqrt{\sum_{jl} \mathcal{J}_{ij} \, \mathcal{K}_{jl} \, (\mathcal{J}^T)_{li}}.$$
(5.33)

 $y_i^{th}$  can be compared with the input value  $y_i^{ab}$ . The smaller the difference  $|y_i^{ab} - y_i^{th}|$ , the better the coupling constants  $\mathbf{C}_{min}$  reproduce the *ab initio* interaction energy.

#### 5.2.1 Constrained regression

We consider valuable to introduce constraints in the linear regression. With the constraints, we aim to drag the coupling constants toward values we expect, primarily to satisfy nuclear matter properties. Linear regression with constrained solution is in the spirit of the Bayesian inference where the prior distribution of the parameters is known.

A technique to include constraints in the regression is represented by the Tikhonov regularization [96] or ridge regression [97], which consists of minimizing a penalty function of the form

$$\chi_T^2(\mathbf{C}) = \frac{1}{d - p + f} \left[ (\mathbf{y} - \mathcal{J}\mathbf{C})^T W(\mathbf{y} - \mathcal{J}\mathbf{C}) + \lambda_T (\mathbf{b} - Q\mathbf{C})^T (\mathbf{b} - Q\mathbf{C}) \right].$$
(5.34)

The Tikhonov parameter  $\lambda_T$  is a real positive number and  $\mathbf{b} = Q\mathbf{C}$  is a system of equations in the parameters  $\mathbf{C}$  with constant terms  $\mathbf{b}$ . The final values of  $\mathbf{C}$  will depend on  $\lambda_T$ . For  $\lambda_T=0$ , the constraints are neglected and Eq.(5.34) reduces to Eq.(5.26). Increasing the value of the Tikhonov parameter, the relevance of the constraints increases, in a way that we can consider  $\lambda_T$  as the weight factor of the constraining equations.

In this formalism, the solution  $\mathbf{C}_T$  of the regression reads

$$(\mathbf{C}_T)_{min} = \left( \begin{bmatrix} \mathcal{J} \\ Q \end{bmatrix}^T \begin{bmatrix} W & 0 \\ 0 & \lambda_T I \end{bmatrix} \begin{bmatrix} \mathcal{J} \\ Q \end{bmatrix} \right)^{-1} \begin{bmatrix} \mathcal{J} \\ Q \end{bmatrix}^T \begin{bmatrix} W & 0 \\ 0 & \lambda I \end{bmatrix} \begin{bmatrix} \mathbf{y} \\ \mathbf{b} \end{bmatrix}, \quad (5.35)$$

with the corresponding covariance matrix

$$(\mathcal{K}_{\mathbf{C}_T})_{ab} = \chi_T^2(\mathbf{C}_T) \left( \begin{bmatrix} \mathcal{J} \\ Q \end{bmatrix}^T \begin{bmatrix} W & 0 \\ 0 & \lambda_T I \end{bmatrix} \begin{bmatrix} \mathcal{J} \\ Q \end{bmatrix} \right)^{-1}.$$
 (5.36)

In the Tikhonov regularization, the constraints are realized at the expenses of the difference  $\mathbf{y}^{ab} - \mathbf{y}^{th}(\mathbf{C}_T)$ . That is, forcing the parameters to satisfy the equations  $\mathbf{b} = Q\mathbf{C}$  produces a deterioration of the  $\chi^2$  in the part related to the data.

Reasonable constraining equations for the parameters **C** regard the properties of the nuclear matter system, described in Appendix B. Particular quantities characteristic of this system, like the energy per particle E/A, effective mass  $m^*/m$ , symmetry energy J, can be expressed in function of the coupling constants of the EDFs.

## 6. Results from *ab initio* calculations

We present the results obtained by applying the technique explained in Chapter 5. The Self-Consistent Green's Function calculations are performed with the solver BoccaDorata [95]. It uses a spherical harmonic oscillator basis, including all the neutron and proton orbitals up to the specified principal quantum number  $N_{max}$ .

Similarly to the proof of principle in Ref. [1], we test the perturbative method at the Hartree-Fock level, with Skyrme SV [98] as interaction, namely  $\hat{H}^{ab} = \hat{T} + \hat{V}_{SV}$ . Such test returns the same parameters of the SV original interaction we started from. Since we limit the calculations to the Hartree-Fock order, the expectation values of the generators produce uncorrelated densities corresponding one-to-one with the densities in the model functional.

This test represents a benchmark among the codes in use for the SCGF solutions, the regression analysis and the spherical Hartree-Fock solver for the model functional (HOSPHE [99]). Details are shown in Appendix F.

We are interested to fit the functional coupling constants to the state-of-art chiral interactions, employing *ab initio* methods beyond the Hartree-Fock approximation. Then, in the following, we discuss principal results.

# 6.1 NNLOsat: chiral interaction optimized for nuclei

Ab initio calculations employ Hamiltonians derived from chiral effective field theory, accounting for the symmetries of QCD. Such Hamiltonians contain coupling constants of the long-range (pion exchange) physics and LECs for the nucleon-nucleon (2N) channel. The three-body (3N) forces are adjusted successively to data from

systems with  $A \leq 4$ . This way of tuning the interaction leads to over binding of medium-mass nuclei and underestimating of charge radii. Furthermore, reproducing binding energy and radii of finite nuclei simultaneously with the empirical nuclear matter saturation point and incompressibility, appears to be an issue for *ab initio* techniques.

To overcome such problems, the authors in Ref. [100] optimized the 3N and 2N forces together, improving the force order by order in the chiral expansion. Their fit includes binding energies and radii of light and medium-mass nuclei as well as deuteron, p-p and p-n scattering data at low energy. The choice of the observables used in the penalty function was made in the spirit of mean-field calculations and energy density functionals.

The obtained interaction called "NNLOsat", performs well to reproduce binding energy and radii of nuclei from He to Ca. The 3N forces play a major role in obtaining saturation of nuclear matter in a way similar to the density dependent term in the EDF theory.

With such derivation, this interaction promises power to extrapolate bulk properties of heavier nuclei.

NNLOsat interaction contains charge symmetry breaking terms other than the Coulomb interaction, and it means that the strength of the interaction is different among neutrons and protons. In our density functional, we neglect the isospinbreaking terms, and generalizations in the spirit of Refs. [74, 101] are left to future work.

### 6.2 Data points from *ab initio* calculations

We performe calculations with the Self-Consistent Green's Function method in the ADC(3) approximation (see Section 4.5), where the chosen interaction NNLOsat (Section 6.1) is included through the two-body and three-body matrix elements. An exploratory study, employing the coupled-cluster-doubles method [102], has investigated the behavior of the ground-state energies in function of the harmonic oscillator energy  $\hbar\omega$  and of the model space, labeled with  $N_{max}$ . It emerges that with NNLOsat interaction the minimum energy for Ca and Ni isotopes is reached at the oscillator energy  $\hbar\omega=20$  MeV. The convergence in term of  $N_{max}$  is not assumed to be exact, nevertheless increasing  $N_{max}$  decreases the binding energy towards the experimental values. In terms of computational resources, even if the present technology allows calculations up to  $N_{max} = 13$ , this would require a too large amount of CPU hours to complete the full set of perturbations. Reducing our model space to  $N_{max} = 11$  or  $N_{max} = 9$  is a necessary compromise between available resources and precision.

With the choice of  $\hbar\omega=20$  MeV, we complete SCGF calculations for 7 semimagic nuclei <sup>16</sup>O, <sup>24</sup>O, <sup>34</sup>Si, <sup>36</sup>S, <sup>40</sup>Ca, <sup>48</sup>Ca and <sup>56</sup>Ni. Each nucleus is formed by a closed level configuration: at least a magic number for one kind of nucleon and a fully filled valence orbital for the other kind. These nuclei represent the available convergent ADC(3) calculations among the semi-magic systems between <sup>16</sup>O and <sup>56</sup>Ni, where the magic numbers are 8, 20 and 28.

The ground state energy per nucleon E/A is plotted in Figure 6.1 for the model spaces  $N_{max} = 7$ ,  $N_{max} = 9$  and  $N_{max} = 11$ . These unperturbed cases ( $\lambda=0$ ) can be compared with the experimental values [103]. The model space  $N_{max} = 7$  appears to be too small to reproduce experimental results. The theoretical predictions improve increasing the oscillator space. For  $N_{max} = 11$  the maximum difference with experiment is at <sup>56</sup>Ni. The difference of 0.25 MeV per nucleon means around 3% error on the total energy that overestimates the assumed 1% error due to the ADC(3) truncation [89]. In absolute value, the calculated <sup>56</sup>Ni binding energy is more than 10 MeV away from the measured value. Such deviation is much larger than the standard deviation of common EDFs (of the order of 1 MeV). The precision of the SCGF method conflicts with the ambition of the novel functionals to reduce the difference with the experimental results. However, in this work, we intend to reproduce the *ab initio* energy irrespective of its agreement with experiments.

In Figure 6.1, we present also the behavior for  $N_{max} = 9$  "nocm", where "nocm" indicates that the two-body center-of-mass correction has been neglected during all the self-consistent calculation. This is our choice of model space. Due to limited computational resources, especially in terms of available CPU memory, we opt for an harmonic oscillator basis truncated to  $N_{max} = 9$ . We decide to neglect the two-body center-of-mass correction from the beginning because, removing it at the end of the calculation, would have introduced a systematic error in the value of the *ab initio* interaction energy<sup>1</sup>. In this way, if on one side the difference with experimental energies becomes larger, on the other side our fit is cleaned from the corresponding systematic error. This choice reflects our focus on the theoretical predictions more than on experimental results.

<sup>&</sup>lt;sup>1</sup>In the SCGF solver, the two-body center-of-mass corrections [104] are implemented through two-body center-of-mass matrix elements, that are added to the two-body potential at every stage of the self-consistent calculation. As a consequence these corrections will be included in the value of the total interaction energy  $V^{tot}(\lambda_i)$ , and they will need to be subtracted from the left-hand side of Eq.(5.20), using the approximated expansion in Fig. 4.6. The subtraction will produce a further contribution to the error associated with  $V_n^{ab}(\lambda_i)$  described in Section 6.3.2. The two-body center-of-mass corrections, if neglected from the beginning, will not contribute to the error on the interaction energy. Furthermore, the two-body center-of-mass corrections are not implemented in the Hartree-Fock solver, then, without these corrections, it is easier to compare ground-state energies from *ab initio* calculations and from the model functionals.



Figure 6.1: Binding energy per nucleon E/A for different nuclei. The theoretical values  $E_{ab}/A$  correspond to the unperturbed cases ( $\lambda = 0$ ). Calculations are made with NNLOsat interaction,  $\hbar\omega=20$  and model space specified by  $N_{max}$  in the legend. Black triangles represent the experimental values taken from Ref. [103].

In our model functional, we consider generators of zero-range contact interaction (Skyrme-like) as in Eq.(C.2). The matrix elements of the two-body terms can be found in Appendix D. They are labeled with the parameters  $t_i$ .  $t_0$  and  $t_0x_0$ describe momentum-independent central interaction (in the power of momentum they represent the leading order  $\mathbf{k}^0$ ).  $t_1$ ,  $t_1x_1$ ,  $t_2$  and  $t_2x_2$  indicates momentumdependent central interaction (order  $\mathbf{k}^2$ ),  $t_e$  and  $t_o$  are tensor interactions (order  $\mathbf{k}^2$ ) and  $w_0$  is the spin-orbit potential (order  $\mathbf{k}^2$ ). The density-dependent term, proportional to  $t_3$ , is replaced by the three-body zero-range interaction (order  $\mathbf{k}^0$ ) as specified in Appendix E.

Using Eq.(C.4), we can replace the central and tensor interaction terms with the generators  $\hat{V}_0^{\rho}$ ,  $\hat{V}_1^{\rho}$ ,  $\hat{V}_0^{\Delta\rho}$ ,  $\hat{V}_1^{\Delta\rho}$ ,  $\hat{V}_0^{\tau}$ ,  $\hat{V}_1^{\tau}$ ,  $\hat{V}_0^{J1}$  and  $\hat{V}_1^{J1}$ .

It is important to consider the meaning of the subscript  $_{T=0}$  and  $_{T=1}$  to indicate respectively the generators associated with isoscalar and isovector densities. Such link between generators and densities is valid only when the average value of
the generators is calculated at the Hartree-Fock level, as in the energy density functional. In fact, already at the next-to-leading order in powers of the interaction, the expectation value of a generator contains contributions not only proportionals to the densities. The Skyrme-like interaction, as shown in Appendix D, is formed by the identity operator  $\mathbb{1}_T$  in the isospin space, then all the generators are isoscalar or isospin invariant.

The studied set of generators consists of 10 elements, the above mentioned  $\hat{V}_T^X$  plus the spin-orbit  $\hat{V}_{w_0}$  and the three-body  $\hat{V}_{t_3}$ .<sup>2</sup>

We use each generator separately as perturbation potential for the system, namely  $\hat{V}^{pert} = \hat{V}^{gen}$ , with 4 different intensity of  $\lambda^{pert}$ . We obtain 284 convergent results, which represent our full database of the perturbed and unperturbed ground state energies. The value of  $\lambda^{pert}$  is selected specifically for each  $\hat{V}^{pert}$  as shown in Table 6.1. The choice of  $\lambda^{pert}$  represents a compromise between large perturbation and convergent results for perturbed nuclei. In fact, the larger is the perturbation strength, the wider is the density space probed. Nevertheless, if the perturbation is excessively strong, the numerical solution of SCGF may diverge.

As motivated in Section 5.1, the parameters of the model EDF are fitted only to the interaction energy  $V_n^{ab}(\lambda_i)$ , given in Eq.(5.20).

**Table 6.1:** The value of  $\lambda_i^{pert}$  used for different  $\hat{V}_i^{pert}$ . The strength of the perturbation parameter is obtained as  $\lambda_i^{pert} = s k_i$  where  $s \in \{-2, -1, 1, 2\}$  and  $k_i$  is tabled below.

i	$\hat{V}_0^{\rho}$	$\hat{V}_1^{\rho}$	$\hat{V}_0^{\Delta \rho}$	$\hat{V}_1^{\Delta \rho}$	$\hat{V}_0^{\tau}$	$\hat{V}_1^{\tau}$	$\hat{V}_0^{J1}$	$\hat{V}_1^{J1}$	$\hat{V}_{w_0}$	$\hat{V}_{t_3}$
$k_i$	2.0	2.0	1.0	1.0	2.0	2.0	2.0	1.0	5.0	100.0

We recall that the NNLOsat interaction is optimized to reproduce ground state properties of finite nuclei as well as saturation of infinite nuclear matter. We will consider the nuclear matter properties as a test of the quality of the parameters obtained in the regression analysis. In fact, the derivation *ab initio* should be able to reproduce the saturation properties included in the *ab initio* interaction. Our interest is to find the most significant selection of generators that can reproduce calculated data and nuclear matter properties.

<sup>&</sup>lt;sup>2</sup>The generators  $\hat{V}_{w_0}$  and  $\hat{V}_{t_3}$  do not have the separation in isoscalar and isovector because the relation between the coupling constants and the parameter (respectively  $C_0^{\nabla J}$ ,  $C_1^{\nabla J}$  and  $w_0$ or  $C_0^{\rho \, dd}$ ,  $C_1^{\rho \, dd}$  and  $t_3$ ) is not invertible.

## 6.3 Criticalities of the method and sources of errors

Before performing the regression to fit the parameters, we address some criticalities that emerge due to the approximation used in the SCGF method.

#### 6.3.1 Hellmann-Feynman theorem

As discussed in Section 5.1, the Routhian in Eq.(5.13) can be seen as a perturbation to the *ab initio* Hamiltonian  $\hat{H}^{ab}$ . In perturbation theory, especially in atomic and molecular physics, the Hellmann-Feynman theorem [105, 106] represents a general approach to evaluate the change of the energy in function of the perturbation. For a system in which the Hamiltonian  $\hat{H}_{\lambda} = \hat{H}_0 + \lambda \hat{V}$  depends explicitly on the parameter  $\lambda$  only in the perturbative term, the theorem states

$$\frac{\mathrm{d}E_{\lambda}}{\mathrm{d}\lambda} \equiv \frac{\mathrm{d}}{\mathrm{d}\lambda} \langle \Psi(\lambda) | \hat{H}_{\lambda} | \Psi(\lambda) \rangle = \langle \Psi(\lambda) | \frac{\partial \hat{H}_{\lambda}}{\partial \lambda} | \Psi(\lambda) \rangle.$$
(6.1)

That is, the first derivative of the total energy with respect to parameter  $\lambda$  of the perturbation is equal to the expectation value of the derivative of the total Hamiltonian operator  $\hat{H}_{\lambda}$  respect to the same perturbation parameter.

Eq.(6.1) is valid under the condition that  $|\Psi(\lambda)\rangle$  is an eigenstate of  $\hat{H}_{\lambda}$ . Ref. [107] shows that also the Hartree-Fock wave function can satisfy the Hellmann-Feynman theorem. Furthermore, Eq.(6.1) can be fulfilled by approximate wave functions that satisfy the variational principle  $\langle \delta \Psi | \hat{H} - E | \Psi \rangle = 0$  for a variation of the form  $|\delta\Psi\rangle = \frac{\partial\Psi}{\partial\lambda}d\lambda$ , as stated in Ref. [108]. However, when the wave function is expanded in a truncated basis [109] or it is a solution of a perturbative expansion [108], the Hellman-Feynman theorem is violated and the gradients of the wave function need to be included as

$$\frac{\mathrm{d}E_{\lambda}}{\mathrm{d}\lambda} = E_{\lambda} \left[ \langle \frac{\mathrm{d}\Psi(\lambda)}{\mathrm{d}\lambda} | \Psi(\lambda) \rangle + \langle \Psi(\lambda) | \frac{\mathrm{d}\Psi(\lambda)}{\mathrm{d}\lambda} \rangle \right] + \langle \Psi(\lambda) | \frac{\partial \hat{H}_{\lambda}}{\partial \lambda} | \Psi(\lambda) \rangle. \tag{6.2}$$

Inserting  $\hat{H}^{ab} + \lambda_i \hat{V}_i^{gen}$  (see Eq.(5.13)) in Eq.(6.1), we obtain that

$$\frac{\mathrm{d}E_{\lambda_j}}{\mathrm{d}\lambda_j} = \langle \Psi(\lambda_j) | \frac{\partial}{\partial\lambda_j} \left[ \hat{H}^{ab} + \lambda_i \hat{V}_i^{gen} \right] | \Psi(\lambda_j) \rangle = \langle \Psi(\lambda_j) | \hat{V}_j^{gen} | \Psi(\lambda_j) \rangle.$$
(6.3)

Here, the first derivative can be calculated with the finite difference method, specifically with the centered-difference formula  $^3$ 

$$\left. \frac{\mathrm{d}E_{\lambda}}{\mathrm{d}\lambda} \right|_{\lambda=0} = \frac{E(\lambda) - E(-\lambda)}{2\lambda} + O(\lambda^2). \tag{6.4}$$

The ground state wave function of the *ab initio* Hamiltonian is not variational, because the SCGF method at the ADC(3) level employes a truncated expansion. We are in the condition discussed above, in which the Hellmann-Feynman theorem is violated. Anyway, we study the case that the perturbation is given by  $\lambda_{ab}\hat{V}^{ab} = \lambda_{ab}(\hat{V}_n^{ab} + \hat{V}^{Coul})$ , i.e., the same potential entering in  $\hat{H}^{ab}$ . The Hellmann-Feynman formula in Eq.(6.3) together with Eq.(6.4) give at the point  $\lambda = 0$  the result

$$\frac{E(\lambda_{ab}) - E(-\lambda_{ab})}{2\lambda_{ab}} \approx \frac{\mathrm{d}E_{\lambda_{ab}}}{\mathrm{d}\lambda_{ab}}\Big|_{\lambda_{ab}=0} = \langle \Psi(0)|\hat{V}_n^{ab} + \hat{V}^{Coul}|\Psi(0)\rangle \equiv V^{ab}(0). \quad (6.5)$$

This compares the finite difference of the energy for the perturbed cases ( $\lambda_{ab}$  and  $-\lambda_{ab}$ ) with the average value of the interaction energy in the unperturbed case ( $\lambda = 0$ ). The quantities in the left-hand and right-hand side of Eq.(6.5) are available from the SCGF solver for a numerical analysis. Such analysis offers an estimate for the difference between the approximated solution in the ADC(3) method and the exact solution, which should satisfy the variational principle and, as a consequence, the Hellmann-Feynman theorem. We can define an error on the *ab initio* energies as

$$\Delta V_H = \left| \frac{\mathrm{d}E_{\lambda_{ab}}}{\mathrm{d}\lambda_{ab}}(0) - V^{ab}(0) \right|,\tag{6.6}$$

where the subscript  $_H$  stands for error extracted from Hellmann-Feynman theorem. This error represents an absolute error on the measure of the interaction energy, due to the truncation in the theoretical method. It is assumed to be dependent on the nucleus but independent from the perturbation, namely the central point value ( $\lambda$ =0) is attributed to all perturbed and unperturbed interaction energies of a certain nucleus.

Figure 6.2 shows the ratio  $\frac{\Delta V_H}{|V^{ab}(0)|}$ , as percentage, in function of the mass number A

<sup>3</sup>For the first derivative, the central finite difference formula

$$\frac{\mathrm{d}f(x_0)}{\mathrm{d}h} = \frac{f(x_0+h) - f(x_0-h)}{2h} + O(h^2),$$

can be further improved using the five-points formula as

$$\frac{\mathrm{d}f(x_0)}{\mathrm{d}h} = \frac{f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)}{12h} + O(h^4).$$

of the nucleus. Such ratio, and consequently the precision of the solution, increases with the increasing of the model space ( $N_{max}$  in the legend). In the case  $N_{max}=9$ "nocm" discussed in the calculation of coupling constants, the imprecision results around 3-4 % of the interaction energy for the heaviest systems. For <sup>16</sup>O and <sup>24</sup>O, it drops down around 1%, which is the expected correction on the total energy due to the ADC(3) truncation.



Figure 6.2: The ratio  $\frac{\Delta V_H}{|V^{ab}(0)|}$  is plotted for different nuclei. Results are relative to the NNLOsat (two and three-body) interaction with the value of  $\lambda_{ab} = 0.005$ . The model space is specified in the legend, for all the cases the oscillator energy is  $\hbar \omega = 20$  MeV. The two-body center-of-mass correction is removed from  $V_{ab}(0)$  (the label "nocm" means that the two-body center-of-mass correction has already been neglected in the calculation of the ab initio solutions).

#### 6.3.2 Minima of the *ab initio* energy

Effects of the approximations made in the SCGF calculation appear also in the ground state energy of perturbed systems.

Figure 6.3 shows the behavior of the *ab initio* energy in function of  $\lambda_i$  for different perturbation  $V_i^{pert}$  explained in the legend. We expect that the case  $\lambda = 0$  (black triangle) is the one with lower binding energy  $E^{ab}(0)$  because  $|\Psi(0)\rangle$  is the solution that minimize the unperturbed case that correspond to the Routhian  $\hat{R} = \hat{H}^{ab}$ . Any other wave function  $|\Psi(\lambda_i \neq 0)\rangle$  represents the solution of a perturbed case, namely it is the minimum for the system described by the Routhian  $\hat{R} = \hat{H}^{ab} + \lambda_i \hat{V}_i^{gen}$ with  $\lambda_i \neq 0$ . For each solution of the perturbed system, it results

$$E^{ab}(\lambda_i) = \langle \Psi(\lambda_i) | \hat{H}^{ab} | \Psi(\lambda_i) \rangle \ge E^{ab}(0), \tag{6.7}$$

if the *ab initio* energy is calculated exactly. From the plot, it is evident that there are cases of energies  $E^{ab}(\lambda_i)$  smaller than  $E^{ab}(0)$ . In these cases, the minimum is shifted at values  $\lambda_i \neq 0$  in constrast with the variational principle. For the perturbation induced by the three-body generator  $\hat{V}_{t_3}$  (orange curve), the energy does not present a minimum but decreases monotonically towards negative  $\lambda_i$ . This effect is partially related to the way the contribution of the three-body interaction is extracted. In fact, we can estimate only the leading order as in Eq.(4.53). Including high order corrections can push the curve to a concavity shape.

It is necessary to study the impact of the uncertainty on the energy minima. In Section 6.3.1, we discussed the Hellmann-Feynman difference as a source of an absolute error associated with the energy. Here, another source of error is due to subtraction of the perturbation energy from the solution of the Routhian, since  $E^{ab}(\lambda_i) = R(\lambda_i) - \lambda_i V_i^{gen}$ . We assume that only the perturbation potential contributes to this uncertainty. Then, the imprecision associated with the value  $E^{ab}(\lambda_i)$  can be estimated from

$$\Delta E_S^{ab}(\lambda_i) = \left| \langle \Psi(\lambda_i) | \lambda_i \hat{V}_i^{gen} | \Psi(\lambda_i) \rangle_{RL} - \langle \Psi(\lambda_i) | \lambda_i \hat{V}_i^{gen} | \Psi(\lambda_i) \rangle_{NLO} \right|, \tag{6.8}$$

where  $\langle \rangle_{RL}$  indicates the full ring and ladder RPA approximation (RL). Such error can be viewed as a relative error between the perturbed solutions and the unperturbed one.

In the bottom panels of Figure 6.3, we present the effect of the subtraction error  $\Delta E_S^{ab}(\lambda_i)$  (left) and of the Hellmann-Feynman error  $\Delta E_H^{ab}$  (right), on the energy minima. For the Hellmann-Feynman uncertainty, we extend the error on the potential to the energy as  $\Delta E_H^{ab} = \Delta V_H$ , assuming that the value of potential is the only source of errors for the total energy. The error bars are visualized as shadows. The case of <sup>16</sup>O, where  $\Delta E_H^{ab}$  value is the smallest among the nuclei, shows that in most of the cases  $\Delta E_H^{ab} > \Delta E_S^{ab}$ . In the other nuclei,  $\Delta E_H^{ab}$  is around one order of magnitude larger than  $\Delta E_S^{ab}$ . In both situations, including the error bars, we can say that  $E^{ab}(\lambda_i \neq 0)$  can be larger than  $E^{ab}(0)$  in the error limit. Then, the variational principle, on which the Levy-Lieb construction is based,



Figure 6.3: (Top) Ab initio energy for the perturbed and unperturbed cases in <sup>16</sup>O. Colors in the legend correspond to the generator used as  $\hat{V}_i^{pert}$ . The black triangle indicates the unperturbed case and the black dashed line shows the reference value  $E^{ab}(0)$ . (Bottom) The shadows represent the error bars associated to the ab initio energy. The same color scheme is employed as in the legend. In the left panel the error is given by Eq.(6.8). In the right panel the error is extracted from the Hellmann-Feynman theorem, corresponding to Eq.(6.6).

continues to hold.

The significant difference in magnitude of  $\Delta E_H^{ab}$  and  $\Delta E_S^{ab}$  suggests to keep separate these errors in the following analysis.

When we move to the *ab initio* (nuclear) interaction energy,  $V_n^{ab}(\lambda_i) = R(\lambda_i) - R(\lambda_i)$ 

 $\lambda_i V_i^{gen}(\lambda_i) - V^{Coul}(\lambda_i) - T^{ab}(\lambda_i)$ , the imprecision due to subtractions becomes

$$[\Delta V_n^{ab}(\lambda_i)]_S = \left[ \left( \langle \lambda_i \hat{V}_i^{gen}(\lambda_i) \rangle_{RL} - \langle \lambda_i \hat{V}_i^{gen}(\lambda_i) \rangle_{NLO} \right)^2 + \left( \langle \hat{V}^{Coul}(\lambda_i) \rangle_{RL} - \langle \hat{V}^{Coul}(\lambda_i) \rangle_{NLO} \right)^2 \right]^{\frac{1}{2}}.$$
(6.9)

It means that the perturbation potential and the Coulomb potential have the larger uncertainties among the removed quantities. The largest contribution in Eq.(6.9) comes from the error associated to the perturbation potential  $\lambda_i \hat{V}_i^{gen}$ . The difference between the expectation value at RL and at NLO is larger for the perturbation potential as well as dependent on the kind of perturbation. The error associated with the Coulomb interaction is, instead, similar for the different perturbations in the same nucleus.

In the Hellmann-Feynman error,  $\Delta V_H$  contains also the contribution from the Coulomb interaction. However, we calculate that the uncertainties associated to the Coulomb potential do not affect significantly (around 1%) the value of the Hellmann-Feynman differences. In this case, we can neglect the Coulomb contributions, and we take  $[\Delta V_n^{ab}]_H = \Delta V_H$ .

### 6.4 Results

We collect the unperturbed and perturbed calculations to organize four smaller databases from the 284 data points available. We select the generators of the model functional according to the expansion in power of the momentum, namely the leading order ( $\mathbf{k}^0$ ) and the next-to-leading order ( $\mathbf{k}^2$ ). We can also identify the generators that produce isoscalar densities or isovector densities at the Hartree-Fock level. In such way, we fit "isoscalar" generators only to energies of N = Z nuclei (<sup>16</sup>O, <sup>40</sup>Ca and <sup>56</sup>Ni), while "isoscalar" and "isovector" generators together are used to describe energies of all the 7 nuclei. The combination of two order in momentum (leading, leading + next-to-leading) and two isospin-like behaviors (isoscalar, isoscalar + isovector) produces the four databases D1, D2, D3 and D4. The inputs and characteristics of each database are summarized in Table 6.2.

We perform the linear regression as described in Section 5.2 to estimate the coupling constants  $C_i$  corresponding to the selected generators. We conduct the analysis using separately  $[\Delta V_n^{ab}(\lambda_i)]_S$  or  $[\Delta V_n^{ab}]_H$  as *ab initio* error  $\Delta y_i^{ab}$  in the weight function.

As guideline for the discussion, in Table 6.3 we present the coupling constants of Skyrme SIII functional [98]. This mean-field functional, including momentum- and density-dependent generators, is a good reference point. Its parameters are in the

Name	D1	D2	D3	D4
nuclei	3 (N = Z)	7	3 (N = Z)	7
datapoints	123	284	123	284
gen. order	$\mathbf{k}^0$	$\mathbf{k}^0$	$\mathbf{k}^0,\mathbf{k}^2$	$\mathbf{k}^0,\mathbf{k}^2$
generators	$\hat{V}_0^{ ho},\hat{V}_{t_3}$	$\hat{V}_0^{ ho},  \hat{V}_1^{ ho},  \hat{V}_{t_3}$	$ \hat{V}_{0}^{\rho}, \hat{V}_{0}^{\Delta\rho}, \hat{V}_{0}^{\tau}, \\ \hat{V}_{0}^{J1}, \hat{V}_{w_{0}}, \hat{V}_{t_{3}}^{\tau} $	$ \begin{array}{c} \hat{V}_{0}^{\rho},  \hat{V}_{1}^{\rho},  \hat{V}_{0}^{\Delta\rho},  \hat{V}_{1}^{\Delta\rho}, \\ \hat{V}_{0}^{\tau},  \hat{V}_{1}^{\tau},  \hat{V}_{0}^{J1},  \hat{V}_{1}^{J1}, \\ \hat{V}_{w_{0}},  \hat{V}_{t_{3}} \end{array} $

Table 6.2: Specific inputs for the databases Ds.

domain of natural units according to Ref. [110], i.e., they scale similarly as the terms of an effective Lagrangian.

**Table 6.3:** Skyrme SIII [98] coupling constants. In the spin-orbit sector  $C_0^{\nabla J} = -90.0$ and  $C_1^{\nabla J} = -30.0$  correspond to  $C_{w_0} = -120.0$ . In the density dependent part  $C_0^{\rho \, dd} = 875.0$  and  $C_1^{\rho \, dd} = -875.0$  are equivalent to  $C_{t_3} = 14000.0$ .  $C_0^{J_1}$  and  $C_1^{J_1}$  are null in this parametrization.

$C_0^{\rho}$	$C_1^{\rho}$	$C_0^{\Delta \rho}$	$C_1^{\Delta \rho}$	$C_0^{\tau}$	$C_1^{\tau}$	$C_0^{J1}$	$C_{1}^{J1}$	$C_0^{\nabla J}$	$C_1^{\nabla J}$	$C_0^{\rho \ dd}$	$C_1^{\rho  dd}$
-423.28	268.08	-62.97	17.03	44.37	-30.62	0	0	-90.00	-30.00	875.00	-875.00

### Case with error from subtraction $[\Delta V_n^{ab}]_S$

We indicate the results corresponding to this prescription with the subscript  $_S$ . The numerical values are presented in Table 6.4 with the associated errors. In the D1<sub>S</sub> and D2<sub>S</sub> database, we fit the *ab initio* potential with only the contact two-body and three-body generators, that are the zero-order terms of the functional. The values we obtained for  $C_0^{\rho}$ ,  $C_1^{\rho}$  and  $C_{t_3}$  are of the same order of magnitude as the corresponding values of SIII.

When the momentum-dependent generators are included in the model, in the database  $D3_S$  and  $D4_S$ , the behavior of the fitted coupling constants changes from SIII values.  $C_{t_3}$  doubles its value compared to the cases  $D1_S$  and  $D2_S$  and the parameters  $C_0^{\Delta\rho}$ ,  $C_0^{\tau}$  and  $C_{w_0}$ , relative to new generators included in the model functional, assume opposite signs with respect to SIII. The  $C_i$  of the isovector generators of the case  $D4_S$  assume values significantly larger than the corresponding isoscalar coupling constants. These oversized numbers are artefacts of the  $\chi^2$  minimization. The expectation values of the isovector generators are generally small,

**Table 6.4:** Values of the parameters for the parametrizations  $D1_S$ ,  $D2_S$ ,  $D3_S$  and  $D4_S$ , with relative errors. In the bottom of the Table, the statistical quantities  $\chi^2$ , model error, Birge factor and BIC are given for each parametrization.

parameter	$D1_S$		$D2_S$		$D3_S$		$D4_S$	
$C_0^{\rho}$	-402.3	$\pm 1.3$	-411.9	$\pm 2.3$	-384.7	$\pm 4.5$	-366.4	$\pm 2.7$
$C_1^{\rho}$	-		183.2	$\pm 6.4$	-		-748.4	$\pm$ 68.0
$C_0^{\Delta  ho}$			-		46.4	$\pm 4.9$	52.0	$\pm 2.7$
$C_1^{\Delta \rho}$	-		-		-		-996.0	$\pm$ 243.4
$C_0^{\tau}$	-		-		-146.2	$\pm$ 11.0	-164.4	$\pm 6.3$
$C_1^{\tau}$	-		-		-		722.9	$\pm$ 79.8
$C_0^{J1}$	-		-		-266.8	$\pm$ 291.5	-1057.4	$\pm$ 213.0
$C_1^{J1}$	-		-		-		-1128.6	$\pm$ 189.1
$C_{w_0}$			-		73.4	$\pm$ 114.7	400.5	$\pm$ 83.8
$C_{t_3}$	13231.5	$\pm$ 146.0	14292.8	$\pm$ 264.5	31448.0	$\pm$ 1267.3	31874.3	$\pm$ 764.9
$\chi^2$	1.000		1.000		1.000		1.000	
model error	1.816		5.448		0.000		0.000	
Birge factor			-		0.399		0.693	
BIC	2693.9		6663.4		2708.8		6483.6	

then the regression push the corresponding coupling constants to large values to reduce the penalty function. The conspicuous errors associated to these parameters reflect the inability of the regression to estimate the parameters themselves.

We consider now statistical quantities that can help us to evaluate the quality of the coupling constants and, as a consequence, the generators of the model. In the regression, the  $\chi^2$ , Eq.(5.26), is normalized adjusting the model error  $\Delta y^{mod}$ . When the *ab initio* error  $\Delta y_i^{ab}$  is large, it can happen that  $\chi^2 < 1$ , then no values of the model error can normalize the penalty function. In this case, we use the Birge factor *b* [111] as universal factor (equal for all the data points) to force the penalty function to 1, namely  $\chi^2(\mathbf{C}) \longrightarrow \frac{\chi^2(\mathbf{C})}{b}$ .

A large model error means that the difference between the observables and the fitted quantities,  $\mathbf{y} - \mathcal{J}\mathbf{C}$ , is large and then the *ab initio* inputs are not accurately reproduced.

It is reasonable to compare  $D1_S$  with  $D3_S$ , both using 123 data points, and separately  $D2_S$  with  $D4_S$ , including 284 data. However,  $D1_S$  and  $D2_S$  normalize the penalty function by the model error, while  $D3_S$  and  $D4_S$  require the Birge factor, as shown in the bottom of Table 6.4. Such distinction makes hard to relate the performance of the different databases.

The Bayesian Information Criterion (BIC) is a statistical quantity useful to study

the relevant number of generators. It is defined as [112]

$$BIC = 2d \ln(\Delta_{RMS}[\text{KeV}]) + p \ln(d), \qquad (6.10)$$

where d is the number of data and p is the number of parameters or equivalently the number of generators.  $\Delta_{RMS} = \sqrt{(\mathbf{y} - \mathcal{J}\mathbf{C})^2}$ , expressed in KeV, represents the root-mean-square deviation of the data points from the fitted values. The smaller the *BIC* value, the more relevant are the parameters to describe the model.

BIC is, then, a proper index to contrast  $D1_S$  with  $D3_S$ . By a little difference,  $D1_S$  seems to carry out more information, since  $BIC(D1_S) < BIC(D3_S)$ . That is, the isoscalar coupling constants of the order  $\mathbf{k}^2$  do not add relevant knowledge to describe the *ab initio* interaction energy.

In the comparison of  $D2_S$  and  $D4_S$ , on the contrary, the addition of the momentumdependent generators in  $D4_S$  reduces the value of *BIC*. As explained before, this database has a larger disposition of unconstrained parameters that the regression can adjust to minimize  $\Delta_{RMS}$ .

The residuals of the Eq.(5.18) are defined as

Residuals 
$$\equiv \frac{\sum_{j} C_{j} \langle V_{j}^{gen}(\lambda_{i}) \rangle_{HF} - V_{n}^{ab}(\lambda_{i})}{V_{n}^{ab}(\lambda_{i})}.$$
 (6.11)

They are presented in Figure 6.4 and Figure 6.5, respectively for <sup>16</sup>O and <sup>56</sup>Ni, the lightest and the heaviest of the calculated systems. A model that fit precisely  $V_n^{ab}(\lambda_i)$  will produce residuals close to zero (black dashed line) for all the perturbation generators. In the present cases, instead, the residual of the unperturbed system ( $\lambda$ =0) is around zero, while, when  $\lambda_i$  moves away from zero, the distance of the residual tends to raise. For <sup>16</sup>O the residuals due to the perturbation  $\hat{V}_1^{J1}$ and  $\hat{V}_1^{\tau}$  pass over 2%. The residuals of <sup>56</sup>Ni are around half the value of the corresponding ones in <sup>16</sup>O, suggesting that the data relative to <sup>56</sup>Ni are reproduced better by the fit. We propagate the error on the residuals, due to the uncertainty  $[\Delta V_n^{ab}(\lambda_i)]_S$ , and we plot the error bars as shadows in Figures 6.4 and 6.5. The propagated errors are similar for the two nuclei, when we take in account the different scale on the *y*-axis.

In the comparison of Figure 6.4 with Figure 6.3, it emerges a similarity between the behavior of  $E^{ab}$  and of the residuals corresponding to the same generators. It means that the fit is hardly able to describe systems that are strongly perturbated. We observe that the most of the residuals lay in the half-plane y > 0, i.e., considering that the interaction energies are negative, the fitted values  $\sum_{j} C_{j} \langle V_{j}^{gen}(\lambda_{i}) \rangle_{HF}$ are smaller than  $V_{n}^{ab}(\lambda_{i})$ .



**Figure 6.4:** Residuals calculated with the parametrization  $D4_S$  in <sup>16</sup>O. In the notation of the linear regression, they read Residuals =  $\frac{\mathcal{J}\mathbf{C}-\mathbf{y}}{\mathbf{y}}$ . The perturbation potential is described by color in the legend and by  $\lambda_i$  on the x-axis. The errors propagated on the residuals are illustrated with shadowed areas of the same color and they are equivalent to  $\Delta \text{Residuals} = \frac{\mathcal{J}\Delta\mathbf{C}}{\mathbf{y}}$ . The reference value 0 is shown with a dashed black line.

Now we will look at the details of the regression to check that the large values of the isovector parameters in  $D4_S$  and their errors are not related with numerical singularities. We study the singular values of the matrix  $\mathcal{J}^T W \mathcal{J}$ . Its inverse enters in the equation for the parameters, Eq.(5.28) and for the covariance matrix, Eq.(5.30). We refer to Appendix A for the definition of singular values and singular value decomposition (SVD).

The singular values  $\alpha_k^2$  of the matrix  $\mathcal{J}^T W \mathcal{J}$  are shown in Figure 6.6 for the case  $D4_s$ . We define the SVD condition number as

$$F_{SVD} = \frac{\max(\alpha_k^2)}{\min(\alpha_k^2)}.$$
(6.12)

It is common practice to assume that  $\mathcal{J}^T W \mathcal{J}$  is singular when  $F_{SVD} \approx 10^{14}$ . In the actual case  $F_{SVD} = 1.3 \times 10^9$ , then the inversion of  $\mathcal{J}^T W \mathcal{J}$  is free from singularities. In Table 6.5, the parametrization D4<sub>S</sub> is compared with the parameters derived from the same database D4 when only the largest 9 singular values out of 10 are



Figure 6.5: Same as in Figure 6.4 for <sup>56</sup>Ni.

kept in  $(\mathcal{J}^T W \mathcal{J})^{-1}$ . We call this new parametrization  $\mathrm{D4}_S(9\mathrm{sv})$ . Reducing the

parameter	$D4_S$		$D4_S(9sv)$	
$C_0^{\rho}$	-366.4	$\pm 2.7$	-362.0	$\pm 5.5$
$C_1^{\rho}$	-748.4	$\pm$ 68.0	-2903.5	$\pm$ 149.3
$C_0^{\Delta  ho}$	52.0	$\pm 2.7$	-18.5	$\pm 3.9$
$C_1^{\Delta \rho}$	-996.0	$\pm$ 243.4	-3224.1	$\pm$ 596.2
$C_0^{\tau}$	-164.4	$\pm 6.3$	56.1	$\pm 4.5$
$C_1^{\tau}$	722.9	$\pm$ 79.8	1463.1	$\pm~165.7$
$C_0^{J1}$	-1057.4	$\pm$ 213.0	52.8	$\pm$ 479.5
$C_{1}^{J1}$	-1128.6	$\pm$ 189.1	-736.9	$\pm$ 420.5
$C_{w_0}$	400.5	$\pm$ 83.8	82.8	$\pm$ 188.6
$C_{t_3}$	31874.3	$\pm$ 764.9	369.1	$\pm 29.4$
$\chi^2$	1.000		1.000	
model error	0.000		4.195	
Birge factor	0.693		-	
BIC	6483.6		6612.5	

**Table 6.5:** The comparison between  $D4_S$  and  $D4_S(9sv)$  parameters.



**Figure 6.6:** Singular values  $\alpha_k^2$  for  $D_{4S}$  and  $D_{4H}$  parametrization. As discussed in Appendix A, they are organized in descending order.

number of singular values means neglecting the smallest contribution to  $\mathcal{J}^T W \mathcal{J}$ . It corresponds to neglect the linear combinations of parameters that influence the fit less or spoil it. In this instance, the smallest contribution comes from the expectation value of the generator of three-body, as the SVD suggests. Ignoring  $\alpha_{10}$  explains the small value  $C_{t_3}$ =369.1 in D4<sub>S</sub>(9sv), when usual value is on the order of 10<sup>4</sup>.

In  $D4_S(9sv)$  the distance between data and fitted values,  $\mathbf{y} - \mathcal{J}\mathbf{C}$ , is large enough to require a model error of 4.195 to normalize the penalty function, on the contrary of the Birge factor in the case  $D4_S$ . This is even more evident when looking at the *BIC* values, that read  $BIC(D4_S) < BIC(D4_S(9sv))$ . In general, we observe that reducing the number of singular values produces a decreasing of the absolute values of the parameters and their errors. This happens because the elements of the matrix  $(\mathcal{J}^T W \mathcal{J})^{-1}$  become smaller at the price of deteriorating the penalty function.

All these evidences suggest that the large value of isovector parameters and errors in  $D4_S$  are not related to numerical issues in the fitting procedure.

We plot the correlation matrix for  $D4_S$  in Figure 6.7, to study if there are evident relation between the parameters. We notice, in particular, the correlation between  $C_0^{J1}$  and  $C_1^{J1}$  and various anti-correlations.



Figure 6.7: Correlation matrix for the parametrizations  $D4_S$ . Full correlation is indicated in yellow, anti-correlation in dark blue.

### Case with error from Hellmann-Feynman difference $[\Delta V_n^{ab}]_H$

We consider the case in which the error  $\Delta y_i^{ab}$  is due to the difference in the Hellmann-Feynman theorem and we indicate the parametrizations with the subscript <sub>H</sub>. Results obtained for the databases D1<sub>H</sub>, D2<sub>H</sub>, D3<sub>H</sub> and D4<sub>H</sub> are presented in Table 6.6.

We have already understood from the bottom panels in Figure 6.3 that, in general,  $[\Delta V_n^{ab}]_H > [\Delta V_n^{ab}]_S$ . This induces in each parametrization  $D_H$  a larger error on the coupling constants, respect to the corresponding  $D_S$ . The huge value of  $\Delta y_i$ makes the weight function smaller and then the normalization of the  $\chi^2$  requires the use of the Birge factor. The Birge factor decreases while increasing the number of parameters (or generators) in the database. This fact suggests an improvement in the fit. The same advise can be extracted by comparing the *BIC* for  $D1_H$  and  $D3_H$ , for  $D2_H$  and  $D4_H$ . In particular, similarly to the  $D_S$  case, the inclusion of all the possible generators,  $D4_H$ , seems to provide the better fit of the *ab initio* interaction energy. We observe also that  $BIC(D4_H) < BIC(D4_S)$ , indicating this parametrization as the best fit.

parameter	$D1_H$		$D2_H$		$D3_H$		$D4_H$	
$C_0^{\rho}$	-397.0	$\pm 8.5$	-392.6	$\pm$ 7.0	-418.0	$\pm 26.3$	-410.7	$\pm 21.3$
$C_1^{\rho}$	-		142.7	$\pm 10.5$	-		-120.2	$\pm$ 708.2
$C_0^{\Delta \rho}$					30.3	$\pm$ 33.7	38.0	$\pm$ 20.0
$C_1^{\Delta \rho}$	-		-		-		-1451.1	$\pm \ 1850.9$
$C_0^{\tau}$			-		-111.5	$\pm$ 69.3	-125.2	$\pm 41.5$
$C_1^{\tau}$	-		-		-		-26.3	$\pm$ 458.5
$C_0^{J1}$	-		-		223.4	$\pm$ 1424.7	506.9	$\pm$ 970.3
$C_1^{J1}$	-		-		-		315.5	$\pm$ 916.0
$C_{w_0}$	-		-		-158.7	$\pm$ 554.6	-267.8	$\pm$ 374.6
$C_{t_3}$	12704.6	$\pm$ 1080.3	12129.2	$\pm$ 882.9	30406.6	$\pm$ 8832.1	31494.8	$\pm$ 6012.6
$\chi^2$	1.000		1.000		1.000		1.000	
model error	0.0		0.0		0.000		0.000	
Birge factor	0.109		0.089		0.049		0.030	
BIC	2717.6		6704.3		2637.0		6360.6	

**Table 6.6:** Values of the parameters for the parametrizations  $D1_H$ ,  $D2_H$ ,  $D3_H$  and  $D4_H$ , with relative errors, and related statistical quantities.

Residuals are shown in Figure 6.8 and 6.9 respectively for <sup>16</sup>O and <sup>56</sup>Ni. In both nuclei the residuals are smaller than 1%, and of the corresponding systems in D4<sub>S</sub> parametrization. It is also evident that the propagated errors are broader than the ones in D4<sub>S</sub>. Including the error bars, almost all the residual are compatible with the value zero.

The singular values for  $D4_H$  are plotted in Figure 6.6. They are more than a factor 10 smaller than the ones for  $D4_S$ , because the large uncertainties make the elements of the weight matrix W smaller. Anyway, the condition number  $F_{SVD} = 9.6 \times 10^8$  keeps the regression away from singularities. Removing the smallest singular values does not improve the fit, in a similar way as we already discussed for  $D4_S$ .

The correlation matrix for  $D4_H$ , in Figure 6.10, points out the correlation between  $C_0^{J1}$  and  $C_1^{J1}$ . The number of anti-correlated parameters seems to be raised but with slightly reduced amplitude respect to  $D4_S$ .

#### 6.4.1 Nuclear matter properties

We test the performance of the obtained parametrizations in the description of nuclear matter.

Appendix B discusses the concept of infinite nuclear matter and shows how to



**Figure 6.8:** Residuals for the parametrization  $D_{4H}$  in <sup>16</sup>O.

extract its properties from a Skyrme-like functional. We derive such quantities for the databases  $D1_S$ ,  $D2_S$ ,  $D3_S$  and  $D4_S$  in Table 6.7, and for  $D1_H$ ,  $D2_H$ ,  $D3_H$  and  $D4_H$  in Table 6.8.

It is interesting to compare them with the properties described by the original NNLOsat interaction. In Ref. [100], the equation of state for the NNLOsat parametrization presents a minimum for the energy at the value of  $E/A \approx -14.5$  MeV. Such minimum is obtained when the Fermi wave vector  $k_F = 1.35$  fm<sup>-1</sup>, i.e., using the relation  $\rho_{sat} = \frac{2}{3\pi^2} k_F^3$ , this value corresponds to  $\rho_{sat} = 0.166$  fm<sup>-3</sup>. The incompressibility is given K = 253 MeV.

Considering the NNLOsat values and the empirical ones (see Table B.1)  $D4_S$  and  $D4_H$  seem to provide a better description of the bulk properties as saturation density  $\rho_{sat}$ , volume radius  $r_0$  and binding energy per particle E/A. This fact agrees with the previous statistical analysis to indicate  $D4_S$  and  $D4_H$  as the best among the respective parametrizations.

The symmetry energy J and its slope L are poorly determined with huge propagated errors. In general, the propagated errors in  $D_H$  are larger than in  $D_S$ , as expected. The effective mass  $m^*/m$  represents an issue for this kind of model. The empirical value is considered between 0.6 and 0.9, with Skyrme-like interactions that often underestimate it (for Skyrme SV  $m^*/m \approx 0.38$ ). In the fitted parametrizations, the closest value appears in the D1 and D2 database, where the value 1 is only due



Figure 6.9: Same as in Figure 6.8 for <sup>56</sup>Ni.



Figure 6.10: Correlation matrix for the parametrizations  $D4_{H}$ .

to the absence of the coupling constant  $C_0^{\tau}$  from the model  $(C_0^{\tau}=0)$ . Including the error bars,  $m^*/m$  for  $\mathrm{D4}_H$  is in the empirical range, but this is not enough to have

**Table 6.7:** Nuclear matter properties extracted for the parametrization  $D1_S$ ,  $D2_S$ ,  $D3_S$ and  $D4_S$ , with relative propagated errors. Empirical values are provided in Table B.1. The properties relative to the NNLOsat interaction are  $\rho_{sat} =$ 0.166 fm <sup>-3</sup>,  $E/A \approx$ -14.5 MeV and K = 253 MeV, given in Ref. [100].

quantity	$D1_S$		$D2_S$		$D3_S$		$D4_S$	
$\rho_{sat}  [\mathrm{fm}^{-3}]$	0.191	$\pm 0.002$	0.181	$\pm 0.002$	0.130	$\pm 0.002$	0.132	$\pm 0.002$
$r_0  [\mathrm{fm}]$	1.078	$\pm 0.003$	1.097	$\pm 0.005$	1.223	$\pm 0.007$	1.219	$\pm 0.005$
E/A [MeV]	-21.79	$\pm 0.09$	-21.28	$\pm 0.13$	-15.19	$\pm 0.34$	-14.56	$\pm 0.20$
$m^*/m$	1	-	1	-	12.52	$\pm 11.02$	-22.72	$\pm 21.95$
$J  [{\rm MeV}]$	-16.3	$\pm 0.3$	17.2	$\pm 1.0$	-32.6	$\pm 2.1$	10.1	$\pm 16.0$
$L [{\rm MeV}]$	-152.9	$\pm 2.0$	-49.5	$\pm 3.3$	-228.6	$\pm$ 11.7	190.4	$\pm$ 79.0
$K [{\rm MeV}]$	491.7	$\pm$ 13.6	479.0	$\pm 21.8$	386.1	$\pm$ 26.9	380.2	$\pm 17.5$

**Table 6.8:** Same as in Table 6.7 for  $D1_H$ ,  $D2_H$ ,  $D3_H$  and  $D4_H$  parametrizations.

quantity	$D1_H$		$D2_H$		$D3_H$		$D4_H$	
$\rho_{sat}  [\mathrm{fm}^{-3}]$	0.196	$\pm 0.012$	0.203	$\pm 0.011$	0.129	$\pm 0.017$	0.128	$\pm 0.012$
$r_0  [\mathrm{fm}]$	1.068	$\pm 0.023$	1.056	$\pm 0.019$	1.227	$\pm 0.055$	1.232	$\pm 0.039$
E/A [MeV]	-21.99	$\pm 0.93$	-22.55	$\pm 0.86$	-16.43	$\pm 2.13$	-15.99	$\pm 1.25$
$m^*/m$	1	-	1	-	3.27	$\pm 4.62$	4.38	$\pm 4.90$
$J  [{\rm MeV}]$	-16.4	$\pm 2.6$	12.1	$\pm 3.1$	-28.4	$\pm$ 13.7	-50.2	$\pm$ 99.2
$L  [{\rm MeV}]$	-154.4	$\pm 15.5$	-71.5	$\pm 15.1$	-205.8	$\pm$ 77.5	-284.1	$\pm$ 436.2
$K \; [MeV]$	497.0	$\pm$ 109.9	509.5	$\pm$ 97.2	399.1	$\pm$ 195.9	393.3	$\pm$ 143.5

a correct distribution of single-particle energies. We aim to improve the effective mass by the constraint of its value with the Tikhonov term.

#### 6.4.2 Constrained results

Following Section 5.2.1, we introduce the Tikhonov term  $\lambda_T$  as Lagrangian parameter of the constraint  $\mathbf{b} = Q\mathbf{C}$ . For our interest to adjust the effective mass  $m^*/m$ , the constraint equation is given by Eq.(B.5) and the target effective mass is set to  $m^*/m=0.70$ .

We vary the value of  $\log_{10}\lambda_T$  from -4 to 2 and we study the changes in the constrained parameters  $\mathbf{C}_T$ , solutions of the constrained regression. In the unconstrained part of  $\chi_T^2$ , we take the inputs used respectively for the databases  $\mathrm{D4}_S$  and  $\mathrm{D4}_H$ , that have provided the best fit of the *ab initio* interaction. For every  $\lambda_T$ ,

we obtain the parametrizations  $D4_S^{lc}(\lambda_T)$  and  $D4_H^{lc}(\lambda_T)$ , where <sup>1c</sup> indicates that one constraint is used. The evolution of the constrained parameters  $\mathbf{C}_T$  in function of the Tikhonov parameter is shown respectively in the top panels of Figure 6.11  $(D4_S^{lc})$  and Figure 6.13  $(D4_H^{lc})$ .



**Figure 6.11:**  $D_{4S}^{1c}(\lambda_T)$  parametrization with  $m^*/m$  constrained to 0.70. (Top) Value of the coupling constants  $\mathbf{C}_T$  in function of  $\lambda_T$ .  $C_{t_3}$  is scaled by a factor 50 as explained in the legend. (Bottom) Contribution of the data points  $\chi^2_{data}$ and contribution of the Tikhonov term  $\chi^2_{constr}$  to the total  $\chi^2_T$  (normalized).

For the case  $D4_S^{1c}$ , the changes in the parameters happen at  $\log_{10}\lambda_T$  between -1 and 0. Out of this region their values are quite stable.  $C_1^{\rho}$ ,  $C_1^{\Delta\rho}$ ,  $C_0^{J1}$ ,  $C_1^{J1}$  and  $C_{t_3}$  are the coupling constants in which the constraint makes the largest impact. We have already noticed that these coupling constants were poorly determined by the regression in the parametrization  $D4_S$ .

In the bottom panel of Figure 6.11, the normalized  $\chi^2_T$  is separated in the contribu-

tion from the data points  $\chi^2_{data}$  and from the constrained part  $\chi^2_{constr}$  (see Eq.(5.34)). It is evident that the contribution of the constrained part to the total  $\chi^2_T$  increases with  $\lambda_T$  up to  $\log_{10}\lambda_T \approx -0.5$ . After that, such contribution drops quickly down to zero. The explanation for this effect is that at the peak of  $\chi^2_{constr}$  the parameters begin to be adjusted to give  $m^*/m$  close to the target value. Increasing  $\lambda_T$  decreases  $\chi^2_{constr}$  because  $\mathbf{b} - Q\mathbf{C} \to 0$ , while the reproduction of the data points deteriorates since the difference  $\mathbf{y} - \mathcal{J}\mathbf{C}$  becomes always more prominent.



Figure 6.12: Infinite nuclear matter properties extracted from  $D4_S^{1c}(\lambda_T)$ . The curves show  $\rho_{sat}$  (top left), E/A (top right),  $m^*/m$  (bottom left) and symmetry energy J (bottom right). The red shadows indicate the propagated error bars. The gray regions illustrate the range of the empirical values in Table B.1.

The kink in the plot of the effective mass  $m^*/m$  is due to numerical instability.

We present the nuclear matter properties  $\rho_{sat}$ , E/A,  $m^*/m$  and symmetry energy J relative to the parametrization  $D4_S^{1c}(\lambda_T)$  in Figure 6.12. For small  $\lambda_T$  the values of such quantities equal the values extracted from  $D4_S$ . In the region of  $\log_{10}\lambda_T$  between -1 and 0, the "active" region of the constraint, the properties change

abruptly and the effective mass is dragged towards the target value. When the target value is reached, at  $\log_{10}\lambda_T$  between 0 and 1, these quantities do not vary any more. We note that the kink in the plot of the effective mass is an artefact of numerical instability, a pole in the Eq.(B.5), and does not have physical significance.

The curves for  $\rho_{sat}$ , E/A and symmetry energy cross their region of empirical values (shown in gray color) before setting to values far away from standard nuclear matter conditions. Such crossing occurs at slightly different value of  $\lambda_T$  for the three quantities and before the effective mass reaches its empirical range. We conclude that there are no values of the Tihkonov parameter in which all the mentioned quantities are in their expected domain, even including the propagated error bars.



**Figure 6.13:** Same as in Figure 6.11 for the parametrization  $D4_{H}^{1c}(\lambda_{T})$ .

A similar analysis is performed for the case  $D4_{H}^{1c}(\lambda_{T})$  in Figure 6.13. Here, the

large variation of the coupling constants can be noticed around  $\log_{10}\lambda_T = -2$ . The largest changes concern, also in this situation, the parameters  $C_1^{\Delta\rho}$ ,  $C_0^{J1}$ ,  $C_1^{J1}$  and  $C_{t_3}$ .

In  $\chi_T^2$ , the separation of the contributions manifests the peak in the curve  $\chi_{constr}^2$ near  $\log_{10} \lambda_T = -2$ . Such peak is smaller in amplitude compared to the case  $\mathrm{D4}_S^{1c}(\lambda_T)$ in Figure 6.11. The reduction is explained by the fact that the unconstrained solution  $\mathrm{D4}_H$  has an effective mass closer to the target value and, then, the distance  $\mathbf{b} - Q\mathbf{C}$  does not grow significantly.



**Figure 6.14:** Same as in Figure 6.12 for the parametrization  $D4_H^{1c}(\lambda_T)$ .

The corresponding variation of the nuclear matter parameters appears smoother in Figure 6.14. However, neither in this case the nuclear matter properties are simultaneously (at the same  $\lambda_T$ ) in agreement with the empirical values. When the effective mass approaches the reference value 0.70, namely around  $\log_{10}\lambda_T \approx$ -1, the energy per particle E/A results over bound and the symmetry energy has become huge.

Both parametrizations,  $D4_S^{1c}(\lambda_T)$  and  $D4_H^{1c}(\lambda_T)$ , fail to reproduce the nuclear

matter properties by constraint of the effective mass. A possible reason for the failure regards the correlation between the parameters. Figure 6.7 (for D4<sub>S</sub>) and Figure 6.10 (for D4<sub>H</sub>) point out a strong anti-correlation between the parameters  $C_0^{\tau}$  and  $C_{t_3}$ . The effective mass depends explicitly and only on  $C_0^{\tau}$ . Trying to adjust the value of this parameters moves  $C_{t_3}$  out of its local minima in the domain of the regression. Since  $C_{t_3}$  is the parameter of the three-body part of the functional, a large reduction of  $C_{t_3}$  value produces strong effect on the saturation properties of the nuclear matter. In fact, the repulsive contribution of the three-body interaction becomes smaller and the nuclear matter system results over bound, with a large saturation density.

Attempts to constraint at the same time the effective mass and the energy per particle have failed to provide reasonable results. The parameters of the model were not able to approach the targeted values of these properties simultaneously.

## 6.5 Model functional

This work aimed to study the feasibility of the derivations based on the *ab initio* interaction to built a model energy density functional. The performed analysis suggested that  $D4_S$  and  $D4_H$  are the most reasonable parametrizations among the set of available generators, namely, the models in which our confidence is higher, also thanks to the prior knowledge on the nuclear matter properties.

We insert the obtained parameters and the corresponding generators in the model EDF in Eq.(5.1), obtaining  $\tilde{E}[\rho]$ . In particular, we construct the functionals  $\tilde{E}[\rho]_{D4_S}$  and  $\tilde{E}[\rho]_{D4_H}$ . We minimize the functionals with respect to all the possible densities (second stage of the Levy-Lieb constrained search). Such minimization, for the case of the parametrization D4<sub>S</sub> as well as for D4<sub>H</sub>, does not converge to a self-consistent solution. That is, the minimum of the functional is not stable and corresponds to densities out of the domain of the densities explored by the perturbations  $\lambda_i$ . It may indicate that the actual information we extracted from the *ab initio* interaction is not extendible to the framework of the EDFs.

We can address possible reasons for the failure of the method.

The derivation assumes that generators of one-body densities are able to fit the *ab initio* interaction energy, which is calculated with the self-energy in approximation ADC(3), well beyond the mean-field order. The coupling constants have the role of absorbing the high order effects in their values. This approach is fully compatible

with the Levy-Lieb construction of exact density functionals. However, if the set of generators is not adequate to describe the original interaction, the minimization of the penalty function can lead values of the coupling constants outside the physical region. Large values of the penalty function relative to NNLOsat interaction, compared to the exact fit of Skyrme SV interaction (Appendix F), can be evidence of that misbehavior.

The introduction of the constraint on the effective mass was not decisive to improve the description of nuclear matter, worsening the bulk properties like saturation density and energy per particle. This can be seen as another indication that the list of parameters and generators is severely limited.

# 7. Summary, conclusions, and perspectives

In this thesis, I studied a link between functional generators employed in the nuclear Energy Density Functionals theory and the chiral interactions used within the *ab initio* calculations.

Applying the technique suggested in Ref. [1], seven semi-magic nuclei in the light-medium mass region were probed with perturbations induced by generators of two- and three-body contact interaction (Skyrme). The perturbations provided a large collection of ground state energies, calculated with the Self-Consistent Green's Functions method in ADC(3) approximation. Such theoretical results formed a database, that extended beyond the limited number of unperturbed solutions normally available, corresponding to the experimental ground state energies.

We used the collection of *ab initio* data points to compare competing models, differing by the selection of generators and by the estimated errors on the data, to describe the *ab initio* interaction energy. For each model or parametrization, we derived the coupling constants of a model functional, to be built by the same generators.

We studied the properties of the obtained coupling constants in relation to their ability to reproduce the potential of the NNLOsat chiral interaction as well as the infinite nuclear matter properties, which the functional is expected to satisfy.

In the Bayesian language, we can say that we had different competing hypotheses, the parametrizations or selection of generators, and we completed the task to determine the set of parameters, in the values of which we placed the largest confidence. Such confidence was also assigned according to the prior best knowledge, namely the nuclear matter properties.

At the end of our analysis, with the help of statistical tools, we preferred two parametrizations  $D4_S$  and  $D4_H$ , both employing all the generators available in our Skyrme-like functional. They differed by the estimated errors on the *ab initio* interaction energies, respectively due to the approximation made on the calculation of the perturbation and Coulomb contributions and due to the estimates obtained by employing the Hellmann-Feynman theorem. The  $D4_H$  parametrization gave slightly better description of the nuclear matter system, including the large propagated error bars.

However, we verified that the fitted parameters were not able to provide a valid model Energy Density Functional since the preferred parametrizations did not lead to convergent functionals.

We discussed possible issues to explain the failure of the approach, pointing towards the conclusion that the set of generators was not adequate to reproduce the *ab initio* interaction. Extension to finite-range and symmetry-breaking generators could be beneficial to establish the suitability of the approach and will be explored in further studies.

Our derivation of the functionals was based only on the information contents of the ground-state energies, in the spirit of the Levy-Lieb construction. It is an open problem whether this information can be sufficient to characterize functionals for nuclear structure calculations. Parametrizations available in the literature usually include such observables as charge radii and nuclear matter properties, together with ground-state energies, in the penalty functions to be optimized.

We also pointed out some limitations of the actual *ab initio* calculations, in particular, related to the SCGF method. In fact, the current approximations, employed to calculate the ground-state energies, seemed to show large uncertainties of the estimated averaged interaction. We could see it by applying the Hellmann-Feynman method or estimating the difference between the highest order and the next-to-leading order contributions. Such uncertainties appeared to be significantly larger than the precision expected at the level of nuclear density functionals.

Appendices

## A. Singular Value Decomposition

We consider a  $m \times n$  matrix A with rank  $r \leq \min(m, n)$ . The Singular Value Decomposition [113] of A allows to write

$$A = L\Sigma R^T. \tag{A.1}$$

L is a  $m \times m$  matrix containing  $\mathbf{l}_1, ..., \mathbf{l}_k$  column vectors that form an orthonormal basis for the column space and  $\mathbf{l}_{k+1}, ..., \mathbf{l}_m$  column vector, orthonormal basis for the left null space  $\mathcal{N}(A^T)$ . R is a  $n \times n$  matrix containing  $\mathbf{r}_1, ..., \mathbf{r}_k$  row vectors that form an orthonormal basis for the row space and  $\mathbf{r}_{k+1}, ..., \mathbf{r}_n$  row vector, orthonormal basis for the left null space  $\mathcal{N}(A)$ .  $\Sigma$  is a  $m \times n$  matrix made with all zeros but the first k matrix elements  $\sigma_i = [\Sigma]_{ii}$ .  $\sigma_1, ..., \sigma_k$  are positive numbers called "singular values".

The decomposition of A appears in vector notation as  $A\mathbf{r}_i = \sigma_i \mathbf{l}_i$  for i = 1, ..., k. Eq.(A.1) can be explicited as

$$\begin{bmatrix} A \end{bmatrix} = \begin{bmatrix} \mathbf{l}_1 & \dots & \mathbf{l}_k & \dots & \mathbf{l}_m \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_k & & \\ & & & 0 & \\ & & & & 0 \end{bmatrix} \begin{bmatrix} \mathbf{r}_1^T & \dots & \mathbf{r}_k^T & \dots & \mathbf{r}_m^T \end{bmatrix}$$
$$= \mathbf{l}_1 \sigma_1 \mathbf{r}_1^T + \dots + \mathbf{l}_k \sigma_k \mathbf{r}_k^T.$$
(A.2)

The singular values  $\sigma_i$  are in descending order ( $\sigma_1 \ge \sigma_i \ge \sigma_k > 0$ ), meaning that the terms in the last line of Eq.(A.2) appear in order of importance.

It is significant to notice that  $\sigma_i^2$  are eigenvalues of  $A^T A$  as well as  $A A^T$ .

Studying the response of the singular values to a small variation in A, Ref. [113] shows that for a small change in one of the matrix elements  $[A]_{ij} \rightarrow [A]_{ij} + \epsilon$ , with  $\epsilon \ll [A]_{ij}$ , the singular values will not be altered more than  $\epsilon$ . That is, the singular values of A are stables.

If eigenvalues of A exist (A is a square matrix), and if A is not normal ( $A^T A \neq A A^T$ ), the same small svariation in a matrix element can lead to a drastic change in the eigenvalues of A (change  $\gg \epsilon$ ). It means that the eigenvalues of a not normal square matrix are unstable, contrarily to the singular values.

### A.1 SVD applied to ill-posed problem

In Section 5.2, we have presented concerns about calculating the inverse of the matrix  $\mathcal{J}^T W \mathcal{J}$ , when it is singular. We can use the SVD to solve this problem. We start with the decomposition of the  $p \times p$  square matrix  $\mathcal{J}^T W \mathcal{J}$ , that results [114]

$$\mathcal{J}^T W \mathcal{J} = \mathcal{R} \; \alpha^2 \mathcal{R}^T, \tag{A.3}$$

where  $\alpha^2$  are q positive (> 0) singular values, with  $q \leq p$ , and  $\mathcal{R}$  is a  $p \times q$  matrix. This is equivalent to assume the decomposition of the rectangular matrix  $\mathcal{J}_{ji}$  as

$$\mathcal{J}_{ji} = \sum_{k=1}^{q} \mathcal{L}_{jk} \alpha_k (\mathcal{R}^T)_{ki}, \qquad (A.4)$$

where  $\mathcal{L}$  is a  $d \times q$  matrix. Outside the null space of  $\mathcal{J}^T W \mathcal{J}$ , its inverse results

$$(\mathcal{J}^T W \mathcal{J})^{-1} = \mathcal{R} \frac{1}{\alpha^2} \mathcal{R}^T.$$
(A.5)

Selecting only the singular values larger than a certain value  $\epsilon$ , we can rewrite the inverse as

$$(\mathcal{J}^T W \mathcal{J})^{-1} = \mathcal{R} \begin{bmatrix} \frac{1}{\alpha_1^2} & & & \\ & \ddots & & \\ & & \frac{1}{\alpha_k^2} & \\ & & & 0 \\ & & & & 0 \end{bmatrix} \mathcal{R}^T,$$
(A.6)

where  $\alpha_{k+1}, ..., \alpha_q < 0$ . In the regression analysis, the fitted parameters are determined by the cut off  $\epsilon$ . In fact, only the first k out of the q singular values influence the value of the parameters as

$$(\mathbf{C}_{min})_{j} = \sum_{l=1}^{k} \sum_{m=1}^{p} \sum_{i=1}^{d} \mathcal{R}_{il} \frac{1}{\alpha_{l}^{2}} (\mathcal{R}^{T})_{lm} (\mathcal{J}^{T})_{mi} w_{i} y_{i}.$$
(A.7)

# B. Infinite nuclear matter properties

Infinite nuclear matter can be viewed as an idealized system made of nucleons, interacting only through nuclear force. The system is considered infinite in the sense that it does not have a surface, and it is invariant for translation.

We are interested to study the Symmetric Nuclear Matter (SNM), assuming that the nuclear matter contains an equal number of protons and neutrons.

For a Skyrme-like functional or interaction the characterizing properties of SNM can be calculated analytically. Such system is described by an energy density in which the terms containing derivatives of the densities are neglected. The energy per nucleon E/A reads

$$\frac{E}{A}(\rho) = \frac{\mathcal{E}}{\rho} = \frac{\hbar^2}{2m} \left(\frac{3\pi^2}{2}\right)^{2/3} \frac{3}{5} \rho^{2/3} + C_0^{\rho} \rho + \frac{1}{16} t_3 \rho^{\gamma+1} + \left(\frac{3\pi^2}{2}\right)^{2/3} \frac{3}{5} C_0^{\tau} \rho^{5/3} \quad (B.1)$$

$$= \frac{\hbar^2}{2m} \left(\frac{3\pi^2}{2}\right)^{2/3} \frac{3}{5} \rho^{2/3} + \frac{3}{8} t_0 \rho + \frac{1}{16} t_3 \rho^{\gamma+1} + \left(\frac{3\pi^2}{2}\right)^{2/3} \frac{3}{80} (3t_1 + 5t_2 + 4t_2 x_2) \rho^{5/3}, \quad (B.2)$$

where the kinetic energy is taken from the Thomas-Fermi model. Eq.(B.1) is expressed with the coupling constants, while Eq.(B.2), in terms of the Skyrme parameters, follows from Ref. [32]. The pression P of the system, equivalent to

$$P(\rho) \equiv \rho^2 \frac{\partial(\mathcal{E}/\rho)}{\partial \rho} = \frac{\hbar^2}{2m} \left(\frac{3\pi^2}{2}\right)^{2/3} \frac{2}{5} \rho^{5/3} + C_0^{\rho} \rho^2 + \frac{1}{16} t_3(\gamma+1) \rho^{\gamma+2} + \left(\frac{3\pi^2}{2}\right)^{2/3} C_0^{\tau} \rho^{8/3},$$
(B.3)

defines the saturation density  $\rho^{sat}$  as the density at which  $P(\rho^{sat}) = 0$  (minimum of the binding energy per nucleon E/A). The volume incompressibility is

$$K(\rho) \equiv 9 \frac{\partial P}{\partial \rho} = \frac{\hbar^2}{2m} \left(\frac{3\pi^2}{2}\right)^{2/3} 6\rho^{2/3} + 18C_0^{\rho}\rho + \frac{9}{16}t_3(\gamma+1)(\gamma+2)\rho^{\gamma+1} + \left(\frac{3\pi^2}{2}\right)^{2/3} 24C_0^{\tau}\rho^{5/3}.$$
(B.4)

The in-medium effective (isoscalar) nucleon mass is given as

$$\frac{m^*}{m}(\rho) = \left[1 + \frac{2m}{\hbar^2} C_0^{\tau} \rho\right]^{-1}.$$
 (B.5)

It is important to notice that it depends explicitly only on the coupling constant  $C_0^{\tau}$ , while the value of  $\rho$  is determined by the saturation condition. The effective mass is related with the density of single-particle levels in the energy space.

The isovector coupling constants enter in the expressions for the symmetry energy J and its derivative L, calculated at the saturation density as

$$J(\rho^{sat}) = \frac{\hbar^2}{2m} \left(\frac{3\pi^2}{2}\right)^{2/3} \frac{1}{3} \rho_{sat}^{2/3} + C_1^{\rho} \rho_{sat} - \frac{1}{48} t_3 (1+2x_3) \rho_{sat}^{\gamma+1} + \left(\frac{3\pi^2}{2}\right)^{2/3} \left(\frac{1}{3} C_0^{\tau} + C_1^{\tau}\right) \rho_{sat}^{5/3},$$
(B.6)

$$L \equiv 3\rho^{sat} \frac{\partial J}{\partial \rho} \Big|_{\rho = \rho^{sat}} = \frac{\hbar^2}{2m} \left( \frac{3\pi^2}{2} \right)^{2/3} \frac{2}{3} \rho^{2/3}_{sat} + C_1^{\rho} \rho_{sat} - \frac{1}{16} t_3 (1 + 2x_3) (\gamma + 1) \rho^{\gamma + 1}_{sat} + \left( \frac{3\pi^2}{2} \right)^{2/3} 10 \left( \frac{1}{3} C_0^{\tau} + C_1^{\tau} \right) \rho^{5/3}_{sat}.$$
(B.7)

Nuclear matter quantities have definite values extrapolated from experimental results or deduced from empirical models (see Table B.1).

In Section 6.4.1, we evaluated the infinite nuclear matter properties for the parametrizations obtained by the regression analysis. Moreover, thanks to Eq.(5.31), we quantified the error propagated on the nuclear matter quantities, helping in the comparison with empirical values. Specifically, the central-difference formula provided the numerical derivatives as

$$G_j^A = \frac{\partial \mathcal{A}}{\partial C_j}\Big|_{\mathbf{C}=\mathbf{C}_{min}} = \frac{\mathcal{A}(\mathbf{C}_{min} + h_j) - \mathcal{A}(\mathbf{C}_{min} - h_j)}{2h_j} + O(h_j^2).$$
(B.8)

**Table B.1:** Typical values for the properties of infinite nuclear matter taken from Ref. [32] and evaluated at  $\rho = \rho^{sat}$ .

quantity	value (or range)	
$\rho_{sat}  [\mathrm{fm}^{-3}]$	$0.17\pm0.03$	
$E/A \; [{\rm MeV}]$	$-16 \pm 0.5$	
$m^*/m$	0.65 - 0.9	
$J \; [{\rm MeV}]$	30 - 35	
$L \; [MeV]$	40 - 76	
$K \; [MeV]$	200 - 260	

# C. Parameters and coupling constants of Skyrme interaction

The interaction part of Skyrme-type EDFs is formed by combinations of density generators  $\mathcal{V}_{j}^{gen}$  and coupling constants  $C_{j}$ , namely  $E_{int}[\rho] = \sum_{j} \int d\mathbf{r} C_{j} \mathcal{V}_{j}^{gen}[\rho]$ . Taking Eq.(2.42) as example,

$$C_j \mathcal{V}_j^{gen}[\rho] = C_T^{\rho} \rho_T^2 + C_T^{\Delta \rho} \rho_T \Delta \rho_T + C_T^{\tau} \rho_T \tau_T + C_T^J \mathbb{J}_T^2 + C_T^{\nabla J} \rho_T \nabla \cdot \mathbf{J}_T.$$
(C.1)

The coupling constants  $C_j$  are connected to linear combinations of the Skyrme parameters  $t_i$ , defining  $\hat{V}_{Skyrme} = \sum_i t_i \hat{V}_{t_i}^{gen}$ . We can distinguish the generators  $\hat{V}_{t_i}^{gen}$  in the standard form of the Skyrme interaction

$$\hat{V}_{Skyrme}(\mathbf{r_1} - \mathbf{r_2}) = t_0(1 + x_0\hat{P}^{\sigma})\delta(\mathbf{r_1} - \mathbf{r_2}) 
+ \frac{1}{2}t_1(1 + x_1\hat{P}^{\sigma}) \left[\hat{\mathbf{k}}'^2\delta(\mathbf{r_1} - \mathbf{r_2}) + \delta(\mathbf{r_1} - \mathbf{r_2})\hat{\mathbf{k}}^2\right] 
+ t_2(1 + x_2\hat{P}^{\sigma})\hat{\mathbf{k}}' \cdot \delta(\mathbf{r_1} - \mathbf{r_2})\hat{\mathbf{k}} 
+ iw_0(\hat{\sigma_1} + \hat{\sigma_2}) \cdot \left[\hat{\mathbf{k}}' \times \delta(\mathbf{r_1} - \mathbf{r_2})\hat{\mathbf{k}}\right] 
+ \frac{t_e}{2}\left\{\left[3(\sigma_1 \cdot \mathbf{k}')(\sigma_2 \cdot \mathbf{k}') - (\sigma_1 \cdot \sigma_2)\mathbf{k}'^2\right]\delta(\mathbf{r_1} - \mathbf{r_2}) 
+ \delta(\mathbf{r_1} - \mathbf{r_2})\left[3(\sigma_1 \cdot \mathbf{k})(\sigma_2 \cdot \mathbf{k}) - (\sigma_1 \cdot \sigma_2)\mathbf{k}'^2\right]\right\} 
+ t_o\left\{3(\sigma_1 \cdot \mathbf{k}')\delta(\mathbf{r_1} - \mathbf{r_2})(\sigma_2 \cdot \mathbf{k}) - (\sigma_1 \cdot \sigma_2)\left[\mathbf{k}' \cdot \delta(\mathbf{r_1} - \mathbf{r_2})\mathbf{k}\right]\right\} 
+ \frac{1}{6}t_3(1 + x_3\hat{P}^{\sigma})\delta(\mathbf{r_1} - \mathbf{r_2})\rho^{\alpha}\left(\frac{\mathbf{r_1} + \mathbf{r_2}}{2}\right), \quad (C.2)$$

which includes also the generators of the tensor part. Using the summation on repeated indices, the Skyrme coupling constants, for an interaction up to the second order in momentum, read

$$C_j = \mathcal{M}_j^i t_i, \tag{C.3}$$

where the matrix  $\mathcal{M}_{j}^{i}$  is obtained explicitly from

Here the  $\frac{1}{2}$  factor in the tensor term  $\sum_{T} \frac{1}{2} C_T^J \mathbf{J}_T^2$  is included in  $C_T^J$ , such that, in spherical symmetry, the corresponding tensor terms give the same results in Ref. [115] as in Ref. [116].

For EDFs derived from an underlying Hamiltonian, holds the relation

$$\int d\mathbf{r} \sum_{j} C_{j} \mathcal{V}_{j}[\rho] = \sum_{j} C_{j} \langle \Phi | \hat{V}_{j}^{gen} | \Phi \rangle = \sum_{i} t_{i} \langle \Phi | \hat{V}_{t_{i}}^{gen} | \Phi \rangle, \quad (C.5)$$

that is,  $C^j \hat{V}_j^{gen} = t^i \hat{V}_{t_i}^{gen}$ . After substituting  $C^j = (C_j)^T = t^i \mathcal{M}_i^j$ , the generators  $\hat{V}_j^{gen}$  are identified as

$$\hat{V}_j^{gen} = (\mathcal{M}_i^j)^{-1} \, \hat{V}_{t_i}^{gen},\tag{C.6}$$

that explicitly reads

$$\begin{bmatrix} \hat{V}_{0}^{\rho} \\ \hat{V}_{1}^{\rho} \\ \hat{V}_{0}^{\rho} \\ \hat{V}_{1}^{\Delta\rho} \\ \hat{V}_{1}^{\Delta\rho} \\ \hat{V}_{1}^{\Delta\rho} \\ \hat{V}_{1}^{\Gamma} \\ \hat{V}_{0}^{\Gamma} \\ \hat{V}_{1}^{\Gamma} \\ \hat{V}_{0}^{J} \\ \hat{V}_{1}^{J} \\ \hat{V}_{0}^{J} \\ \hat{V}_{1}^{J} \\ \hat{V}_{0}^{J} \\ \hat{V}_{1}^{J} \\ \hat{V}_{0}^{J} \\ \hat{V}_{1}^{J} \\ \hat{V}_{0} \\ \hat{V}_{1}^{J} \\ \hat{V}_{1}^{J} \\ \hat{V}_{0} \\ \hat{V}_{1}^{J} \\ \hat{V}_{2}^{J} \\ \hat{V}_{1}^{J} \\ \hat{V}_{$$

The notation  $\hat{V}_{(t)w_0}$  distinguishes the generator of the spin-orbit term associated with the parameter  $w_0$  from the generator  $\hat{V}_{w_0}$  associated to the coupling constant  $C_{w_0}$ .

Eq.(C.7) considers the vector contribution  $V_T^J \equiv V_T^{J1}$  to the tensor term, which is the only non-zero contribution to the tensor interaction in spherical symmetry. For the spin-orbit interaction, the only relation available is

$$C_{w_0}\langle\Phi|\hat{V}_{w_0}|\Phi\rangle = w_0\langle\Phi|\hat{V}_{(t)w_0}|\Phi\rangle = \int d\mathbf{r} \left(C_0^{\nabla J}\rho_0(\mathbf{r})\nabla\cdot\mathbf{J}_0(\mathbf{r}) + C_1^{\nabla J}\rho_1(\mathbf{r})\nabla\cdot\mathbf{J}_1(\mathbf{r})\right),$$
(C.8)

making not possible to separate the contribution of the isoscalar generator from the isovector one.

The derivation of the two-body matrix elements for the Skyrme interaction is presented in Appendix D.

Similarly, when deriving the term proportional to  $t_3$  from a zero-range three-body interaction (see Appendix E) with  $x_3 = 1$  fixed, the isospin components are not separable, and it results

$$C_{t_3}\langle\Phi|\hat{V}_{t_3}|\Phi\rangle = t_3\langle\Phi|\hat{V}_{t_3}|\Phi\rangle = \int d\mathbf{r} \left(C_0^{\rho\,dd}\rho_0^2(\mathbf{r}) + C_1^{\rho\,dd}\rho_1^2(\mathbf{r})\right). \tag{C.9}$$
# D. Skyrme two-body zero-range interaction

We present the expressions for the matrix elements of the two-body zero-range Skyrme interaction, Eq. $(C.2)^1$ , derived with the help of Ref. [117]. We consider the antisymmetrized<sup>2</sup> JT-coupled matrix element

$$\langle ab; J'M'; T'M'_T | V | cd; JM; TM_T \rangle_{as}$$

$$= \mathcal{N}_{ab}(J'T')\mathcal{N}_{cd}(JT) \Big[ \langle ab; J'M'; T'M'_T | \hat{V} | cd; JM; TM_T \rangle$$

$$+ (-1)^{j_c+j_d-J-T} \langle ab; J'M'; T'M'_T | \hat{V} | dc; JM; TM_T \rangle \Big],$$

$$(D.1)$$

where the normalization of the two-particle state reads

$$\mathcal{N}_{ab}(JT) = \frac{\sqrt{1 - \delta_{ab}(-1)^{J+T}}}{1 + \delta_{ab}}.$$
 (D.2)

In the following, we first concentrate on the part  $\langle ab; J'M'; T'M'_T | \hat{V} | cd; JM; TM_T \rangle$ and then we provide the complete expression, Eq.(D.1), for the distinct components of the interaction.

Since interested in a scalar potential  $\hat{V}$ , the angular momentum rules impose the condition  $\delta_{JJ'}\delta_{MM'}$ , such that

$$\langle ab; J'M'; T'M'_T | \hat{V} | cd; JM; TM_T \rangle = \langle ab; JM; T'M'_T | \hat{V} | cd; JM; TM_T \rangle.$$
(D.3)

<sup>&</sup>lt;sup>1</sup>The density-dependent part, last line in Eq.(C.2), is derived from the three-body zero-range interaction in Appendix E.

<sup>&</sup>lt;sup>2</sup>In Appendices D and E, we explicitly use the subscript " $_{as}$ " to distinguish the antisymmetrized matrix elements from the ones that are not. In the other parts of the thesis, we referred to antisymmetric matrix elements omitting the subscript for simplicity of notation.

After introducing the relative coordinates  $\mathbf{X} = \frac{1}{\sqrt{2}}(\mathbf{r}_1 + \mathbf{r}_2)$  and  $\mathbf{x} = \frac{1}{\sqrt{2}}(\mathbf{r}_1 - \mathbf{r}_2)$ , the space part of the interaction becomes

$$\langle \mathbf{r}_1' \mathbf{r}_2' | \hat{V} | \mathbf{r}_1 \mathbf{r}_2 \rangle = \delta \left( \frac{1}{\sqrt{2}} (\mathbf{X}' - \mathbf{X}) \right) v(\mathbf{x}', \mathbf{x}).$$
 (D.4)

In this relative coordinates, the  $\delta$ -interaction results

$$\langle \mathbf{r}_1' \mathbf{r}_2' | \delta(\mathbf{r}_1 - \mathbf{r}_2) | \mathbf{r}_1 \mathbf{r}_2 \rangle = \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_1 - \mathbf{r}_1') \delta(\mathbf{r}_2 - \mathbf{r}_2')$$
(D.5)

$$= \delta \left( \frac{1}{\sqrt{2}} (\mathbf{X}' - \mathbf{X}) \right) \delta(\sqrt{2}\mathbf{x}) \delta(\sqrt{2}\mathbf{x}').$$
 (D.6)

The corresponding relative momenta are

$$\mathbf{k_x} = \sqrt{2}\mathbf{k_r} = \sqrt{2}\left[-\frac{i}{2}\left(\nabla_{\mathbf{r_1}} - \nabla_{\mathbf{r_2}}\right)\right],\tag{D.7}$$

$$\mathbf{k}_{\mathbf{x}'}' \equiv \sqrt{2} \left[ \frac{i}{2} \left( \nabla_{\mathbf{r}_1'} - \nabla_{\mathbf{r}_2'} \right) \right].$$
(D.8)

The JT-coupled matrix elements can be written as

$$\begin{aligned} \langle ab; JM; T'M_T' | \hat{V} | cd; JM; TM_T \rangle \\ &= \langle n_a l_a j_a m_a, n_b l_b j_b m_b; JM; \frac{1}{2} \tau_a, \frac{1}{2} \tau_b; T'M_T' | \hat{V} | n_c l_c j_c m_c, n_d l_d j_d m_d; JM; \frac{1}{2} \tau_c, \frac{1}{2} \tau_d; TM_T \rangle \\ &= \sum_{\lambda' S'T'M_T'} \hat{\lambda}' \hat{S}' \hat{j}_a \hat{j}_b \left\{ \begin{array}{c} l_a & l_b & \lambda' \\ \frac{1}{2} & \frac{1}{2} & S' \\ j_a & j_b & J \end{array} \right\} C_{\frac{1}{2} \tau_a \frac{1}{2} \tau_b}^{T'M_T'} \sum_{N'L'n'l'} M_{n_a l_a n_b l_b, \lambda'}^{N'L'n'l'} * \\ &\times \sum_{\lambda STM_T} \hat{\lambda} \hat{S} \hat{j}_c \hat{j}_d \left\{ \begin{array}{c} l_c & l_d & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_c & j_d & J \end{array} \right\} C_{\frac{1}{2} \tau_c \frac{1}{2} \tau_d}^{TM_T} \sum_{NLnl} M_{n_c l_c n_d l_d, \lambda}^{NLnl} \\ &\times \langle N'L', n'l'\lambda'; \frac{1}{2} \frac{1}{2} S'M_S'; JM; \frac{1}{2} \frac{1}{2} T'M_T' | \delta \left( \frac{1}{\sqrt{2}} (\mathbf{X}' - \mathbf{X}) \right) v(\mathbf{x}', \mathbf{x}) f(\sigma_1, \sigma_2) f(\tau_1, \tau_2) \\ &\times |NL, nl\lambda; \frac{1}{2} \frac{1}{2} SM_S; JM; \frac{1}{2} \frac{1}{2} TM_T \rangle, \end{aligned}$$

with the coupled orbital angular momentum  $\lambda$  ( $\lambda'$ ), the coupled spin S (S') and the notation  $\hat{j} = \sqrt{2j+1}$ .  $M_{n_1 l_1 n_2 l_2, \lambda}^{NLnl} = \langle 2n_1 + l_1, l_1, 2n_2 + l_2, l_2; \lambda | 2N + L, L, 2n + l, l; \lambda \rangle_{d=1}$  are the coefficients of the Talmi-Moshinski transformations for the harmonic oscillator brackets [118]. The dependence on space-spin-isospin coordinates appears in

$$\langle N'L', n'l'\lambda'; \frac{1}{2}\frac{1}{2}S'M'_{S}; JM; \frac{1}{2}\frac{1}{2}T'M'_{T}|\delta\left(\frac{1}{\sqrt{2}}(\mathbf{X}'-\mathbf{X})\right)v(\mathbf{x}',\mathbf{x})f(\sigma_{1},\sigma_{2})f(\tau_{1},\tau_{2})$$

$$\times |NL, nl\lambda; \frac{1}{2}\frac{1}{2}SM_{S}; JM; \frac{1}{2}\frac{1}{2}TM_{T}\rangle$$

$$= \sum_{M_{\lambda}M_{S}M'_{\lambda}M'_{S}}C_{\lambda'M'_{\lambda}S'M'_{S}}^{JM}C_{\lambda M_{\lambda}SM_{S}}\sum_{M_{L}m_{l}M'_{L}m'_{l}}C_{LM_{L}lm_{l}}^{\lambda M_{\lambda}}C_{L'M'_{L}l'm'_{l}}^{\lambda'M'_{\lambda}}$$

$$\times \langle N'L'M'_{L}|\delta\left(\frac{1}{\sqrt{2}}(\mathbf{X}'-\mathbf{X})\right)|NLM_{L}\rangle\langle n'l'm'_{l}|v(\mathbf{x}',\mathbf{x})|nlm_{l}\rangle$$

$$\times \langle \frac{1}{2}\frac{1}{2}S'M'_{S}|f(\sigma_{1},\sigma_{2})|\frac{1}{2}\frac{1}{2}SM_{S}\rangle\langle \frac{1}{2}\frac{1}{2}T'M'_{T}|f(\tau_{1},\tau_{2})|\frac{1}{2}\frac{1}{2}TM_{T}\rangle.$$

$$(D.10)$$

The center-of-mass motion results

$$\langle N'L'M'_L|\delta\left(\frac{1}{\sqrt{2}}(\mathbf{X}'-\mathbf{X})\right)|NLM_L\rangle = (\sqrt{2})^3\delta_{LL'}\delta_{M_LM'_L}\delta_{NN'}.$$
 (D.11)

The Skyrme interaction in relative coordinates reads

$$\begin{aligned} v(\mathbf{x}', \mathbf{x}) f(\sigma_{\mathbf{1}}, \sigma_{\mathbf{2}}) &= t_0 (1 + x_0 P_{\sigma}) \delta(\sqrt{2} \mathbf{x}') \delta(\sqrt{2} \mathbf{x}) \\ &+ \frac{t_1}{2} (1 + x_1 P_{\sigma}) \left[ \frac{1}{2} \mathbf{k}'_{\mathbf{x}'}{}^2 \delta(\sqrt{2} \mathbf{x}') \delta(\sqrt{2} \mathbf{x}) + \delta(\sqrt{2} \mathbf{x}') \delta(\sqrt{2} \mathbf{x}) \frac{1}{2} \mathbf{k}_{\mathbf{x}}{}^2 \right] \\ &+ t_2 (1 + x_2 P_{\sigma}) \left[ \frac{1}{\sqrt{2}} \mathbf{k}'_{\mathbf{x}'} \cdot \delta(\sqrt{2} \mathbf{x}') \delta(\sqrt{2} \mathbf{x}) \frac{1}{\sqrt{2}} \mathbf{k}_{\mathbf{x}} \right] \\ &- i w_0 \left( \sigma_{\mathbf{1}} + \sigma_{\mathbf{2}} \right) \cdot \left[ \frac{1}{\sqrt{2}} \mathbf{k}'_{\mathbf{x}'} \times \delta(\sqrt{2} \mathbf{x}') \delta(\sqrt{2} \mathbf{x}) \frac{1}{\sqrt{2}} \mathbf{k}_{\mathbf{x}} \right] \\ &+ \frac{t_e}{2} \left\{ 3 (\sigma_{\mathbf{1}} \cdot \frac{1}{\sqrt{2}} \mathbf{k}'_{\mathbf{x}'}) (\sigma_{\mathbf{2}} \cdot \frac{1}{\sqrt{2}} \mathbf{k}'_{\mathbf{x}'}) \delta(\sqrt{2} \mathbf{x}) \frac{1}{\sqrt{2}} \mathbf{k}_{\mathbf{x}} \right] \\ &- \delta(\sqrt{2} \mathbf{x}') \delta(\sqrt{2} \mathbf{x}) (\sigma_{\mathbf{1}} \cdot \sigma_{\mathbf{2}}) \frac{1}{2} \mathbf{k}'_{\mathbf{x}'}{}^2 \\ &+ 3 \delta(\sqrt{2} \mathbf{x}') \delta(\sqrt{2} \mathbf{x}) (\sigma_{\mathbf{1}} \cdot \frac{1}{\sqrt{2}} \mathbf{k}_{\mathbf{x}}) (\sigma_{\mathbf{2}} \cdot \frac{1}{\sqrt{2}} \mathbf{k}_{\mathbf{x}}) \\ &- \delta(\sqrt{2} \mathbf{x}') \delta(\sqrt{2} \mathbf{x}) (\sigma_{\mathbf{1}} \cdot \sigma_{\mathbf{2}}) \frac{1}{2} \mathbf{k}_{\mathbf{x}}{}^2 \right\} \\ &+ t_o \left\{ 3 (\sigma_{\mathbf{1}} \cdot \frac{1}{\sqrt{2}} \mathbf{k}'_{\mathbf{x}'}) \delta(\sqrt{2} \mathbf{x}') \delta(\sqrt{2} \mathbf{x}) (\sigma_{\mathbf{2}} \cdot \frac{1}{\sqrt{2}} \mathbf{k}_{\mathbf{x}}) \\ &- \left( \sigma_{\mathbf{1}} \cdot \sigma_{\mathbf{2}} \right) \left[ \frac{1}{\sqrt{2}} \mathbf{k}'_{\mathbf{x}'} \cdot \delta(\sqrt{2} \mathbf{x}') \delta(\sqrt{2} \mathbf{x}) \frac{1}{\sqrt{2}} \mathbf{k}_{\mathbf{x}} \right] \right\}, \end{aligned}$$
(D.12)

while the isospin independence of the interaction gives

$$\langle \frac{1}{2} \frac{1}{2} T' M'_T | \mathbb{1}_T | \frac{1}{2} \frac{1}{2} T M_T \rangle = \delta_{TT'} \delta_{M_T M'_T}.$$
 (D.13)

The tensor part in Eq.(D.12) can be rewritten as

$$\begin{aligned} v(\mathbf{x}', \mathbf{x}) f(\sigma_{1}, \sigma_{2}) \Big|_{tensor} &= \frac{3}{2} t_{e} \frac{1}{2} \Biggl\{ \sum_{M_{\sigma}=-2}^{2} (-1)^{2-M_{\sigma}} [\sigma_{1} \otimes \sigma_{2}]_{2M_{\sigma}} [\mathbf{k}'_{\mathbf{x}'} \otimes \mathbf{k}'_{\mathbf{x}'}]_{2,-M_{\sigma}} \\ &\times \delta(\sqrt{2}\mathbf{x}') \delta(\sqrt{2}\mathbf{x}) + \delta(\sqrt{2}\mathbf{x}') \delta(\sqrt{2}\mathbf{x}) \\ &\times \sum_{M_{\sigma}=-2}^{2} (-1)^{2-M_{\sigma}} [\sigma_{1} \otimes \sigma_{2}]_{2M_{\sigma}} [\mathbf{k}_{\mathbf{x}} \otimes \mathbf{k}_{\mathbf{x}}]_{2,-M_{\sigma}} \Biggr\} \\ &+ 3t_{o} \frac{1}{2} \Biggl\{ \sum_{M_{\sigma}=-2}^{2} (-1)^{2-M_{\sigma}} [\sigma_{1} \otimes \sigma_{2}]_{2M_{\sigma}} [\mathbf{k}'_{\mathbf{x}'} \otimes \mathbf{k}_{\mathbf{x}}]_{2,-M_{\sigma}} \\ &\times \delta(\sqrt{2}\mathbf{x}') \delta(\sqrt{2}\mathbf{x}) \Biggr\}. \end{aligned}$$
(D.14)

In the spin sector, we can distinguish different contributions. The spin identity gives

$$\langle \frac{1}{2} \frac{1}{2} S' M'_S | \mathbb{1}_S | \frac{1}{2} \frac{1}{2} S M_S \rangle = \delta_{SS'} \delta_{M_S M'_S}, \tag{D.15}$$

the spin-exchange operator reads

$$\left\langle \frac{1}{2} \frac{1}{2} S' M'_{S} | P^{\sigma} | \frac{1}{2} \frac{1}{2} S M_{S} \right\rangle = (-1)^{S+1} \delta_{SS'} \delta_{M_{S}M'_{S}}.$$
 (D.16)

The term entering the spin-orbit part results

$$\left\langle \frac{1}{2} \frac{1}{2} S' M'_{S} \right| \left[ \sigma_{1} + \sigma_{2} \right]_{1M_{\sigma}} \left| \frac{1}{2} \frac{1}{2} S M_{S} \right\rangle = \left( (-1)^{S'} + (-1)^{-S} \right) \sqrt{6} \hat{S}' (-1)^{M_{\sigma}} C^{SM_{S}}_{S'M'_{S}1, -M_{\sigma}} \\ \times \left\{ \frac{1}{2} \frac{1}{2} S'_{S'1} \right\} \\ = \delta_{SS'=1} 2 \sqrt{6} \hat{S} (-1)^{S+M_{\sigma}} C^{SM_{S}}_{SM'_{S}1, -M_{\sigma}} \left\{ \frac{1}{2} \frac{1}{2} S_{S'1} \right\},$$

$$(D.17)$$

where we used that  $((-1)^{S'} + (-1)^{-S}) = 2(-1)^S \delta_{SS'}$ , with the triangular rule in  $C^{SM_S}_{S'M'_S 1-M_{\sigma}} \neq 0$  giving S=S'=1, and the relations

$$\langle \frac{1}{2} \frac{1}{2} S' M'_{S} | [\sigma_{1}]_{1M_{\sigma}} | \frac{1}{2} \frac{1}{2} SM_{S} \rangle = \sum_{m'_{1}m'_{2}m_{1}m_{2}} C^{S'M'_{S}}_{\frac{1}{2}m'_{1}\frac{1}{2}m'_{2}} C^{SM_{S}}_{\frac{1}{2}m_{1}\frac{1}{2}m_{2}} \sqrt{3} C^{\frac{1}{2}m'_{1}}_{\frac{1}{2}m_{1}M_{\sigma}} \delta_{m'_{2}m_{2}}$$
$$= (-1)^{S'} \sqrt{6} \hat{S}' (-1)^{M_{\sigma}} C^{SM_{S}}_{S'M'_{S}1, -M_{\sigma}} \left\{ \begin{array}{c} \frac{1}{2} & \frac{1}{2} & S' \\ S & 1 & \frac{1}{2} \end{array} \right\},$$
(D.18)

$$\langle \frac{1}{2} \frac{1}{2} S' M'_{S} | [\sigma_{2}]_{1M_{\sigma}} | \frac{1}{2} \frac{1}{2} SM_{S} \rangle = \sum_{m'_{1}m'_{2}m_{1}m_{2}} C^{S'M'_{S}}_{\frac{1}{2}m'_{1}\frac{1}{2}m'_{2}} C^{SM_{S}}_{\frac{1}{2}m_{1}\frac{1}{2}m_{2}} \sqrt{3} C^{\frac{1}{2}m'_{2}}_{\frac{1}{2}m_{2}1M_{\sigma}} \delta_{m'_{1}m_{1}}$$

$$= (-1)^{S} \sqrt{6} \hat{S}' (-1)^{M_{\sigma}} C^{SM_{S}}_{S'M'_{S}1, -M_{\sigma}} \left\{ \begin{array}{c} \frac{1}{2} & \frac{1}{2} & S' \\ S & 1 & \frac{1}{2} \end{array} \right\}.$$

$$(D.19)$$

The spin contribution in the tensor part is

$$\langle \frac{1}{2} \frac{1}{2} S' M'_{S} | [\sigma_{1} \otimes \sigma_{2}]_{2M_{\sigma}} | \frac{1}{2} \frac{1}{2} SM_{S} \rangle = \hat{S}'^{-1} C_{SM_{S}2M_{\sigma}}^{S'M'_{S}} (S'|| [\sigma_{1} \otimes \sigma_{2}]_{2} ||S)$$

$$= \hat{S}'^{-1} C_{SM_{S}2M_{\sigma}}^{S'M'_{S}} \hat{S}' \hat{S}_{2} \begin{cases} \frac{1}{2} & \frac{1}{2} & S' \\ \frac{1}{2} & \frac{1}{2} & S \\ 1 & 1 & 2 \end{cases}$$

$$\times \left( \frac{1}{2} || [\sigma_{1}]_{1} || \frac{1}{2} \right) \left( \frac{1}{2} || [\sigma_{2}]_{1} || \frac{1}{2} \right)$$

$$= \delta_{SS'=1} 2 \sqrt{\frac{5}{3}} C_{1M_{S}2M_{\sigma}}^{1M'_{S}},$$

$$(D.20)$$

where, for the triangular rule, S=S'=1 is necessary to have  $C_{SM_S2M_{\sigma}}^{S'M'_S} \neq 0$ , and we used that  $\left(\frac{1}{2}|| [\sigma_1]_1 || \frac{1}{2}\right) = \sqrt{6}$ ,  $\hat{S} = \sqrt{3}$  and  $\left\{\begin{array}{cc} \frac{1}{2} & \frac{1}{2} & 1\\ \frac{1}{2} & \frac{1}{2} & 1\\ 1 & 1 & 2\end{array}\right\} = \frac{1}{9}$ .

For the spatial part of the interaction, we calculate the integral in the momuntum space as

$$\langle n'l'm_l'|v(\mathbf{x}',\mathbf{x})|nlm_l\rangle \equiv \int d\mathbf{x} d\mathbf{x}' \phi^*_{n'l'm_l'}(\mathbf{x}')v(\mathbf{x}',\mathbf{x})\phi_{nlm_l}(\mathbf{x})$$
  
= 
$$\int d\mathbf{q} d\mathbf{q}' \tilde{\phi}^*_{n'l'm_l'}(\mathbf{q}')\tilde{v}(\mathbf{q}',-\mathbf{q})\tilde{\phi}_{nlm_l}(\mathbf{q}),$$
 (D.21)

thanks to the Fourier transform

$$\tilde{v}(\mathbf{q}', -\mathbf{q}) = \frac{1}{(2\pi)^3} \int d\mathbf{x} d\mathbf{x}' v(\mathbf{x}', \mathbf{x}) e^{-i\mathbf{q}' \cdot \mathbf{x}'} e^{i\mathbf{q} \cdot \mathbf{x}}.$$
 (D.22)

The separation of the momentum dependence in radial and angular part reads

$$\tilde{v}(\mathbf{q}',-\mathbf{q}) \propto c_k' g'(q') Y_{k'M_k'}(\mathbf{\Omega}') g(q) c_k Y_{kM_k}(\mathbf{\Omega}), \qquad (D.23)$$

where the coefficient  $c_k$  are such that  $1 = \sqrt{4\pi} Y_{00}(\Omega)$ ,  $\mathbf{q}_{\mu} = \sqrt{\frac{4\pi}{3}} q Y_{1\mu}(\Omega)$ ,  $\mathbf{q}^2 = \sqrt{4\pi} Y_{00}(\Omega)$ .

From the coupling of the spherical harmonics  $^3$ 

$$\{Y_{l_1m_1}(\mathbf{\Omega}) \otimes Y_{l_2m_2}(\mathbf{\Omega})\}_{LM} = \frac{\hat{l}_1\hat{l}_2}{\sqrt{4\pi}\hat{L}} C^{L0}_{l_10l_20} Y_{LM}(\mathbf{\Omega}),$$
(D.24)

we obtain

$$\mathbf{q}^{2} = \mathbf{q} \cdot \mathbf{q} = (-\sqrt{3})q^{2} \frac{4\pi}{3} \left\{ Y_{1m_{1}}(\mathbf{\Omega}) \otimes Y_{1m_{2}}(\mathbf{\Omega}) \right\}_{00}$$
  
=  $(-\sqrt{3})q^{2} \frac{4\pi}{3} \frac{3}{\sqrt{4\pi}} \left( -\sqrt{\frac{1}{3}} \right) Y_{00}(\mathbf{\Omega}) = q^{2} \sqrt{4\pi} Y_{00}(\mathbf{\Omega}),$  (D.25)

and

$$\{\mathbf{q} \otimes \mathbf{q}\}_{2,-M_{\sigma}} = q^{2} \frac{4\pi}{3} \{Y_{1m_{1}}(\mathbf{\Omega}) \otimes Y_{1m_{2}}(\mathbf{\Omega})\}_{2,-M_{\sigma}}$$
  
=  $q^{2} \frac{4\pi}{3} \frac{3}{\sqrt{5}\sqrt{4\pi}} \sqrt{\frac{2}{3}} Y_{2,-M_{\sigma}}(\mathbf{\Omega}) = q^{2} \sqrt{4\pi} \sqrt{\frac{2}{15}} Y_{2,-M_{\sigma}}(\mathbf{\Omega}).$  (D.26)

Inserting Eq.(D.23) in the integral in Eq.(D.21) leads to the simplified expression

$$\int d\mathbf{q} d\mathbf{q}' \, \tilde{\phi}_{n'l'm_l}^*(\mathbf{q}') \left[ g'(q') Y_{k'M_k'}(\mathbf{\Omega}') g(q) Y_{kM_k}(\mathbf{\Omega}) \right] \, \tilde{\phi}_{nlm_l}(\mathbf{q})$$

$$= \int dq' \, q'^2 g'(q') \tilde{R}_{n'l'}^*(q') \int dq \, q^2 g(q) \tilde{R}_{nl}(q)$$

$$\times \int d\mathbf{\Omega}' \, Y_{l'm_l'}^*(\mathbf{\Omega}') Y_{k'M_k'}(\mathbf{\Omega}') \int d\mathbf{\Omega} \, (-1)^{-M_k} Y_{k,-M_k}^*(\mathbf{\Omega}) Y_{lm_l}(\mathbf{\Omega})$$

$$= (-1)^{-M_k} \delta_{l'k'} \delta_{m_lM_k'} \delta_{lk} \delta_{m_l,-M_k} r_{n'l'}^*(g') r_{nl}(g),$$
(D.27)

with  $r_{nl}(g) \equiv \int dq \, q^2 g(q) \tilde{R}_{nl}(q)$ . The radial part of the harmonic oscillator solution is defined as

$$R_{nl}(x) \equiv b^{\frac{3}{2}} \sqrt{\frac{2(n!)}{\Gamma(n+l+\frac{3}{2})}} (bx)^{l} L_{n}^{(l+\frac{1}{2})} ((bx)^{2}) e^{-\frac{1}{2}(bx)^{2}}$$
$$\equiv b^{\frac{3}{2}} F_{nl}(bx) e^{-\frac{1}{2}(bx)^{2}},$$
(D.28)

 ${}^{3}$ Eq.(14) page 144 of Ref. [119].

where  $b = \frac{\sqrt{\hbar \omega m_N c^2}}{\hbar c}$  is the harmonic oscillator lenght (in fm<sup>-1</sup>). The Fourier transform,

$$\tilde{R}_{nl}(q) = \frac{(-i)^{2n+l}}{b^3} R_{nl}\left(\frac{q}{b^2}\right) = b^{-\frac{3}{2}}(-i)^{2n+l} F_{nl}\left(\frac{q}{b}\right) e^{-\frac{1}{2}(\frac{q}{b})^2},\tag{D.29}$$

leads (after defining  $y \equiv \frac{q}{b}$ ) to

$$r_{nl}(g) = \int dy \, y^2 b^{\frac{3}{2}} g(by)(-i)^{2n+l} F_{nl}(y) \, e^{-\frac{1}{2}(y)^2}.$$
 (D.30)

When building the antisymmetrized matrix element, we consider the property of the particle exchange symmetry. In fact, the matrix element with exchanged particles  $c \leftrightarrow d$  results

$$\langle ab; JM; T'M'_{T} | \hat{V} | dc; JM; TM_{T} \rangle$$
  
=  $(-1)^{\lambda - L} (-1)^{l_{c} + l_{d} + \lambda + \frac{1}{2} + \frac{1}{2} + S + j_{c} + j_{d} + J} \langle ab; JM; T'M'_{T} | \hat{V} | cd; JM; TM_{T} \rangle,$  (D.31)

due to the symmetries for particle exchanging, respectively in the Talmi-Moshinski transformations

$$M_{n_d l_d n_c l_c, \lambda}^{NLnl} = (-1)^{\lambda - L} M_{n_c l_c n_d l_d, \lambda}^{NLnl}, \tag{D.32}$$

and in the 9j-symbols

$$\left\{ \begin{array}{cc} l_d & l_c & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_d & j_c & J \end{array} \right\} = (-1)^{l_c + l_d + \lambda + \frac{1}{2} + \frac{1}{2} + S + j_c + j_d + J} \left\{ \begin{array}{cc} l_c & l_d & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_c & j_d & J \end{array} \right\}.$$
(D.33)

#### D.1 Central part

**Term**  $\hat{V} = t_0 \hat{V}_{t_0} + t_0 x_0 \hat{V}_{t_0 x_0}$ The coupling of momentum space and spin parts of the interaction,

$$\tilde{v}(\mathbf{q}',-\mathbf{q})f(\sigma_1,\sigma_2) = t_0(1+x_0P^{\sigma})\frac{1}{(2\pi)^3}\frac{1}{(\sqrt{2})^6}4\pi Y_{00}(\mathbf{\Omega}')Y_{00}(\mathbf{\Omega})g'(1)g(1), \quad (D.34)$$

gives the coupled matrix element as

$$\begin{split} \langle ab; JM; T'M_{T}'|\hat{V}|cd; JM; TM_{T} \rangle \\ &= \sum_{\lambda'S'} \hat{\lambda}' \hat{S}' \hat{j}_{a} \hat{j}_{b} \begin{cases} l_{a} & l_{b} & \lambda \\ \frac{1}{2} & \frac{1}{2} & S' \\ j_{a} & j_{b} & J \end{cases} \sum_{\lambda'L'n'l'} M_{nalanblb,\lambda'}^{N'L'n'l'} * \\ &\times \sum_{\lambda S} \hat{\lambda} \hat{S} \hat{j}_{c} \hat{j}_{d} \begin{cases} l_{c} & l_{d} & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{c} & j_{d} & J \end{cases} \sum_{NLnl} M_{nclcndld,\lambda}^{NLnl} \\ &\times \sum_{M_{\lambda}M_{S}M_{\lambda}'M_{S}'} C_{\lambda'M_{\lambda}'S'M_{S}}^{JM} C_{\lambda M_{\lambda}SM_{S}}^{JM} \sum_{M_{Lml}} C_{LM_{L}lm_{l}}^{\lambda M_{\lambda}} C_{L'M_{L}l'm_{l}'}^{\lambda'M_{\lambda}'} \\ &\times (\sqrt{2})^{3} \delta_{LL'} \delta_{M_{L}M_{L}'} \delta_{NN'} \delta_{TT'} \delta_{M_{T}M_{T}'} \delta_{SS'} \delta_{M_{S}M_{S}'} t_{0} (1 + x_{0} (-1)^{S+1}) \\ &\times (\sqrt{2})^{3} \frac{1}{(\sqrt{2})^{6}} 4\pi \delta_{l'0} \delta_{m_{l}'0} \delta_{m_{l}0} r_{n'l'}^{*} (1) r_{nl} (1) \\ &= \sum_{NLS} \hat{L} \hat{L} \hat{S} \hat{S} \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \begin{cases} l_{a} & l_{b} & L \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{a} & j_{b} & J \end{cases} \begin{cases} l_{c} & l_{d} & L \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{c} & j_{d} & J \end{cases} \\ &\times \left( \sum_{n'} M_{nalanblb,L}^{NLn'0} * r_{n'0}^{*} (1) \right) \left( \sum_{n} M_{nclcndl,L}^{NLn0} r_{n0} (1) \right) \delta_{TT'} \delta_{M_{T}M_{T}'} \\ &\times \frac{1}{(4\pi)^{2}} 2\sqrt{2} t_{0} (1 + x_{0} (-1)^{S+1}). \end{split}$$

The antisymmetrized matrix element is

$$\begin{aligned} \langle ab; JM; TM_{T} | \hat{V} | cd; JM; TM_{T} \rangle_{as} \\ &= \mathcal{N}_{ab} (JT) \mathcal{N}_{cd} (JT) \sum_{NLS} \hat{L} \hat{L} \hat{S} \hat{S} \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \left\{ \begin{array}{cc} l_{a} & l_{b} & L \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{a} & j_{b} & J \end{array} \right\} \left\{ \begin{array}{cc} l_{c} & l_{d} & L \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{c} & j_{d} & J \end{array} \right\} \\ &\times \left( \sum_{n'} M_{nal_{a}nbl_{b},L}^{NLn'0} * r_{n'0}^{*}(1) \right) \left( \sum_{n} M_{ncl_{c}ndl_{d},L}^{NLn0} r_{n0}(1) \right) \frac{1}{(4\pi)^{2}} 2\sqrt{2} t_{0} (1+x_{0}(-1)^{S+1}) \\ &\times \left[ 1+(-1)^{j_{c}+j_{d}-J-T}(-1)^{l_{c}+l_{d}+L+\frac{1}{2}+\frac{1}{2}+S+j_{c}+j_{d}+J} \right]. \end{aligned}$$
(D.36)

**Term**  $\hat{V} = t_1 \hat{V}_{t_1} + t_1 x_1 \hat{V}_{t_1 x_1}$ The coupling of momentum space and spin parts of the interaction,

$$\tilde{v}(\mathbf{q}', -\mathbf{q})f(\sigma_{1}, \sigma_{2}) = \frac{t_{1}}{2}(1 + x_{1}P^{\sigma})\frac{1}{2}\frac{1}{(2\pi)^{3}}\frac{1}{(\sqrt{2})^{6}}4\pi Y_{00}(\mathbf{\Omega}')Y_{00}(\mathbf{\Omega}) \times [g'(q'^{2})g(1) + g'(1)g(q^{2})],$$
(D.37)

gives the coupled matrix element as

$$\begin{split} \langle ab; JM; T'M_{T}'|\hat{V}|cd; JM; TM_{T} \rangle \\ &= \sum_{\lambda'S'} \hat{\lambda}' \hat{S}' \hat{j}_{a} \hat{j}_{b} \begin{cases} l_{a} & l_{b} & \lambda \\ \frac{1}{2} & \frac{1}{2} & S' \\ j_{a} & j_{b} & J \end{cases} \sum_{N'L'n'l'} M_{nalanblb,\lambda'}^{N'L'n'l'} * \\ &\times \sum_{\lambda S} \hat{\lambda} \hat{S} \hat{j}_{c} \hat{j}_{d} \begin{cases} l_{c} & l_{d} & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{c} & j_{d} & J \end{cases} \sum_{NLnl} M_{nclcnd_{d,\lambda}}^{NLnl} \\ &\times \sum_{M_{\lambda}M_{S}M_{\lambda}'M_{S}'} C_{\lambda'M_{\lambda}S'M_{S}}^{JM} C_{\lambda'M_{\lambda}SM_{S}}^{JM} \sum_{M_{L}m_{l}M_{L}'m_{l}'} C_{LM_{L}lm_{l}}^{\lambda'M_{\lambda}} C_{L'M_{L}}^{\lambda'M_{\lambda}'} \\ &\times (\sqrt{2})^{3} \delta_{LL'} \delta_{M_{L}M_{L}'} \delta_{NN'} \delta_{TT'} \delta_{M_{T}M_{T}'} \delta_{SS'} \delta_{M_{S}M_{S}'} \frac{t_{1}}{2} (1 + x_{1}(-1)^{S+1}) \\ &\times \frac{1}{2} \frac{1}{(2\pi)^{3}} \frac{1}{(\sqrt{2})^{6}} 4\pi \delta_{l'0} \delta_{m_{l}'0} \delta_{l_{0}} \delta_{m_{l}0} \left[ r_{n'l'}^{*}(q'^{2}) r_{nl}(1) + r_{n'l'}^{*}(1) r_{nl}(q^{2}) \right] \\ &= \sum_{NLS} \hat{L} \hat{L} \hat{S} \hat{S} \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \begin{cases} l_{a} & l_{b} & L \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{a} & j_{b} & J \end{cases} \begin{cases} l_{c} & l_{d} & L \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{c} & j_{d} & J \end{cases} \delta_{TT'} \delta_{M_{T}M_{T}'} \\ &\times \sum_{n'n} M_{nalanble,L}^{NLn'0} * M_{nclcnd_{l,L}}^{NLn0} \left[ r_{n'0}^{*}(q'^{2}) r_{n0}(1) + r_{n'0}^{*}(1) r_{n0}(q^{2}) \right] \\ &\times \frac{1}{(4\pi)^{2}} \sqrt{2} \frac{t_{1}}{2} (1 + x_{1}(-1)^{S+1}). \end{split}$$

The antisymmetrized matrix element is

$$\langle ab; JM; TM_{T} | \hat{V} | cd; JM; TM_{T} \rangle_{as}$$

$$= \mathcal{N}_{ab}(JT) \mathcal{N}_{cd}(JT) \sum_{NLS} \hat{L} \hat{L} \hat{S} \hat{S} \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \left\{ \begin{array}{cc} l_{a} & l_{b} & L \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{a} & j_{b} & J \end{array} \right\} \left\{ \begin{array}{cc} l_{c} & l_{d} & L \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{c} & j_{d} & J \end{array} \right\}$$

$$\times \sum_{n'n} M_{nal_{a}n_{b}l_{b},L}^{NLn'0} * M_{ncl_{c}n_{d}l_{d},L}^{NLn0} \left[ r_{n'0}^{*}(q'^{2})r_{n0}(1) + r_{n'0}^{*}(1)r_{n0}(q^{2}) \right]$$

$$\times \frac{1}{(4\pi)^{2}} \frac{2\sqrt{2}}{2} \frac{t_{1}}{2} (1 + x_{1}(-1)^{S+1}) \left[ 1 + (-1)^{j_{c}+j_{d}-J-T}(-1)^{l_{c}+l_{d}+L+\frac{1}{2}+\frac{1}{2}+S+j_{c}+j_{d}+J} \right].$$

$$(D.39)$$

**Term**  $\hat{V} = t_2 \hat{V}_{t_2} + t_2 x_2 \hat{V}_{t_2 x_2}$ The coupling of momentum space and spin parts of the interaction gives

$$\tilde{v}(\mathbf{q}', -\mathbf{q})f(\sigma_{1}, \sigma_{2}) = \frac{t_{2}}{2}(1 + x_{2}P^{\sigma})\frac{1}{2}\frac{1}{(2\pi)^{3}}\frac{1}{(\sqrt{2})^{6}}\frac{4\pi}{3} \times (-\sqrt{3})\sum_{M'_{k}M_{k}}C^{00}_{1M'_{k}1M_{k}}Y_{1M'_{k}}(\mathbf{\Omega}')Y_{1M_{k}}(\mathbf{\Omega})g'(q')g(q),$$
(D.40)

where the factor  $(-\sqrt{3})$  arises from the definition of the scalar product in terms of irreducible tensors (L=1),

$$\mathbf{A}_{L} \cdot \mathbf{B}_{L} = (-1)^{L} \sqrt{2L+1} \left[ \mathbf{A}_{L} \mathbf{B}_{L} \right]_{00} = (-1)^{L} \sqrt{2L+1} \sum_{m_{1}m_{2}} C_{Lm_{1}Lm_{2}}^{00} A_{Lm_{1}} B_{Lm_{2}}$$
$$= \sum_{m} (-1)^{m} A_{Lm} B_{L,-m}.$$
(D.41)

The coupled matrix element results

$$\begin{split} \langle ab; JM; T'M'_{T}|\hat{V}|cd; JM; TM_{T} \rangle \\ &= \sum_{\lambda'S'} \hat{\lambda}' \hat{S}' \hat{j}_{a} \hat{j}_{b} \begin{cases} l_{a} \quad l_{b} \quad \lambda \\ \frac{1}{2} \quad \frac{1}{2} \quad S' \\ j_{a} \quad j_{b} \quad J \end{cases} \sum_{\lambda'L'n'l'} M_{nalanbl_{b},\lambda'}^{N'L'n'l'} * \\ &\times \sum_{\lambda S} \hat{\lambda} \hat{S} \hat{j}_{c} \hat{j}_{d} \begin{cases} l_{c} \quad l_{d} \quad \lambda \\ \frac{1}{2} \quad \frac{1}{2} \quad S \\ j_{c} \quad j_{d} \quad J \end{cases} \sum_{NLnl} M_{nclcnl_{d,\lambda}}^{NLnl} \\ &\times \sum_{\lambda S} \hat{\lambda} \hat{S} \hat{j}_{c} \hat{j}_{d} \begin{cases} L_{c} \quad l_{d} \quad \lambda \\ \frac{1}{2} \quad \frac{1}{2} \quad S \\ j_{c} \quad j_{d} \quad J \end{cases} \sum_{NLnl} M_{nclcnl_{d,\lambda}}^{NLnl} \\ &\times \sum_{M_{\lambda}M_{S}M'_{\lambda}M'_{S}} C_{\lambda'M'_{\lambda}S'M'_{S}}^{JM} C_{\lambda M_{\lambda}SM_{S}}^{JM} \sum_{M_{L}m_{l}M'_{L}m'_{l}} C_{LM_{\lambda}lm_{l}}^{\lambda'M'_{\lambda}} \\ &\times (\sqrt{2})^{3} \delta_{LL'} \delta_{M_{L}M'_{L}} \delta_{NN'} \delta_{TT'} \delta_{M_{T}M'_{T}} \delta_{SS'} \delta_{M_{S}M'_{S}} t_{2} (1 + x_{2} (-1)^{S+1}) \\ &\times \frac{1}{2} \frac{1}{(2\pi)^{3}} \frac{1}{(\sqrt{2})^{6}} \frac{4\pi}{3} (-\sqrt{3}) \sum_{M'_{k}M_{k}} C_{1M'_{k}1M_{k}}^{00} (-1)^{-M_{k}} \delta_{l'1} \delta_{m'_{l}M'_{k}} \delta_{l1} \delta_{m_{l},-M_{k}} r_{n'l'}^{*}(q') r_{nl}(q) \\ &= \sum_{\lambda S} \hat{\lambda} \hat{\lambda} \hat{S} \hat{S} \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \begin{cases} l_{a} \quad l_{b} \quad \lambda \\ \frac{1}{2} \quad \frac{1}{2} \quad S \\ j_{a} \quad j_{b} \quad J \end{cases} \begin{cases} l_{c} \quad l_{d} \quad \lambda \\ \frac{1}{2} \quad \frac{1}{2} \quad S \\ j_{c} \quad j_{d} \quad J \end{cases} \delta_{TT'} \delta_{M_{T}M'_{T}} \\ &\times \sum_{NL} \left( \sum_{n'} M_{nalanb_{b},\lambda}^{NLn'_{1}} r_{n''_{1}}(q') \right) \left( \sum_{n} M_{ncl_{c}nd_{d},\lambda}^{NLn1} \\ n_{c}l_{c}n_{d}l_{d},\lambda} r_{n1}(q) \right) \\ &\times \frac{1}{(4\pi)^{2}} \frac{\sqrt{2}}{3} t_{2} (1 + x_{2} (-1)^{S+1}). \end{split}$$
(D.42)

The antisymmetrized matrix element is

$$\langle ab; JM; TM_{T} | \hat{V} | cd; JM; TM_{T} \rangle_{as}$$

$$= \mathcal{N}_{ab} (JT) \mathcal{N}_{cd} (JT) \sum_{\lambda S} \hat{\lambda} \hat{\lambda} \hat{S} \hat{S} \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \begin{cases} l_{a} & l_{b} & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{a} & j_{b} & J \end{cases} \begin{cases} l_{c} & l_{d} & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{c} & j_{d} & J \end{cases}$$

$$\times \sum_{NL} \left( \sum_{n'} M_{nalanblb,\lambda}^{NLn'1} * r_{n'1}^{*}(q') \right) \left( \sum_{n} M_{nclcndld,\lambda}^{NLn1} r_{n1}(q) \right)$$

$$\times \frac{1}{(4\pi)^{2}} \frac{2\sqrt{2}}{6} t_{2} (1 + x_{2} (-1)^{S+1})$$

$$\times \left[ 1 + (-1)^{j_{c}+j_{d}-J-T} (-1)^{\lambda-L} (-1)^{l_{c}+l_{d}+\lambda+\frac{1}{2}+\frac{1}{2}+S+j_{c}+j_{d}+J} \right].$$

$$(D.43)$$

#### D.2Spin-orbit part

**Term**  $\hat{V} = w_0 \hat{V}_{(t)w_0}$ The coupling of momentum space and spin parts of the interaction gives

$$\tilde{v}(\mathbf{q}', -\mathbf{q})f(\sigma_{\mathbf{1}}, \sigma_{\mathbf{2}}) = -i w_{0} \frac{1}{2} \frac{1}{(2\pi)^{3}} \frac{1}{(\sqrt{2})^{6}} \frac{4\pi}{3} (-\sqrt{3}) \sum_{M_{\sigma}M_{r}} C^{00}_{1M_{\sigma}1M_{r}} (\sigma_{\mathbf{1}} + \sigma_{\mathbf{2}})_{1M_{\sigma}} \times (-i\sqrt{2}) \sum_{M'_{k}M_{k}} C^{1M_{r}}_{1M'_{k}1M_{k}} Y_{1M'_{k}}(\mathbf{\Omega}') Y_{1M_{k}}(\mathbf{\Omega}) g'(q')g(q),$$
(D.44)

where the factor  $(-i\sqrt{2})$  arises from

$$(\mathbf{A}_1 \times \mathbf{B}_1)_{1m} = -i\sqrt{2} \sum_{m_1m_2} C^{1m}_{1m_11m_2} A_{1m_1} B_{1m_2}.$$
 (D.45)

The coupled matrix element results

$$\begin{split} \langle ab; JM; T'M_{T}'|\hat{V}|cd; JM; TM_{T} \rangle \\ &= \sum_{\lambda'S'} \hat{\lambda}' \hat{S}' \hat{j}_{a} \hat{j}_{b} \begin{cases} l_{a} & l_{b} & \lambda \\ \frac{1}{2} & \frac{1}{2} & S' \\ j_{a} & j_{b} & J \end{cases} \sum_{\lambda'L'n'l'} M_{nalanbl_{b}\lambda'}^{N'L'n'l'} * \\ &\times \sum_{\lambda S} \hat{\lambda} \hat{S} \hat{j}_{c} \hat{j}_{d} \begin{cases} l_{c} & l_{d} & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{c} & j_{d} & J \end{cases} \sum_{NLnl} M_{ncl_{c}nd_{d},\lambda}^{NLnl} \\ &\times \sum_{M_{\lambda}M_{S}M_{\lambda}'M_{S}'} C_{\lambda'M_{\lambda}S'M_{S}'}^{JM} C_{\lambda'M_{\lambda}SM_{S}}^{JM} \sum_{M_{L}m_{l}M_{L}'m'_{l}} C_{LM_{L}lm_{l}}^{\lambda'M_{\lambda}} \\ &\times (\sqrt{2})^{3} \delta_{LL'} \delta_{M_{L}M_{L}'} \delta_{NN'} \delta_{TT'} \delta_{M_{T}M_{T}'} (-i w_{0}) \frac{1}{2} \frac{1}{(2\pi)^{3}} \frac{1}{(\sqrt{2})^{6}} \frac{4\pi}{3} \\ &\times (-\sqrt{3}) \sum_{M_{\sigma}M_{r}} C_{1M_{\sigma}1M_{r}}^{0M} \delta_{SS'=1} 2\sqrt{6} \hat{S}(-1)^{S+M_{\sigma}} C_{SM_{S}',1-M_{\sigma}}^{SM_{S}} \left\{ \frac{1}{2} & \frac{1}{2} & S \\ S & (-i\sqrt{2}) \sum_{M_{\kappa}'M_{k}} C_{1M_{\sigma}1M_{r}}^{1M_{r}} \delta_{SS'=1} 2\sqrt{6} \hat{S}(-1)^{S+M_{\sigma}} C_{SM_{S}',1-M_{\sigma}}^{SM_{S}} \left\{ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ S & (-i\sqrt{2}) \sum_{M_{\kappa}'M_{k}} C_{1M_{\sigma}}^{1M_{r}} (-1)^{-M_{k}} \delta_{l'1} \delta_{m_{l}M_{\kappa}'} \delta_{l1} \delta_{m_{l},-M_{k}} r_{n'l'}^{*} (q') r_{nl}(q) \\ &= \sum_{\lambda\lambda'} \hat{\lambda} \hat{\lambda} \hat{\lambda}' \hat{\lambda}' \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \left\{ \frac{l_{a}}{2} & \frac{l_{b}}{2} & \lambda' \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 1 \\ j_{a} & j_{b} & J \end{array} \right\} \left\{ \frac{l_{c}} & l_{d} & \lambda \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_{c} & j_{d} & J \end{array} \right\} \delta_{TT'} \delta_{M_{T}M_{T}'} \\ &\times \sum_{NL} \left( \sum_{n'} M_{nalanbl_{b},\lambda'}^{NLn'_{1}} r_{n''_{1}}(q') \right) \left( \sum_{n} M_{ncl_{n}d_{d},\lambda}^{NLn1} r_{n}(q) \right) \\ &\times (-1)^{L+\lambda+\lambda'+J} \frac{1}{(4\pi)^{2}} (-12\sqrt{2}) w_{0} \left\{ \begin{array}{l} 1 & L & \lambda \\ \lambda' & 1 & 1 \end{array} \right\} \left\{ \begin{array}{l} 1 & \lambda' & J \\ \lambda & 1 & 1 \end{array} \right\}. \end{split}$$

The antisymmetrized matrix element is

$$\langle ab; JM; TM_T | \hat{V} | cd; JM; TM_T \rangle_{as}$$

$$= \mathcal{N}_{ab}(JT) \mathcal{N}_{cd}(JT) \sum_{\lambda\lambda'} \hat{\lambda} \hat{\lambda} \hat{\lambda}' \hat{\lambda}' \hat{j}_a \hat{j}_b \hat{j}_c \hat{j}_d \begin{cases} l_a & l_b & \lambda' \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_a & j_b & J \end{cases} \begin{cases} l_c & l_d & \lambda \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_c & j_d & J \end{cases}$$

$$\times \sum_{NL} \left( \sum_{n'} M_{nalanblb,\lambda'}^{NLn'1} r_{n'1}^*(q') \right) \left( \sum_{n} M_{nclcndld,\lambda}^{NLn1} r_{n1}(q) \right)$$

$$\times (-1)^{L+\lambda+\lambda'+J} \frac{1}{(4\pi)^2} 2\sqrt{2}(-6) w_0 \begin{cases} 1 & L & \lambda \\ \lambda' & 1 & 1 \end{cases} \begin{cases} 1 & \lambda' & J \\ \lambda & 1 & 1 \end{cases}$$

$$\times \left[ 1 + (-1)^{j_c+j_d-J-T}(-1)^{\lambda-L}(-1)^{l_c+l_d+\lambda+j_c+j_d+J} \right].$$

$$(D.47)$$

## D.3 Tensor part

## $\mathbf{Term} \ \hat{V} = t_e \hat{V}_{t_e}$

The coupling of momentum space and spin parts of the interaction gives  $\frac{1}{2}$ 

$$\tilde{v}(\mathbf{q}', -\mathbf{q})f(\sigma_{1}, \sigma_{2}) = \frac{3}{2} t_{e} \frac{1}{2} \frac{1}{(2\pi)^{3}} \frac{1}{(\sqrt{2})^{6}} 4\pi \sqrt{\frac{2}{15}} \\ \times \sum_{M_{\sigma}m_{1}m_{2}} (-1)^{2-M_{\sigma}} C_{1m_{1}1m_{2}}^{2M_{\sigma}} (\sigma_{1})_{1m_{1}} (\sigma_{2})_{1m_{2}} \\ \times \left[ Y_{2,-M_{\sigma}}(\mathbf{\Omega}') Y_{00}(\mathbf{\Omega}) g'(q'^{2}) g(1) + Y_{00}(\mathbf{\Omega}') Y_{2,-M_{\sigma}}(\mathbf{\Omega}) g'(1) g(q^{2}) \right] .$$
(D.48)

The coupled matrix element results

$$\begin{aligned} \langle ab; JM; T'M'_{T} | \hat{V} | cd; JM; TM_{T} \rangle \\ &= \sum_{\lambda'S'} \hat{\lambda}' \hat{S}' \hat{j}_{a} \hat{j}_{b} \begin{cases} l_{a} & l_{b} & \lambda' \\ \frac{1}{2} & \frac{1}{2} & S' \\ j_{a} & j_{b} & J \end{cases} \sum_{N'L'n'l'} M_{nalanblb,\lambda'}^{N'L'n'l' *} \\ &\times \sum_{\lambda S} \hat{\lambda} \hat{S} \hat{j}_{c} \hat{j}_{d} \begin{cases} l_{c} & l_{d} & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_{c} & j_{d} & J \end{cases} \sum_{NLnl} M_{nclcnl_{d,\lambda}}^{NLnl} \\ &\times \sum_{M_{\lambda}M_{S}M'_{\lambda}M'_{S}} C_{\lambda'M'_{\lambda}S'M'_{S}}^{JM} C_{\lambda M_{\lambda}SM_{S}}^{JM} \sum_{M_{L}m_{l}M'_{L}m'_{l}} C_{LM_{L}lm_{l}}^{\lambda M_{\lambda}} C_{L'M'_{L}l'm'_{l}}^{\lambda'M'_{\lambda}} \\ &\times (\sqrt{2})^{3} \delta_{LL'} \delta_{M_{L}M'_{L}} \delta_{NN'} \delta_{TT'} \delta_{M_{T}M'_{T}} \frac{3}{2} t_{e} \frac{1}{2} \frac{1}{(2\pi)^{3}} \frac{1}{(\sqrt{2})^{6}} 4\pi \sqrt{\frac{2}{15}} \\ &\times \sum_{M_{\sigma}} (-1)^{2-M_{\sigma}} \delta_{SS'=1} \hat{S} 6 \sqrt{5} C_{SM_{S}2M_{\sigma}}^{S'M'_{S}} \begin{cases} \frac{1}{2} & \frac{1}{2} & S' \\ 1 & 1 & 2 \end{cases} \\ &\times \left[ \delta_{l'2} \delta_{m'_{l}-M_{\sigma}} \delta_{l0} \delta_{m_{l}0} r_{n'l'}^{*}(q'^{2}) r_{nl}(1) + (-1)^{M_{\sigma}} \delta_{l'0} \delta_{m'_{l}0} \delta_{l2} \delta_{m_{l}M_{\sigma}} r_{n'l'}^{*}(1) r_{nl}(q^{2}) \right]. \end{aligned}$$
(D.49)

Looking at the total spin quantum numbers, we rewrite

$$\sum_{S'S} \hat{S}' \hat{S} \delta_{SS'=1} \hat{S} 6\sqrt{5} C_{SM_S 2M_\sigma}^{S'M_S'} \left\{ \begin{array}{ccc} \frac{1}{2} & \frac{1}{2} & S' \\ \frac{1}{2} & \frac{1}{2} & S \\ 1 & 1 & 2 \end{array} \right\} = 2\sqrt{15} C_{SM_S 2M_\sigma}^{S'M_S'}, \qquad (D.50)$$

keeping in mind that S and S' in the Clebsch-Gordan have value 1.

We start by studying the first case, corresponding to  $\{\mathbf{q}' \otimes \mathbf{q}'\}_{2,-M_{\sigma}}$ :

$$\begin{split} \langle ab; JM; T'M'_{T} | \hat{V} | cd; JM; TM_{T} \rangle_{1} \\ &= \delta_{TT'} \delta_{M_{T}M'_{T}} \sum_{\lambda\lambda'} \hat{\lambda} \hat{\lambda}' \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \begin{cases} l_{a} l_{b} \lambda' \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_{a} & j_{b} & J \end{cases} \begin{cases} l_{c} l_{d} \lambda \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_{c} & j_{d} & J \end{cases} \\ &\times (\sqrt{2})^{3} \frac{3}{2} t_{e} \frac{1}{2} \frac{1}{(2\pi)^{3}} \frac{1}{(\sqrt{2})^{6}} 4\pi \sqrt{\frac{2}{15}} 2\sqrt{15} \\ &\times \sum_{NL} \left( \sum_{n'} M_{nal_{a}n_{b}l_{b},\lambda'}^{NLn'_{2}} * r_{n'2}^{*}(q'^{2}) \right) \left( \sum_{n} M_{ncl_{c}n_{d}l_{d},\lambda} r_{n0}(1) \right) \\ &\times \sum_{N_{\lambda}M_{\lambda}M_{\lambda}M'_{\lambda}M'_{\lambda}M_{L}M_{\sigma}} (-1)^{-M_{\sigma}} C_{\lambda'M'_{\lambda}S'M'_{\lambda}}^{JM} C_{\lambda M_{\lambda}SM_{\lambda}}^{\lambda M_{\lambda}} C_{\lambda M_{\lambda}DO}^{\lambda M_{\lambda}} C_{\lambda M_{\lambda}2D}^{\lambda M_{\lambda}} C_{\lambda M_{\lambda}SM_{\lambda}}^{\lambda M_{\lambda}} C_{\lambda M_{\lambda}}^{\lambda M_{\lambda}} \int_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \begin{cases} l_{a} l_{b} \lambda' \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_{a} j_{b} J \end{cases} \begin{cases} l_{c} l_{d} \lambda \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_{c} j_{d} J \end{cases} \end{cases} \\ &\times (\sqrt{2})^{3} \frac{3}{2} t_{e} \frac{1}{2} \frac{1}{(2\pi)^{3}} \frac{1}{(\sqrt{2})^{6}} 4\pi \sqrt{\frac{2}{15}} 2\sqrt{15} (-1)^{1+\lambda+J} \hat{\lambda}' \sqrt{3} \begin{cases} 1 \lambda' J \\ \lambda & 1 2 \end{cases} \\ &\times \sum_{N} \left( \sum_{n'} M_{nal_{a}n_{b}l_{b},\lambda'}^{Nn'2} * r_{n'2}^{*}(q'^{2}) \right) \left( \sum_{n} M_{ncl_{c}n_{d}l_{d},\lambda}^{Nn0}(1) \right). \end{split}$$

We consider now the second case, corresponding to  $\{\mathbf{q}\otimes\mathbf{q}\}_{2,-M_{\sigma}}$ :

$$\begin{split} \langle ab; JM; T'M'_{T} | \hat{V} | cd; JM; TM_{T} \rangle_{2} \\ &= \delta_{TT'} \delta_{M_{T}M'_{T}} \sum_{\lambda\lambda'} \hat{\lambda} \hat{\lambda}' \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \left\{ \begin{array}{l} l_{a} & l_{b} & \lambda' \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_{a} & j_{b} & J \end{array} \right\} \left\{ \begin{array}{l} l_{c} & l_{d} & \lambda \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_{c} & j_{d} & J \end{array} \right\} \\ &\times (\sqrt{2})^{3} \frac{3}{2} t_{e} \frac{1}{2} \frac{1}{(2\pi)^{3}} \frac{1}{(\sqrt{2})^{6}} 4\pi \sqrt{\frac{2}{15}} 2\sqrt{15} \\ &\times \sum_{NL} \left( \sum_{n'} M_{nalanblb,\lambda'}^{NLn'0} * r_{n'0}^{*}(1) \right) \left( \sum_{n} M_{nclcndld,\lambda}^{NLn2} r_{n2}(q^{2}) \right) \\ &\times \sum_{M_{\lambda}M_{S}M_{\lambda}'M'_{S}M_{L}M_{\sigma}} (-1)^{-M_{\sigma}+M_{\sigma}} C_{\lambda'M'_{\lambda}S'M'_{S}}^{JM} C_{\lambda M_{\lambda}SM_{S}}^{\lambda M_{\lambda}} C_{LM_{L}2M_{\sigma}}^{\lambda'M'_{\lambda}} C_{SM_{S}2M_{\sigma}}^{S'M'_{S}} \\ &= \delta_{TT'} \delta_{M_{T}M'_{T}} \sum_{\lambda\lambda'} \hat{\lambda} \hat{\lambda}' \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \left\{ \begin{array}{l} l_{a} & l_{b} & \lambda' \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_{a} & j_{b} & J \end{array} \right\} \left\{ \begin{array}{l} l_{c} & l_{d} & \lambda \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_{c} & j_{d} & J \end{array} \right\} \\ &\times (\sqrt{2})^{3} \frac{3}{2} t_{e} \frac{1}{2} \frac{1}{(2\pi)^{3}} \frac{1}{(\sqrt{2})^{6}} 4\pi \sqrt{\frac{2}{15}} 2\sqrt{15} (-1)^{1+\lambda'+J} \hat{\lambda} \sqrt{3} \left\{ \begin{array}{l} 1 & \lambda' & J \\ \lambda & 1 & 2 \end{array} \right\} \\ &\times \sum_{N} \left( \sum_{n'} M_{nalanblb,\lambda'}^{N\lambda'n'0} * r_{n'0}^{*}(1) \right) \left( \sum_{n} M_{nclcnd_{d,\lambda}}^{N\lambda'n2} r_{n2}(q^{2}) \right). \end{split}$$

Then, including both cases, we obtain

$$\langle ab; JM; T'M'_{T} | \hat{V} | cd; JM; TM_{T} \rangle$$

$$= \delta_{TT'} \delta_{M_{T}M'_{T}} \sum_{\lambda\lambda'} \hat{\lambda} \hat{\lambda}' \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \left\{ \begin{array}{c} l_{a} & l_{b} & \lambda' \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_{a} & j_{b} & J \end{array} \right\} \left\{ \begin{array}{c} l_{c} & l_{d} & \lambda \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_{c} & j_{d} & J \end{array} \right\}$$

$$\times (-1)^{1+J} (\sqrt{2})^{3} \frac{3}{2} t_{e} \frac{1}{2} \frac{1}{(2\pi)^{3}} \frac{1}{(\sqrt{2})^{6}} 4\pi \sqrt{\frac{2}{15}} 2\sqrt{15} \sqrt{3} \left\{ \begin{array}{c} 1 & \lambda' & J \\ \lambda & 1 & 2 \end{array} \right\}$$

$$\times \sum_{N} \left[ (-1)^{\lambda} \hat{\lambda}' \left( \sum_{n'} M_{nalanbl_{b},\lambda'}^{N\lambda n'2} * r_{n'2}^{*}(q'^{2}) \right) \left( \sum_{n} M_{ncl_{c}ndl_{d},\lambda}^{N\lambda n0} r_{n0}(1) \right)$$

$$+ (-1)^{\lambda'} \hat{\lambda} \left( \sum_{n'} M_{nalanbl_{b},\lambda'}^{N\lambda' n'0} * r_{n'0}^{*}(1) \right) \left( \sum_{n} M_{ncl_{c}ndl_{d},\lambda}^{N\lambda' n2} r_{n2}(q^{2}) \right) \right].$$

The antisymmetrized matrix element is

$$\langle ab; JM; TM_{T} | \hat{V} | cd; JM; TM_{T} \rangle_{as}$$

$$= \mathcal{N}_{ab} (JT) \mathcal{N}_{cd} (JT) \sum_{\lambda\lambda'} \hat{\lambda} \hat{\lambda}' \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \begin{cases} l_{a} & l_{b} & \lambda' \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_{a} & j_{b} & J \end{cases} \begin{cases} l_{c} & l_{d} & \lambda \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_{c} & j_{d} & J \end{cases}$$

$$\times (-1)^{1+J} (2\sqrt{2}) \frac{3}{2} t_{e} \frac{1}{(4\pi)^{2}} \sqrt{6} \begin{cases} 1 & \lambda' & J \\ \lambda & 1 & 2 \end{cases}$$

$$\times \sum_{N} \left[ (-1)^{\lambda} \hat{\lambda}' \left( \sum_{n'} M_{nalanblb,\lambda'}^{N\lambda n'2} * r_{n'2}^{*} (q'^{2}) \right) \left( \sum_{n} M_{nclcndl,\lambda}^{N\lambda n0} r_{n0} (1) \right) \right]$$

$$\times \left[ 1 + (-1)^{j_{c}+j_{d}-J-T} (-1)^{\lambda-\lambda} (-1)^{l_{c}+l_{d}+\lambda+j_{c}+j_{d}+J} \right]$$

$$+ (-1)^{\lambda'} \hat{\lambda} \left( \sum_{n'} M_{nalanblb,\lambda'}^{N\lambda' n'0} * r_{n'0}^{*} (1) \right) \left( \sum_{n} M_{nclcndl,\lambda}^{N\lambda' n2} r_{n2} (q^{2}) \right)$$

$$\times \left[ 1 + (-1)^{j_{c}+j_{d}-J-T} (-1)^{\lambda-\lambda'} (-1)^{l_{c}+l_{d}+\lambda+j_{c}+j_{d}+J} \right]$$

**Term**  $\hat{V} = t_o \hat{V}_{t_o}$ The coupling of momentum space and spin parts of the interaction gives

$$\tilde{v}(\mathbf{q}', -\mathbf{q})f(\sigma_{\mathbf{1}}, \sigma_{\mathbf{2}}) = 3 t_{o} \frac{1}{2} \frac{1}{(2\pi)^{3}} \frac{1}{(\sqrt{2})^{6}} \frac{4\pi}{3} \\ \times \sum_{M_{\sigma}} (-1)^{2-M_{\sigma}} \sum_{m_{1}m_{2}} C^{2M_{\sigma}}_{1m_{1}1m_{2}} (\sigma_{\mathbf{1}})_{1m_{1}} (\sigma_{\mathbf{2}})_{1m_{2}}$$

$$\times \sum_{M'_{k}M_{k}} C^{2,-M_{\sigma}}_{1M'_{k}1M_{k}} Y_{1M'_{k}} (\mathbf{\Omega}') Y_{1M_{k}} (\mathbf{\Omega}) g'(q') g(q).$$
(D.55)

The coupled matrix element results

$$\begin{split} \langle ab; JM; T'M_{T}'|\hat{V}|cd; JM; TM_{T} \rangle \\ &= \sum_{\lambda'S'} \hat{\lambda}' \hat{S}' \hat{j}_{a} \hat{j}_{b} \begin{cases} l_{a} \quad l_{b} \quad \lambda \\ \frac{1}{2} \quad \frac{1}{2} \quad S' \\ j_{a} \quad j_{b} \quad J \end{cases} \sum_{N'L'n'l'} M_{nalanblb,\lambda'}^{N'L'n'l'} * \\ &\times \sum_{\lambda S} \hat{\lambda} \hat{S} \hat{j}_{c} \hat{j}_{d} \begin{cases} l_{c} \quad l_{d} \quad \lambda \\ \frac{1}{2} \quad \frac{1}{2} \quad S \\ j_{c} \quad j_{d} \quad J \end{cases} \sum_{NLnl} M_{nclcndl_{d},\lambda}^{NLnl} \\ &\times \sum_{M_{\lambda}M_{S}M_{\lambda}M_{S}'} C_{\lambda'M_{\lambda}S'M_{S}}^{JM} C_{\lambda M_{\lambda}SM_{S}}^{JM} \sum_{M_{L}m_{l}M_{L}'m_{l}'} C_{LM_{L}lm_{l}}^{\lambda M_{\lambda}} \\ &\times \sum_{M_{\lambda}M_{S}M_{\lambda}M_{S}'} C_{\lambda'M_{\lambda}S'M_{S}}^{JM} C_{\lambda M_{\lambda}SM_{S}}^{JM} \sum_{M_{L}m_{l}M_{L}'m_{l}'} C_{LM_{L}lm_{l}}^{\lambda M_{\lambda}} C_{L'M_{L}'l'n_{l}'}^{\lambda'M_{\lambda}'} \\ &\times (\sqrt{2})^{3} \delta_{LL'} \delta_{M_{L}M_{L}'} \delta_{NN'} \delta_{TT'} \delta_{M_{T}M_{T}'} 3 t_{o} \frac{1}{2} \frac{1}{(2\pi)^{3}} \frac{1}{(\sqrt{2})^{6}} \frac{4\pi}{3} \\ &\times \sum_{M_{\sigma}} (-1)^{2-M_{\sigma}} \delta_{SS'=1} \hat{S} 6 \sqrt{5} C_{SM_{S}2M_{\sigma}}^{S'M_{S}'} \left\{ \frac{1}{2} \quad \frac{1}{2} \quad S' \\ 1 \quad 1 \quad 2 \end{cases} \\ &\times \sum_{M_{\sigma}} C_{1M_{k}'}^{2,-M_{\sigma}} (-1)^{-M_{k}} \delta_{l'1} \delta_{m_{l}'M_{k}'} \delta_{l1} \delta_{m_{l},-M_{k}} r_{n'l'}^{*}(q') r_{nl}(q) \\ &= \sum_{\lambda\lambda\lambda'} \hat{\lambda} \hat{\lambda} \hat{\lambda}' \hat{\lambda}' \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \left\{ \frac{l_{a} \quad l_{b} \quad \lambda'}{\frac{1}{2} \quad \frac{1}{2}} \\ \frac{1}{2} \quad \frac{1}{2} \quad 1 \\ j_{a} \quad j_{b} \quad J \end{cases} \left\{ \frac{l_{c} \quad l_{d} \quad \lambda}{\frac{1}{2} \quad \frac{1}{2}} \\ j_{c} \quad j_{d} \quad J \end{array} \right\} \delta_{TT'} \delta_{M_{T}M_{T}'} \\ &\times \sum_{NL} \left( \sum_{n'} M_{nalanbl_{b},\lambda'}^{NLn'_{1}} r_{n'1}^{*}(q') \right) \left( \sum_{n} M_{nclcnd_{d},\lambda}^{NLn1}(q) \right) \\ &\times (-1)^{L+\lambda+\lambda'+J+1} 3 t_{o} \frac{1}{(4\pi)^{2}} 10\sqrt{2} \left\{ \begin{array}{c} 1 \quad L \quad \lambda \\ \lambda' \quad 2 \quad 1 \end{array} \right\} \left\{ \begin{array}{c} 1 \quad \lambda' \quad J \\ \lambda \quad 1 \quad 2 \end{array} \right\}. \end{array} \right\}$$

The antisymmetrized matrix element is

$$\langle ab; JM; TM_{T} | \hat{V} | cd; JM; TM_{T} \rangle_{as}$$

$$= \mathcal{N}_{ab}(JT) \mathcal{N}_{cd}(JT) \sum_{\lambda\lambda'} \hat{\lambda} \hat{\lambda} \hat{\lambda}' \hat{\lambda}' \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \begin{cases} l_{a} & l_{b} & \lambda' \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_{a} & j_{b} & J \end{cases} \begin{cases} l_{c} & l_{d} & \lambda \\ \frac{1}{2} & \frac{1}{2} & 1 \\ j_{c} & j_{d} & J \end{cases}$$

$$\times \sum_{NL} \left( \sum_{n'} M_{nal_{a}n_{b}l_{b},\lambda'}^{NLn'1} r_{n'1}^{*}(q') \right) \left( \sum_{n} M_{ncl_{c}n_{d}l_{d},\lambda}^{NLn1} r_{n1}(q) \right)$$

$$\times (-1)^{L+\lambda+\lambda'+J+1} 3t_{o} \frac{1}{(4\pi)^{2}} 10\sqrt{2} \begin{cases} 1 & L & \lambda \\ \lambda' & 2 & 1 \end{cases} \begin{cases} 1 & \lambda' & J \\ \lambda & 1 & 2 \end{cases}.$$

$$(D.57)$$

# E. Three-body zero-range contact interaction

We study the case of the generators of three-body force. We consider an antisymmetric three-body zero-range contact interaction, represented by the operator

$$\hat{V}_{t_3} = \delta(\mathbf{r_1} - \mathbf{r_2})\delta(\mathbf{r_2} - \mathbf{r_3}) \ \mathcal{A}_{123}(\hat{P}^{\sigma}, \hat{P}^{\tau}) \equiv \hat{V}_{\delta} \ \mathcal{A}_{123}(\hat{P}^{\sigma}, \hat{P}^{\tau}), \qquad (E.1)$$

where the antisymmetric part is described by

$$\mathcal{A}_{123} = \left[ 1 - \hat{P}_{12}^{\sigma} \hat{P}_{12}^{\tau} - \hat{P}_{23}^{\sigma} \hat{P}_{23}^{\tau} - \hat{P}_{31}^{\sigma} \hat{P}_{31}^{\tau} + \hat{P}_{12}^{\sigma} \hat{P}_{12}^{\tau} \hat{P}_{23}^{\sigma} \hat{P}_{23}^{\tau} + \hat{P}_{13}^{\sigma} \hat{P}_{13}^{\tau} \hat{P}_{23}^{\sigma} \hat{P}_{23}^{\tau} \right]. \quad (E.2)$$

Its contribution to the interaction potential is  $\hat{V}^{3B} = t_3 \hat{V}_{t_3}$ .

### E.1 Three-body matrix elements

In the JT coupling, we indicate a three-body antisymmetric matrix element with  $\langle ab(J_{ab}T_{ab})c; JM; TM_T | \hat{V}_{t_3} | de(J_{de}T_{de})f; JM; TM_T \rangle_{as}$ . The JT-coupling can be translated in the LST-coupling as

$$\langle ab(J_{ab}T_{ab})c; JM; TM_{T}|V_{t_{3}}|de(J_{de}T_{de})f; JM; TM_{T}\rangle_{as} = \\ \sum_{L_{ab}L_{de}LL'} \sum_{S_{ab}S_{de}SS'} \hat{S}_{ab}\hat{S}_{de}\hat{L}_{ab}\hat{L}_{de}\hat{J}_{ab}\hat{J}_{de}\hat{L}\hat{L}\hat{L}\hat{S}\hat{S}\hat{j}_{a}\hat{j}_{b}\hat{j}_{c}\hat{j}_{d}\hat{j}_{e}\hat{j}_{f} \\ \times \left\{ \begin{array}{ccc} l_{a} & \frac{1}{2} & j_{a} \\ l_{b} & \frac{1}{2} & j_{b} \\ L_{ab} & S_{ab} & J_{ab} \end{array} \right\} \left\{ \begin{array}{ccc} L_{ab} & S_{ab} & J_{ab} \\ l_{c} & \frac{1}{2} & j_{c} \\ L & S & J \end{array} \right\} \left\{ \begin{array}{ccc} l_{d} & \frac{1}{2} & j_{d} \\ l_{e} & \frac{1}{2} & j_{e} \\ L_{de} & S_{de} & J_{de} \end{array} \right\} \left\{ \begin{array}{ccc} L_{de} & S_{de} & J_{de} \\ l_{f} & \frac{1}{2} & j_{f} \\ L' & S' & J \end{array} \right\} \\ \times \sum_{M_{L}M_{L'}M_{S}M_{S'}} C_{LM_{L}SM^{S}}C_{L'M_{L'}S'M_{S'}}^{JM} \\ \times \langle ab(L_{ab}S_{ab}T_{ab})c; LM_{L}; SM_{S}; TM_{T}|\hat{V}_{t_{3}}|de(L_{de}S_{de}T_{de})f; L'M_{L'}; S'M_{S'}; TM_{T}\rangle_{as}, \\ (E.3) \end{array} \right\}$$

where the 9j-symbols recouple four angular momenta (see Sections 1.3 and 1.4 of Ref. [120]) in the form

$$|l_{a}s_{a}(j_{a})l_{b}s_{b}(j_{b}); J_{ab}M_{ab}\rangle = \sum_{L_{ab}S_{ab}} \hat{S}_{ab}\hat{L}_{ab}\hat{j}_{a}\hat{j}_{b} \begin{cases} l_{a} & \frac{1}{2} & j_{a} \\ l_{b} & \frac{1}{2} & j_{b} \\ L_{ab} & S_{ab} & J_{ab} \end{cases} \\ \times |l_{a}l_{b}(L_{ab})s_{a}s_{b}(S_{ab}); J_{ab}M_{ab}\rangle.$$
(E.4)

The single-particle state  $|a\rangle$  is labeled as

$$|a\rangle = |n_{a}l_{a}m_{a}^{l}\frac{1}{2}m_{a}^{s}\frac{1}{2}m_{a}^{t}\rangle = R_{n_{a}l_{a}}(r)Y_{l_{a}m_{a}^{l}}(\theta,\phi)\chi_{\frac{1}{2}m_{a}^{s}}^{S}(\sigma)\chi_{\frac{1}{2}m_{a}^{t}}^{T}(\tau),$$
(E.5)

and the single-particle coordinates are expressed by  $\mathbf{x} \equiv (r, \theta, \phi, \sigma, \tau)$ . In our case, the direct (i.e. not antisymmetrized) *LST*-coupled matrix element is written explicitly as

$$\begin{aligned} &\langle ab(L_{ab}S_{ab}T_{ab})c; LM_{L}; SM_{S}; TM_{T}|\hat{V}_{\delta}|de(L_{de}S_{de}T_{de})f; L'M_{L'}; S'M_{S'}; TM_{T}\rangle_{dir} \\ &= \sum_{\substack{m_{a}^{l}m_{b}^{l}m_{a}^{l}M_{a}^{l}m_{b}^{l}m_{b}^{l}M_{de}^{l}m_{b}^{l}m_{b}^{l}M_{de}^{l}m_{b}^{m}m_{b}^{l}M_{de}^{l}m_{b}^{m}m_{b}^{l}M_{de}^{l}m_{b}^{m}m_{b}^{l}M_{de}^{l}m_{b}^{m}m_{b}^{l}M_{de}^{l}m_{b}^{m}m_{b}^{l}M_{de}^{l}m_{b}^{m}m_{b}^{l}M_{de}^{l}m_{b}^{l}M_{de}^{l}m_{b}^{l}M_{de}^{l}m_{b}^{l}M_{de}^{l}m_{b}^{l}M_{de}^{l}m_{b}^{l}m_{b}^{l}M_{de}^{l}m_{b}^{l}m_{b}^{l}M_{de}^{l}m_{b}^{l}m_{b}^{l}m_{b}^{l}m_{b}^{l}m_{b}^{l}m_{b}^{l}m_{b}^{l}m_{b}^{l}m_{b}^{l}m_{b}^{l}m_{b}^{l}m_{b}^{l}m_{b}^{l}m_{b}^{l}m_{b}^{l}cm_{c}^{l}C_{lam_{d}^{l}am_{b}^{l}m_{b}^{l}}C_{Lam_{d}^{l}de}^{LM_{d}M_{de}^{l}m_{b}^{l}}C_{lam_{d}^{l}de}^{l}m_{b}^{l}C_{lam_{d}^{l}m_{d}^{l}}^{l}m_{b}^{l}C_{lam_{d}^{l}m_{d}^{l}m_{d}^{l}}^{l}m_{d}^{l}C_{lam_{d}^{l}m_{d}^{l}m_{d}^{l}}^{l}m_{d}^{l}C_{lam_{d}^{l}m_{d}^{l}m_{d}^{l}}^{l}m_{d}^{l}C_{lam_{d}^{l}m_{d}^{l}m_{d}^{l}}^{l}m_{d}^{l}C_{lam_{d}^{l}m_{d}^{l}m_{d}^{l}}^{l}m_{d}^{l}C_{lam_{d}^{l}m_{d}$$

where the  $\delta$ -functions in the round parentheses mean the particle number conservation before and after the interaction.

## E.2 Spin and isospin sectors

In Eq.(E.6) the spin and isospin parts can be separated from the orbital and radial parts, namely

$$\langle ab(L_{ab}S_{ab}T_{ab})c; LM_{L}; SM_{S}; TM_{T}|\hat{V}_{\delta}|de(L_{de}S_{de}T_{de})f; L'M_{L'}; S'M_{S'}; TM_{T}\rangle_{dir}$$

$$= \sum_{m_{a}^{l}m_{b}^{l}m_{c}^{l}M_{ab}^{L}} \sum_{m_{a}^{l}m_{b}^{l}m_{e}^{l}m_{f}^{l}M_{de}^{L}} C_{l_{a}m_{a}^{l}l_{b}m_{b}^{l}}^{LM_{L}} C_{L_{ab}M_{ab}^{L}l_{c}m_{c}^{l}}^{Lde_{d}M_{de}^{l}} C_{L_{de}M_{de}^{l}l_{f}m_{f}^{l}}^{L'M_{L'}}$$

$$\times \int d\mathbf{r}_{1}d\mathbf{r}_{2}d\mathbf{r}_{3}d\mathbf{r}_{4}d\mathbf{r}_{5}d\mathbf{r}_{6} R_{nala}^{*}(r_{1})R_{nblb}^{*}(r_{2})R_{nclc}^{*}(r_{3})R_{ndld}(r_{4})R_{nele}(r_{5})R_{nflf}(r_{6})$$

$$\times \frac{\delta(r_{1}-r_{2})}{r_{2}^{2}} \frac{\delta(r_{1}-r_{3})}{r_{3}^{2}} \left( \frac{\delta(r_{1}-r_{4})}{r_{4}^{2}} \frac{\delta(r_{2}-r_{5})}{r_{5}^{2}} \frac{\delta(r_{3}-r_{6})}{r_{6}^{2}} \right)$$

$$\times Y_{l_{a}m_{a}^{l}}^{*}(\theta_{1},\phi_{1})Y_{l_{b}m_{b}^{l}}^{*}(\theta_{2},\phi_{2})Y_{l_{c}m_{c}^{l}}^{*}(\theta_{3},\phi_{3})Y_{l_{d}m_{d}^{l}}(\theta_{4},\phi_{4})Y_{l_{e}m_{e}^{l}}(\theta_{5},\phi_{5})Y_{l_{f}m_{f}^{l}}(\theta_{6},\phi_{6})$$

$$\times \frac{\delta(\theta_{1}-\theta_{2})\delta(\phi_{1}-\phi_{2})}{\sin\theta_{2}} \frac{\delta(\theta_{1}-\theta_{3})\delta(\phi_{1}-\phi_{3})}{\sin\theta_{3}}$$

$$\times \left( \frac{\delta(\theta_{1}-\theta_{4})\delta(\phi_{1}-\phi_{4})}{\sin\theta_{4}} \frac{\delta(\theta_{2}-\theta_{5})\delta(\phi_{2}-\phi_{5})}{\sin\theta_{5}} \frac{\delta(\theta_{3}-\theta_{6})\delta(\phi_{3}-\phi_{6})}{\sin\theta_{6}} \right)$$

$$\times \langle ab(S_{ab})c; SM_{S}|V_{\delta}|de(S_{de})f; S'M_{S'}\rangle_{dir} \langle ab(T_{ab})c; TM_{T}|V_{\delta}|de(T_{de})f; TM_{T}\rangle_{dir}.$$

$$(E.7)$$

Using the following relation in the spin (and isospin) channel,

$$\sum_{\sigma_1 \sigma_2} \chi_{\frac{1}{2} m_a^s}^{S*}(\sigma_1) \chi_{\frac{1}{2} m_b^s}^S(\sigma_2) \delta_{\sigma_1 \sigma_2} = \delta_{\frac{1}{2} \frac{1}{2}} \delta_{m_a^s m_b^s}, \tag{E.8}$$

we obtain respectively

$$\langle ab(S_{ab})c; SM_S|\mathbb{1}_S|de(S_{de})f; S'M_{S'}\rangle_{dir} = \delta_{S_{ab}S_{de}}\delta_{SS'}\delta_{M_SM_{S'}},\tag{E.9}$$

$$\langle ab(T_{ab})c; TM_T | \mathbb{1}_T | de(T_{de})f; TM_T \rangle_{dir} = \delta_{T_{ab}T_{de}} \delta_{TT} \delta_{M_T M_T}.$$
 (E.10)

#### E.2.1 Antisymmetrization of spin and isospin

The antisymmetric  $|ket\rangle$  can be written as

$$|def\rangle_{as} = |def\rangle_{dir} - |edf\rangle + |fde\rangle - |dfe\rangle + |efd\rangle - |fed\rangle.$$
(E.11)

We use Eq.(3) from Ref. [121] to re-write the coupling of the third nucleon to the antisymmetric state of the other two nucleons. We also consider that the orbital

part does not affect the antisymmetrization of the  $|ket\rangle$  because of the spatial symmetry of the  $\delta$ -interaction. Then, it results

$$\langle ab(S_{ab}T_{ab})c; SM_{S}; TM_{T} | \hat{V}_{t_{3}} | de(S_{de}T_{de})f; S'M_{S'}; TM_{T} \rangle_{as}$$

$$= \left[ \delta_{S_{ab}S_{de}} \delta_{T_{ab}T_{de}} - \left[ 1 - (-1)^{S_{de}+T_{de}} \right] \hat{S}_{ab} \hat{S}_{de} \hat{T}_{ab} \hat{T}_{de} \left\{ \begin{array}{cc} \frac{1}{2} & \frac{1}{2} & S_{ab} \\ \frac{1}{2} & S & S_{de} \end{array} \right\} \left\{ \begin{array}{cc} \frac{1}{2} & \frac{1}{2} & T_{ab} \\ \frac{1}{2} & T & T_{de} \end{array} \right\} \right]$$

$$\times \left[ 1 - (-1)^{S_{ab}+T_{ab}} \right].$$

$$(E.12)$$

## E.3 Radial and orbital sectors

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For the radial and angular part in Eq.(E.6), redefined as

$$\begin{split} V_{\delta}^{space} &\equiv \sum_{m_{a}^{l}m_{b}^{l}m_{c}^{l}M_{ab}^{L}} \sum_{m_{a}^{l}m_{b}^{l}m_{b}^{l}M_{de}^{L}} C_{l_{a}m_{a}^{l}l_{b}m_{b}^{l}}^{L_{ab}M_{ab}^{L}l_{c}m_{c}^{l}} C_{l_{d}m_{d}^{l}l_{e}m_{e}^{l}}^{L_{de}M_{de}^{L}} C_{L_{de}M_{de}^{L}l_{f}m_{f}^{l}}^{L_{de}M_{de}^{L}l_{f}m_{f}^{l}} \\ &\times \int d\mathbf{r}_{1} d\mathbf{r}_{2} d\mathbf{r}_{3} d\mathbf{r}_{4} d\mathbf{r}_{5} d\mathbf{r}_{6} R_{n_{a}l_{a}}^{*}(r_{1}) R_{n_{b}l_{b}}^{*}(r_{2}) R_{n_{c}l_{c}}^{*}(r_{3}) R_{n_{d}l_{d}}(r_{4}) R_{n_{e}l_{e}}(r_{5}) R_{n_{f}l_{f}}(r_{6}) \\ &\times \frac{\delta(r_{1}-r_{2})}{r_{2}^{2}} \frac{\delta(r_{1}-r_{3})}{r_{3}^{2}} \left( \frac{\delta(r_{1}-r_{4})}{r_{4}^{2}} \frac{\delta(r_{2}-r_{5})}{r_{5}^{2}} \frac{\delta(r_{3}-r_{6})}{r_{6}^{2}} \right) \\ &\times Y_{l_{a}m_{a}^{l}}^{*}(\theta_{1},\phi_{1}) Y_{l_{b}m_{b}^{l}}^{*}(\theta_{2},\phi_{2}) Y_{l_{c}m_{c}^{l}}^{*}(\theta_{3},\phi_{3}) Y_{l_{d}m_{d}^{l}}(\theta_{4},\phi_{4}) Y_{l_{e}m_{e}^{l}}(\theta_{5},\phi_{5}) Y_{l_{f}m_{f}^{l}}(\theta_{6},\phi_{6}) \\ &\times \frac{\delta(\theta_{1}-\theta_{2})\delta(\phi_{1}-\phi_{2})}{\sin\theta_{2}} \frac{\delta(\theta_{1}-\theta_{3})\delta(\phi_{1}-\phi_{3})}{\sin\theta_{3}} \\ &\times \left( \frac{\delta(\theta_{1}-\theta_{4})\delta(\phi_{1}-\phi_{4})}{\sin\theta_{4}} \frac{\delta(\theta_{2}-\theta_{5})\delta(\phi_{2}-\phi_{5})}{\sin\theta_{5}} \frac{\delta(\theta_{3}-\theta_{6})\delta(\phi_{3}-\phi_{6})}{\sin\theta_{6}} \right), \end{split}$$
(E.13)

we use the separation of radial and angular coordinates in spherical symmetry  $\int d\mathbf{r} = \int r^2 dr \int \sin\theta \, d\theta \int d\phi$ . After coupling the spherical harmonics and applying angular momentum algebra,

$$V_{\delta}^{space} = \frac{\hat{l}_{a}\hat{l}_{b}\hat{l}_{c}\hat{l}_{d}\hat{l}_{e}\hat{l}_{f}}{16\pi^{2}\hat{L}^{2}}C_{l_{a}0l_{b}0}^{L_{ab}0}C_{L_{ab}0l_{c}0}^{L0}C_{l_{d}0l_{e}0}^{L_{de}0}C_{L_{de}0l_{f}0}^{L'0}(-1)^{l_{a}+l_{b}+l_{c}-L}\delta_{LL'}\delta_{M_{L}M_{L'}}$$

$$\times \int \mathrm{d}r \, r^{2}R_{n_{a}l_{a}}^{*}(r)R_{n_{b}l_{b}}^{*}(r)R_{n_{c}l_{c}}^{*}(r)R_{n_{d}l_{d}}(r)R_{n_{e}l_{e}}(r)R_{n_{f}l_{f}}(r).$$
(E.14)

## E.4 JT-coupled matrix elements

Inserting Eqs.(E.6), (E.12) and (E.14) in the JT-coupled matrix element, Eq.(E.3) reads

 $\langle ab(J_{ab}T_{ab})c; JM; TM_T | \hat{V}_{t_3} | de(J_{de}T_{de})f; JM; TM_T \rangle_{as}$ 

$$= \sum_{L_{ab}L_{de}LL'} \sum_{S_{ab}S_{de}SS'} (-1)^{l_{a}+l_{b}+l_{c}-L} \hat{S}_{ab} \hat{S}_{de} \hat{L}_{ab} \hat{L}_{de} \hat{J}_{ab} \hat{J}_{de} \hat{L} \hat{L}' \hat{S} \hat{S}' \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \hat{l}_{e} \hat{l}_{d} \hat{l$$

The sum over  $S_{ab}$  and  $S_{de}$ , and the conditions  $\delta_{(T_{ab}+S_{ab},1)}\delta_{(T_{de}+S_{de},1)}$  produce four different cases. In the following, we use also that  $(-1)^{S_{ab}+S_{de}} = (-1)^{T_{ab}+T_{de}}$ .

Case  $S_{ab}=0$ ,  $S_{de}=0$ ,  $T_{ab}=1$  and  $T_{de}=1$ With the help of Eq.(1.97) in Ref. [120], that is

$$\hat{l}_{1}\hat{l}_{2}\left(\begin{array}{ccc}l_{1} & l_{2} & l_{12}\\ 0 & 0 & 0\end{array}\right)\left\{\begin{array}{ccc}l_{1} & l_{2} & l_{12}\\ j_{1} & j_{2} & l_{12}\\ \frac{1}{2} & \frac{1}{2} & 0\end{array}\right\} = \frac{1 + (-1)^{l_{1} + l_{2} + L_{12}}}{2}\frac{(-1)^{l_{2} + j_{2} + \frac{1}{2}}}{\sqrt{2}\hat{l}_{12}}\left(\begin{array}{ccc}j_{1} & j_{2} & l_{12}\\ -\frac{1}{2} & \frac{1}{2} & 0\end{array}\right),$$

$$(E.16)$$

and with the relation between Clebsch-Gordan coefficients and 3j-symbols,

$$C_{l_10l_20}^{l_120} = (-1)^{l_1 - l_2} \hat{l}_{12} \begin{pmatrix} l_1 & l_2 & l_{12} \\ 0 & 0 & 0 \end{pmatrix},$$
(E.17)

we obtain

$$\langle ab(J_{ab}1)c; J; \frac{1}{2} | \hat{V}_{t_3} | de(J_{de}1)f; J; \frac{1}{2} \rangle_{as} = \frac{3}{2} (-1)^{T_{ab}+T_{de}} \hat{J}_{ab} \hat{J}_{de} \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \hat{j}_{e} \hat{j}_{f} \frac{(-1)^{l_b+l_e+j_b-j_e+J_{ab}+J_{de}}}{16\pi^2} \times \left( \begin{array}{cc} j_a & j_b & J_{ab} \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{array} \right) \left( \begin{array}{cc} j_c & J & J_{ab} \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{array} \right) \left( \begin{array}{cc} j_d & j_e & J_{de} \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{array} \right) \left( \begin{array}{cc} j_d & j_e & J_{de} \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{array} \right) \left( \begin{array}{cc} j_f & J & J_{de} \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{array} \right) \\ \times \int dr \, r^2 R^*_{n_a l_a}(r) R^*_{n_b l_b}(r) R^*_{n_c l_c}(r) R_{n_d l_d}(r) R_{n_e l_e}(r) R_{n_f l_f}(r).$$
(E.18)

The conditions  $\delta_{L_{ab}J_{ab}}$ ,  $\delta_{L_{de}J_{de}}$ ,  $l_a + l_b + L_{ab} = \text{even}$ ,  $l_c + L_{ab} + L = \text{even}$ ,  $l_d + l_e + L_{de} = \text{even}$ ,  $l_f + L_{de} + L = \text{even}$  appear during the derivation.

Case  $S_{ab}=1$ ,  $S_{de}=0$ ,  $T_{ab}=0$  and  $T_{de}=1$ Using Eq.(1.98) in Ref. [120],

$$\hat{l}_{1}\hat{l}_{2}\begin{pmatrix} l_{1} & l_{2} & l_{12} \\ 0 & 0 & 0 \end{pmatrix} \begin{cases} l_{1} & l_{2} & l_{12} \\ j_{1} & j_{2} & j_{12} \\ \frac{1}{2} & \frac{1}{2} & 1 \end{cases}$$

$$= \frac{(-1)^{l_{12}}}{\sqrt{6}} \frac{1 + (-1)^{l_{1}+l_{2}+l_{12}}}{2} \begin{pmatrix} j_{1} & j_{2} & j_{12} \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}$$

$$\times \left[ \frac{\hat{j}_{1}^{2} + (-1)^{j_{1}+j_{2}+j_{12}} \hat{j}_{2}^{2}}{\sqrt{2j_{12}(j_{12}+1)}} \begin{pmatrix} j_{12} & 1 & l_{12} \\ 1 & -1 & 0 \end{pmatrix} + (-1)^{l_{1}+j_{1}+\frac{1}{2}} \begin{pmatrix} j_{12} & 1 & l_{12} \\ 0 & 0 & 0 \end{pmatrix} \right],$$

$$(E.19)$$

the matrix element results

$$\begin{aligned} \langle ab(J_{ab}0)c; J; \frac{1}{2} | \hat{V}_{t_3} | de(J_{de}1)f; J; \frac{1}{2} \rangle_{as} = \\ \sum_{L_{ab}} \frac{\sqrt{3}}{2} (-1)^{T_{ab}+T_{de}} \hat{L}_{ab}^2 \hat{J}_{ab} \hat{J}_{de} \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \hat{j}_{e} \hat{j}_{f} \frac{(-1)^{l_{e}+l_{f}+j_{a}+j_{b}+j_{c}+j_{e}+L_{ab}}}{16\pi^2} \\ \times \left( \frac{j_{a}}{\frac{1}{2}} - \frac{j_{b}}{-\frac{1}{2}} 0 \right) \left( \frac{j_{c}}{\frac{1}{2}} - \frac{J}{-\frac{1}{2}} 0 \right) \left( \frac{j_{d}}{\frac{1}{2}} - \frac{j_{e}}{-\frac{1}{2}} 0 \right) \left( \frac{j_{f}}{\frac{1}{2}} - \frac{J}{-\frac{1}{2}} 0 \right) \\ \times \left[ \frac{\hat{j}_{a}^{2} + (-1)^{j_{a}+j_{b}+J_{ab}} \hat{j}_{b}^{2}}{\sqrt{2J_{ab}(J_{ab}+1)}} \left( \frac{J_{ab}}{1} - 1 - \frac{L_{ab}}{0} \right) + (-1)^{l_{a}+j_{a}+\frac{1}{2}} \left( \frac{J_{ab}}{0} - 1 - \frac{L_{ab}}{0} \right) \right] \\ \times \left[ \frac{\hat{j}_{c}^{2} + (-1)^{j_{c}+J+J_{ab}} \hat{J}^{2}}{\sqrt{2J_{ab}(J_{ab}+1)}} \left( \frac{J_{ab}}{1} - 1 - \frac{L_{ab}}{0} \right) + (-1)^{l_{c}+j_{c}+\frac{1}{2}} \left( \frac{J_{ab}}{0} - 1 - \frac{L_{ab}}{0} \right) \right] \\ \times \int dr \, r^{2} R_{n_{a}l_{a}}^{*}(r) R_{n_{b}l_{b}}^{*}(r) R_{n_{c}l_{c}}^{*}(r) R_{n_{d}l_{d}}(r) R_{n_{e}l_{e}}(r) R_{n_{f}l_{f}}(r), \end{aligned}$$
(E.20)

with the conditions  $\delta_{L_{de}J_{de}}$ , and  $l_a + l_b + L_{ab} = \text{even}$ ,  $l_c + L_{ab} + L = \text{even}$ ,  $l_d + l_e + L_{de} = \text{even}$ ,  $l_f + L_{de} + L = \text{even}$ .

Case  $S_{ab}=0$ ,  $S_{de}=1$ ,  $T_{ab}=1$  and  $T_{de}=0$ The matrix element results

$$\begin{aligned} \langle ab(J_{ab}1)c; J; \frac{1}{2} | \hat{V}_{t_3} | de(J_{de}0)f; J; \frac{1}{2} \rangle_{as} = \\ \sum_{L_{de}} \frac{\sqrt{3}}{2} (-1)^{T_{ab}+T_{de}} \hat{L}_{de}^2 \hat{J}_{ab} \hat{J}_{de} \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \hat{j}_{e} \hat{j}_{f} \frac{(-1)^{l_{b}+l_{c}+j_{b}+j_{d}+j_{e}+j_{f}+L_{de}}}{16\pi^2} \\ \times \left( \frac{j_{a}}{\frac{j_{b}}{2}} - \frac{j_{ab}}{2} \right) \left( \frac{j_{c}}{\frac{1}{2}} - \frac{J}{2} - \frac{J}{2} \right) \left( \frac{j_{d}}{\frac{j_{e}}{2}} - \frac{J}{2} - \frac{J}{2} \right) \left( \frac{j_{f}}{\frac{1}{2}} - \frac{J}{2} - \frac{J}{2} \right) \\ \times \left[ \frac{\hat{j}_{d}^2 + (-1)^{j_{d}+j_{e}+J_{de}} \hat{j}_{e}^2}{\sqrt{2J_{de}(J_{de}+1)}} \left( \frac{J_{de}}{1} - \frac{L_{de}}{1} \right) + (-1)^{l_{d}+j_{d}+\frac{1}{2}} \left( \frac{J_{de}}{2} - \frac{1}{2} \right) \right) \right] \\ \times \left[ \frac{\hat{j}_{f}^2 + (-1)^{j_{f}+J+J_{de}} \hat{j}_{e}^2}{\sqrt{2J_{de}(J_{de}+1)}} \left( \frac{J_{de}}{1} - \frac{L_{de}}{2} \right) + (-1)^{l_{f}+j_{f}+\frac{1}{2}} \left( \frac{J_{de}}{2} - \frac{1}{2} \right) \right) \right] \\ \times \int dr \, r^2 R_{n_{a}l_{a}}^*(r) R_{n_{b}l_{b}}^*(r) R_{n_{c}l_{c}}^*(r) R_{n_{d}l_{d}}(r) R_{n_{e}l_{e}}(r) R_{n_{f}l_{f}}(r), \end{aligned}$$
(E.21)

with the conditions  $\delta_{L_{ab}J_{ab}}$ , and  $l_a + l_b + L_{ab} = \text{even}$ ,  $l_c + L_{ab} + L = \text{even}$ ,  $l_d + l_e + L_{de} = \text{even}$ ,  $l_f + L_{de} + L = \text{even}$ .

Case  $S_{ab}=1$ ,  $S_{de}=1$ ,  $T_{ab}=0$  and  $T_{de}=0$ The matrix element results

$$\begin{split} \langle ab(J_{ab}0)c; J; \frac{1}{2} |\hat{V}_{t_{3}}| de(J_{de}0)f; J; \frac{1}{2} \rangle_{as} = \\ \sum_{L_{ab}L_{de}} \frac{1}{2} (-1)^{T_{ab}+T_{de}} \hat{L}_{ab}^{2} \hat{L}_{de}^{2} \hat{J}_{ab} \hat{J}_{de} \hat{j}_{a} \hat{j}_{b} \hat{j}_{c} \hat{j}_{d} \hat{j}_{e} \hat{j}_{f} \frac{(-1)^{j_{a}+j_{b}+j_{c}+j_{d}+j_{e}+j_{f}+L_{ab}+L_{de}+1}}{16\pi^{2}} \\ \times \left( \begin{array}{cc} j_{a} & j_{b} & J_{ab} \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{array} \right) \left( \begin{array}{cc} j_{c} & J & J_{ab} \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{array} \right) \left( \begin{array}{cc} j_{d} & j_{e} & J_{de} \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{array} \right) \left( \begin{array}{cc} j_{f} & J & J_{de} \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{array} \right) \\ \times \left[ \frac{\hat{j}_{a}^{2} + (-1)^{j_{a}+j_{b}+J_{ab}} \hat{j}_{b}^{2}}{\sqrt{2J_{ab}(J_{ab}+1)}} \left( \begin{array}{cc} J_{ab} & 1 & L_{ab} \\ 1 & -1 & 0 \end{array} \right) + (-1)^{l_{a}+j_{a}+\frac{1}{2}} \left( \begin{array}{cc} J_{ab} & 1 & L_{ab} \\ 0 & 0 & 0 \end{array} \right) \right] \\ \times \left[ \frac{\hat{j}_{c}^{2} + (-1)^{j_{c}+J+J_{ab}} \hat{j}_{c}^{2}}{\sqrt{2J_{ab}(J_{ab}+1)}} \left( \begin{array}{cc} J_{ab} & 1 & L_{ab} \\ 1 & -1 & 0 \end{array} \right) + (-1)^{l_{c}+j_{c}+\frac{1}{2}} \left( \begin{array}{cc} J_{ab} & 1 & L_{ab} \\ 0 & 0 & 0 \end{array} \right) \right] \\ \times \left[ \frac{\hat{j}_{d}^{2} + (-1)^{j_{d}+j_{d}+J_{de}} \hat{j}_{e}^{2}}{\sqrt{2J_{ab}(J_{de}+1)}}} \left( \begin{array}{cc} J_{de} & 1 & L_{de} \\ 1 & -1 & 0 \end{array} \right) + (-1)^{l_{d}+j_{d}+\frac{1}{2}} \left( \begin{array}{cc} J_{de} & 1 & L_{de} \\ 0 & 0 & 0 \end{array} \right) \right] \\ \times \left[ \frac{\hat{j}_{f}^{2} + (-1)^{j_{f}+J+J_{de}} \hat{j}_{e}^{2}}{\sqrt{2J_{de}(J_{de}+1)}} \left( \begin{array}{cc} J_{de} & 1 & L_{de} \\ 1 & -1 & 0 \end{array} \right) + (-1)^{l_{f}+j_{f}+\frac{1}{2}} \left( \begin{array}{cc} J_{de} & 1 & L_{de} \\ 0 & 0 & 0 \end{array} \right) \right] \right] \\ \times \int dr \, r^{2} R_{nal_{a}}^{*}(r) R_{nbl_{b}}^{*}(r) R_{ncl_{c}}^{*}(r) R_{ndl_{d}}(r) R_{nel_{e}}(r) R_{nfl_{f}}(r), \end{split}$$
(E.22)

with the conditions  $l_a + l_b + L_{ab} =$  even,  $l_c + L_{ab} + L =$  even,  $l_d + l_e + L_{de} =$  even,  $l_f + L_{de} + L =$  even.

## F. Tests and benchmarks

Here we present results of tests and benchmarks performed to check the numerical consistency of the different solvers used in this work. In fact, we employ a code for the SCGF solutions (Boccadorata [95]), an Hartree-Fock solver in spherical harmonic oscillator basis for the model EDFs (HOSPHE [99]) and a code to perform the regression analysis of the data.

All the solvers use the same values of physical constants relevant for the nuclear many-body problem. These values are collected in Table F.1.

 Table F.1: Physical constants used in the calculations.

constant	value
$m_N c^2 \; [{\rm MeV}]$	938.918267
$\hbar c  [\text{MeV} \cdot \text{fm}]$	197.326972

## F.1 Test of the functional derivation at Hartree-Fock level

We apply the method described in Section 5 to Hartree-Fock calculations, that is, the quantities entering in the regression come from not correlated solutions. In the reference Hamiltonian  $\hat{H}^{ab}{}^{1}$ , we choose to describe the system with Skyrme SV [98] interaction, namely  $\hat{H}^{ab} = \hat{T} + \hat{V}_{SV}$ , where the Coulomb interaction is neglected for simplicity. The potential is formed by generators commonly used to build the EDF at the mean-field level and then gives stable binding energies for

<sup>&</sup>lt;sup>1</sup>The subscript  $^{ab}$  is used to keep the same notation as in Section 5 even if in this Appendix the Hamiltonian includes a phenomenological effective interaction.

Hartree-Fock calculations. The specific form of the interaction is

$$\hat{V}_{SV} = (t_0 + t_0 x_0 \hat{P}^{\sigma}) \delta(\mathbf{r}_1 - \mathbf{r}_2) + \frac{1}{2} (t_1 + t_1 x_1 \hat{P}^{\sigma}) \left[ \hat{\mathbf{k}}^{\prime 2} \delta(\mathbf{r}_1 - \mathbf{r}_2) + \delta(\mathbf{r}_1 - \mathbf{r}_2) \hat{\mathbf{k}}^2 \right] + (t_2 + t_2 x_2 \hat{P}^{\sigma}) \left[ \hat{\mathbf{k}}^{\prime 2} \cdot \delta(\mathbf{r}_1 - \mathbf{r}_2) \hat{\mathbf{k}}^2 \right] + i \, w_0 (\hat{\sigma_1} + \hat{\sigma_2}) \cdot \left[ \hat{\mathbf{k}}^{\prime} \times \delta(\mathbf{r}_1 - \mathbf{r}_2) \hat{\mathbf{k}}^2 \right] \equiv t_0 \hat{V}_{t_0} + t_0 x_0 \hat{V}_{t_0 x_0} + t_1 \hat{V}_{t_1} + t_1 x_1 \hat{V}_{t_1 x_1} + t_2 \hat{V}_{t_2} + t_2 x_2 \hat{V}_{t_2 x_2} + w_0 \hat{V}_{(t) w_0}, \quad (F.1)$$

where the density-dependent term ( $\propto t_3$ ) is absent in the SV parametrization. The last line of Eq.(F.1) defines the generators  $\hat{V}_j^{gen}$ . Note that in this Section we work with the parameters  $t_j$ , instead of the coupling constants  $C_j$ , and their relative generators.

In our choice, the perturbations are induced by the same generators,  $\hat{V}_i^{pert} = \hat{V}_i^{gen}$ , acting one at a time with a certain Lagrange multiplier  $\lambda_i$ . We are interested, for testing purposes, to construct a model functional  $\tilde{E} = \langle \Phi | \hat{T} + \sum_j t_j \hat{V}_j^{gen} | \Phi \rangle$ , with the model Hamiltonian analogous to the reference Hamiltonian.

The independent-particle nature of the Hartree-Fock solution  $|\Phi(\lambda_i)\rangle$  allows us to directly evaluate the expectation value of the interaction energy as

$$V^{ab}(\lambda_i) \equiv V_{SV}(\lambda_i) = \langle \Phi(\lambda_i) | \hat{V}_{SV} | \Phi(\lambda_i) \rangle.$$
 (F.2)

More important, since we built the model functional with the same generators used in the *ab initio*-like interaction energy, and we perform a calculation at the Hartree-Fock level, we expect an exact fulfillment of Eq.(5.18), that is

$$V^{ab}(\lambda_i) = \sum_j t_j \langle \Phi(\lambda_i) | \hat{V}_j^{gen} | \Phi(\lambda_i) \rangle_{HF} = \sum_j t_j \langle \Phi(\lambda_i) | \hat{V}_j^{gen} | \Phi(\lambda_i) \rangle.$$
(F.3)

In the following, we indicate the Hartree-Fock average value of the generators as  $V_j^{gen}(\lambda_i) \equiv \langle \Phi(\lambda_i) | \hat{V}_j^{gen} | \Phi(\lambda_i) \rangle_{HF}$ .

The kinetic energy results  $\langle \Phi(\lambda_i) | \hat{T} | \Phi(\lambda_i) \rangle = T[\rho(\lambda_i)]$ , such that the model functional in Eq.(5.1) appears equivalent to the standard functional for Skyrme SV.

We consider a small model space, the spherical harmonic oscillator basis is restricted to  $N_{max} = 5$ , with oscillator energy  $\hbar \omega = 14$  MeV. The calculations employ the matrix elements defined in Appendix D for the generators. The same matrix elements provide the Skyrme SV potential, using the parameter values given in Ref. [98] and shown in Table F.2. We use the solver BoccaDorata [95], with the Hartree-Fock (*HF*) option.

The regression analysis (see Section 5.2) involves results calculated for 7 closed-shell nuclei (<sup>16</sup>O, <sup>24</sup>O, <sup>34</sup>Si, <sup>36</sup>S, <sup>40</sup>Ca, <sup>48</sup>Ca and <sup>56</sup>Ni), each one perturbed with 7 different interactions  $V_i^{gen}$  and 10 possible values of  $\lambda_i$  for each i ( $\lambda_i = -9, -7, -5, -3, -1, 1, 3, 5, 7, 9$ ).



**Figure F.1:** Plot of the average value of the Skyrme SV energy  $E_{ab}$  for <sup>16</sup>O. The solutions  $|\Phi(\lambda_i)\rangle$ , corresponding to the perturbations  $(\lambda_i)$ , are identified by the markers color and the strength shown on the x-axis.

In total, we collect 496 data points, corresponding to convergent solutions, including the unperturbed ground states ( $\lambda_i = 0$ ). Each data point contains the observables  $V^{ab}(\lambda_i)$  and the variables  $V_j^{gen}(\lambda_i)$  as inputs. Data relative to the nucleus <sup>16</sup>O are presented in Figure F.1, where the plot shows

Data relative to the nucleus <sup>16</sup>O are presented in Figure F.1, where the plot shows that the unperturbed solution  $\lambda = 0$  represents the minimum for the *ab initio*-like energy  $E_{ab}$ , in agreement with the variational principle.

This exercise does not offer any physical argument of discussion about the interaction, because we fit a mean-field interaction using its own generators. However, apart the goal of testing the numerical coherence of the codes, it is interesting to study some general features of the regression analysis.

First of all, the results of the fit are strongly deteriorated removing the smallest singular values as described in Appendix A. It means that the corresponding  $\chi^2(\mathbf{t})$  increases significantly when reducing the number of singular values, because the Eq.(F.3) is not exact any more. This fact suggests that all the singular values are important to determine the parameters  $t_i$  or, equivalently, there are not singular

values small enough to make the matrix  $\mathcal{J}^T W \mathcal{J}$  singular.

More interesting point, it is the discussion of the generators relevant to reproduce the *ab initio*-like interaction. Skyrme SV potential presents only 5 non-zero parameters out of the 7 available ones for the central and spin-orbit parts (see the column  $\hat{V}_{SV}$  in Table F.2). We observe that using the 5 non-zero generators (5p) or using all 7 of them (7p) does not change significantly the  $\chi^2(\mathbf{t})$ . However, as one of the 5 original generators is substituted with one of the zero ones, for example  $\hat{V}_{(t)w0}$  is replaced with  $\hat{V}_{t_1x_1}$  (5p\*), the  $\chi^2(\mathbf{t})$  becomes much larger than zero and the values of the parameters change completely from the value of the original interaction  $\hat{V}_{SV}$ . These results are summarized in Table F.2, including the associated errors obtained from regression.

**Table F.2:** Comparison between the value of the parameters used in the Skyrme SV interaction  $(\hat{V}_{SV})$  and the ones obtained from the regression analysis (fit). Also the errors associated with the fitted parameters are displayed. The different selection of parameters and relative generators (5p, 7p and 5p\*) are explained in the text.

parameter	$\hat{V}_{SV}$	fit (5p)		fit $(7p)$		fit $(5p^*)$	
$t_0$	-1248.29	-1248.291	$\pm 0.003$	-1248.294	$\pm 0.004$	-1193.0	$\pm 21.7$
$t_0 x_0$	212.21	212.209	$\pm 0.002$	212.160	$\pm 0.028$	-2120.2	$\pm$ 119.7
$t_1$	970.56	970.560	$\pm 0.005$	970.566	$\pm 0.006$	861.5	$\pm$ 37.4
$t_1x_1$	-	-	-	0.065	$\pm 0.042$	3930.6	$\pm$ 173.6
$t_2$	107.22	107.221	$\pm 0.001$	107.237	$\pm 0.018$	110.1	$\pm 4.0$
$t_2 x_2$	-	-	-	-0.019	$\pm 0.022$	-	-
$w_0$	150.00	150.001	$\pm 0.001$	150.000	$\pm 0.001$	-	-
$\chi^2$		$2.22 \times 10^{-7}$		$2.21 \times 10^{-7}$		7.70	
BIC		2357.7		2366.9		10969.2	

In Table F.2, the comparison of the BIC value, Eq.(6.10), for (5p) and (7p) shows that the interaction energy  $V_{SV}$  can be reproduced better with the 5 generators (the ones which are, in fact, used to build the Skyrme SV potential) than the 7 generators. That is, among the 7 generators, 2 are redundant and do not improve the information content.

We need to clarify that we have used the weight  $w_i=1$  in the  $\chi^2$  because the theoretical uncertainties, associated with the interaction energy, are around 1 eV and then negligible. The  $\chi^2$  is not normalized.

Figure F.2 offers a graphical representation of Eq.(F.3), where data points relative to nucleus <sup>56</sup>Ni are displayed. The parametrization (5p) shows a great agreement between the average value  $V_{ab}$  of the interaction energy (markers) and the right-



Figure F.2: Plot of Eq.(F.3) for the nucleus <sup>56</sup>Ni and parametrization (5p). The average values  $V_{ab}(\lambda_i)$  of the Skyrme SV interaction energy are represented with markers ("ab" in the legend), while the lines describe the right-hand side of Eq.(F.3), dependent on the fitted parameters  $t_j$  ("fit"). Different colors indicates different perturbation potentials  $\hat{V}_i^{gen} = \hat{V}_{t_i}$ , with the value of  $\lambda_i$  shown on the x-axis. The shadowed areas identify the propagated errors on the interaction energies, associated with the error on the fitted parameters.

hand side of Eq.(F.3), with the parameters obtained from the regression analysis. The parametrization (5p<sup>\*</sup>), instead, gives an appreciable difference between the Skyrme SV average value and the product of the expectation value of the generators and the corresponding parameters. Such difference is responsible for the large value of the  $\chi^2$  in the (5p<sup>\*</sup>) case. Figure F.3 points out that, if the selected generators are not adapt to describe the interaction energy, the behavior of the fitted values can be tilted respect to the data. Furthermore, since the regression fits the data points from all the nuclei at once, for some nuclei it can happen a vertical shift between markers and lines. That is, the parameters underestimate or overestimate the average value of the potential systematically for all the data points of the nucleus, including the unperturbed case ( $\lambda = 0$ ). As mentions, not shown here, in



**Figure F.3:** Same as Figure F.2 for the nucleus  ${}^{56}Ni$  and parametrization  $(5p^*)$ .

 $^{24}$ O ( $^{34}$ Si) the fitted values underestimate (overestimate) the inputs data. The propagated errors (shadowed areas) are large for the (5p<sup>\*</sup>) case while negligible for the (5p) case.

The parametrization (5p) allows to calculate the infinite nuclear matter quantities described in Appendix B. The values are collected in Table F.3. The standard properties of Skyrme SV interaction are reproduced as in particular the small isoscalar effective mass  $m^*/m$  and the large incompressibility K, due to the lack of the density-dependent term.

The previous analysis is performed including  $\hat{V}_{t_3}$ , the generators of the threebody contact term, among the possible generators. The obtained parametrization (8p) extends the parametrization (7p) to include the  $t_3$  parameter. As shown in Table F.4, the larger number of parameters does not provide an improvement in the fit of the Skyrme SV potential since the BIC is larger than in the case of (5p). The parametrization (5p<sup>\*\*</sup>) considers the parameters  $t_0,t_1,t_2,w_0$  and  $t_3$ , i.e., replaces the  $t_0x_0$  parameter in the original Skyrme SV with the parameter relative to the three-body zero-range interaction. In the case (5p<sup>\*\*</sup>) as in the case (5p<sup>\*</sup>),

**Table F.3:** Values of infinite nuclear matter quantities for the parametrization (5p) of the Skyrme SV model functional (compare with Table B.1 for standard value).

quantity	value	
$\rho_{sat}  [\mathrm{fm}^{-3}]$	0.15509	$\pm 0.00001$
$r_0$ [fm]	1.15463	$\pm 0.00001$
$E/A \; [{\rm MeV}]$	-16.04774	$\pm 0.00001$
$m^*/m$	0.38289	$\pm 0.00001$
$J \; [MeV]$	32.82451	$\pm 0.00016$
$L \; [MeV]$	96.09112	$\pm 0.00052$
$K \; [MeV]$	305.67449	$\pm 0.00380$

replacing one of the original generators corresponds to a large increase of the  $\chi^2$ , and a decreasing quality to reproduce Eq.(F.3).

**Table F.4:** Same as in Table F.2, but with the generator of the three-body contact interaction  $t_3$  included in the regression analysis. (8p) is the extension of (7p) to include  $t_3$ . (5p\*\*) parametrization uses  $t_0$ ,  $t_1$ ,  $t_2$ ,  $w_0$  and  $t_3$  as generators.

parameter	$\hat{V}_{SV}$	fit $(8p)$		fit $(5p^{**})$	
$t_0$	-1248.29	-1248.295	$\pm 0.004$	-1429.26	$\pm$ 7.85
$t_0 x_0$	212.21	212.162	$\pm 0.028$	-	-
$t_1$	970.56	970.567	$\pm 0.007$	1263.70	$\pm 15.85$
$t_1x_1$	-	0.065	$\pm 0.042$	-	-
$t_2$	107.22	107.237	$\pm 0.018$	121.02	$\pm 2.63$
$t_2 x_2$	-	-0.018	$\pm 0.023$	-	-
$w_0$	150.00	150.000	$\pm 0.001$	197.36	$\pm 2.26$
$t_3$	-	-0.018	$\pm 0.028$	652.56	$\pm$ 100.61
$\chi^2$		$2.22 \times 10^{-7}$		3.123	
BIC		2372.7		10521.8	

#### F.2 Benchmarks for the matrix elements

The matrix elements for the generators  $\hat{V}_{j}^{gen}$  corresponding to the coupling constant  $C_{j}$  are obtained from the generators  $\hat{V}_{t_{j}}$ , derived in Appendix D, and from Eq.(C.7). To check the correctness of the matrix elements, we can consider that, for a Hartree-Fock state  $|\Phi(\lambda_{i})\rangle$ , it results

$$\langle \Phi(\lambda_i) | \hat{T} + \hat{V}_{SV} + \lambda_i \hat{V}_i^{gen} | \Phi(\lambda_i) \rangle = T[\rho(\lambda_i)] + V_{SV}[\rho(\lambda_i)] + \lambda_i V_i^{gen}[\rho(\lambda_i)], \quad (F.4)$$

where the Coulomb interaction is neglected on both sides. The left-hand side can be calculated with the SCGF method, at the Hartree-Fock level, and the matrix elements  $\hat{V}_i^{gen}$  we are interested to test. The right-hand side can be obtained from an energy density functional solver after rescaling the coupling constants as  $C_j \to C_j$  for  $j \neq i$  and  $C_i \to C_i + \lambda_i$ . Specifically we compare the results from the SCGF code Boccadorata [95] and the EDFs code HOSPHE [99]. Both use a basis of spherical harmonic oscillator wave function, and we choose a model space limited to  $N_{max} = 9$  and energy  $\hbar\omega = 20$  MeV. We select value of  $\lambda_i$  such that the differences in total energy respect to the  $\lambda = 0$  case are of the order of few MeV. The agreement between the perturbed energy from Green's functions and from EDFs is at the eV level for all the generators  $\hat{V}_0^{\rho}$ ,  $\hat{V}_1^{\rho}$ ,  $\hat{V}_0^{\Delta\rho}$ ,  $\hat{V}_1^{\tau}$ ,  $\hat{V}_0^{J1}$ ,  $\hat{V}_1^{J1}$ and  $\hat{V}_{w_0}$ .

#### F.2.1 Benchmarks for the three-body matrix elements

The three-body matrix elements for a zero-range potential are given in Eq.(E.15). For an Hartree-Fock state that describes the ground state of a spin saturated system, Ref. [44] shows that the expectation value of the three-body generator  $\hat{V}_{t_3}$  (see Eq.(E.1)) is equivalent to the expectation value of the two-body density dependent operator

$$\hat{V}_{dd} = (1 + x_3 \hat{P}^{\sigma}) \,\delta(\mathbf{r_1} - \mathbf{r_2}) \,\rho\left(\frac{\mathbf{r_1} + \mathbf{r_2}}{2}\right),\tag{F.5}$$

with the parameter  $x_3 = 1$  fixed <sup>2</sup>. We use this fact to benchmark the three-body matrix elements, namely

$$\langle \Phi(\lambda_{t_3}) | \hat{T} + \hat{V}_{SV} + \lambda_{t_3} \hat{V}_{t_3} | \Phi(\lambda_{t_3}) \rangle = T[\rho(\lambda_{t_3})] + V_{SV}[\rho(\lambda_{t_3})] + \lambda_{t_3} V_{dd}[\rho(\lambda_{t_3})].$$
(F.6)

We compare the results from the SCGF code Boccadorata [95], for the left-hand side, and the EDFs code HOSPHE [99], for the right-hand side. For testing purpose, we

<sup>&</sup>lt;sup>2</sup>We remind that  $\hat{V}_{t_3}$  and  $\hat{V}_{dd}$  are multiplied by the parameter  $t_3$ , respectively in the contributions to the three-body  $\delta$ -interaction and to the density-dependent potential.

select a model space limited to  $N_{max} = 5$  and energy  $\hbar \omega = 14$  MeV. The reduction to  $N_{max} = 5$  is necessary in order to have no truncation in the two particles basis  $N_{max}(2) = 10$  and in the three particles basis  $N_{max}(3) = 15$ . Otherwise the model space is limited to  $N_{max}(2) = N_{max}(3) = 16$  for larger single-particle model space,  $N_{max} > 5$ , due to memory limitations.

The agreement between the perturbed energies is at the order of the eV, proving the equivalence between the three-body zero-range interaction and the two-body density-dependent potential.

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