DEPARTMENT OF PHYSICS
UNIVERSITY OF JYVÄSKYLÄ
RESEARCH REPORT No. 10/2010

HIGHER-ORDER ENERGY DENSITY FUNCTIONALS IN NUCLEAR SELF-CONSISTENT THEORY

by

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Academic Dissertation
for the Degree of
Doctor of Philosophy

To be presented, by permission of the
Faculty of Mathematics and Science
of the University of Jyväskylä,
for public examination in Auditorium FYS1 of the
University of Jyväskylä on December 14, 2011
at 12 o'clock noon

Jyväskylä, Finland
December 2011

Preface

"...there is no scientific work which only one man can write", says Galileo Galilei in the 14th scene of Bertolt Brecht's *The life of Galileo*. He refers to his own work, the *Discorsi* [Gal38], that opened the era of the modern science, suggesting that any scientific activity can be really meaningful only when it is considered within a tradition, a community, a society. If this is true for the milestone works that marked the history of the physics, it is not less true for a doctoral dissertation.

The work presented in this thesis is not an isolated achievement, but it was carried out at the Department of Physics of the University of Jyväskylä during the years 2008-2011, within the Finland Distinguished Professor Programme (FIDIPRO) [FID07]. The project, having for its objectives advanced studies in theoretical nuclear structure physics and being linked with similar project of research worldwide [UNE], has been for me the ideal stepping stone to educate myself and get the necessary skills to enter more deeply in the fascinating field of the nuclear structure.

I would like to express my gratitude to Prof. Jacek Dobaczewski for supervising me, with competence and high professionalism, during this project. It has been said that the learning process is a tree whose roots are bitter and fruit sweet: now that I am very close to taste the fruit of my work, I understand how was important to have a stimulating and professional support to my studies.

There are many other people from whom I learnt. First of all, I would like to mention here the members of the FIDIPRO that influenced and supported me, sharing with generosity their ideas and skills: Gillis Carlsson, Markus Kortelainen, Nicholas Michel, Alessandro Pastore, Jussi Toivanen, Pekka Toivanen, Petr Vesely. All this people played an important role in completion of this work and their support in all situations, coffee breaks (espresso!) included, contributed to increase the enthusiasm for the topics of my research. Also the staff members of the department of physics at Jyväskylä university deserve a big thank, in particular several lecturers, such as Prof. Jouni Suhonen, Prof. Robert van Leeuwen, Dr. Kimmo Kainulainen, and Dr. Markku Lehto.

Finally, I wish to thank Alice, my family in Italy, and all my friends for their

encouragement during these years.

Jyväskylä, 2011 Francesco Raimondi

Abstract

In this thesis consisting of two publications and an overview part, a study of two aspects of energy density functionals has been performed.

Firstly, we have linked the next-to-next-to-next-to-leading order nuclear energy density functional to a zero-range pseudopotential that includes all possible terms up to sixth order in derivatives. Within the Hartree-Fock approximation, the quasi-local nuclear Energy Density Functional (EDF) has been calculated as the average energy obtained from the pseudopotential. The direct reference of the EDF to the pseudopotential acts as a constraint that allows for expressing the isovector coupling constants functional in terms of the isoscalar ones, or *vice versa*. The constraints implemented in this way imply a reduction by a factor of two of the number of the free coupling constants in the functional. Three main applications have been studied: we have considered the functional restricted by the Galilean symmetry, gauge symmetry, and again Galilean symmetry along with the spherical symmetry.

As second aspect concerning the next-to-next-to-next-to-leading order nuclear energy density functional, we analyzed conditions under which the continuity equation is valid for functionals or pseudopotentials built of higher-order derivatives. We derived constraints on the coupling constant of the energy density functional that guarantee the validity of the continuity equation in all spin-isospin channels. We also linked these constraints to local gauge symmetries for abelian and non-abelian groups.

Keywords: nuclear energy density functionals, pseudopotentials, continuity equation

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List of Publications

I F. Raimondi, B.G. Carlsson and J. Dobaczewski, *Effective pseudopotential for energy density functionals with higher-order derivatives*, Phys. Rev. C **83**, 054311 (2011)

II F. Raimondi, B.G. Carlsson, J. Dobaczewski and J. Toivanen, *Continuity equation and local gauge invariance for the N^3LO nuclear Energy Density Functionals*, arXiv:1110.3027v1 [nucl-th]

Both paper I and II are focused on some particular aspects concerning the nuclear EDF developed in Refs. [CDK08,CDT10]. The idea to proceed in the development of the nuclear N^3LO functional as the research project of the author's doctoral studies, by performing an analysis of the N^3LO pseudopotential (paper I) and continuity equation (paper II), have been suggested by the supervisor Prof. Jacek Dobaczewski. The supervisor and coauthors have also contributed in critical evaluation of the obtained results, from the early stage of the provisional results until the final results presented in both publications.

In paper I, the author has derived the two forms (central-like and tensor) of the N^3LO pseudopotential and listed all the significant terms, included the relation of conversion between the parameters of the zero- and second-order pseudopotential and those of the Skyrme interaction. The derivation concerning the time-reversal invariance and hermiticity of the pseudopotential has been carried out by the author, with an independent check by the supervisor. The author has derived the condition of invariance of the N^3LO pseudopotential under the gauge transformation, and calculated the corresponding relations defining the gauge-invariant pseudopotential. The entire analysis concerning the relations between the pseudopotential and the EDF, from the averaging of the pseudopotential over the uncorrelated wave function to the relations connecting the isoscalar and isovector parts of the functional, have been performed by the author, both for the Galilean and gauge invariance cases. The author has carried out the analogous analysis, performed for the case of assumed spherical, space-inversion, and time-reversal symmetries of the EDF. Gillis Carlsson has been a decisive guidance, with many practical pieces of advice, in implementing the symbolic programming.

In paper II, the theoretical link between the continuity equation and local gauge invariance of the potential energy density has been established by the supervisor and Gillis Carlsson. The author has extended this link for the special case of the N^3LO quasilocal functional, by deriving and implementing the general condition that the N^3LO potential must fulfill in order to obtain the continuity equations in the four spin and isospin channels. The author has then proceeded with the calculation of the constraints on the coupling constants of the functional, which verify the general condition derived for the N^3LO one-body pseudopotential. The constraints in the four channels have been calculated by the author with the use of symbolic programming. In this respect, Gillis Carlsson and Jussi Toivanen have been a precious guidance in solving some practical issues concerning the implementation of the codes.

Finally, in both publications the leading author's role is underlined by him being the first author, with broken alphabetical order.

Contents

Chapter 1

Introduction

The ongoing theoretical efforts in nuclear structure physics have all in common the main target to bridge the gap with the experiments, by improving the quality of description and predictability of the methods and approximations. In particular, significative progress in deriving nuclear properties in *ab initio* approach have been achieved for light nuclei, like for instance the no-core shell model (NCSM) [NQS09], and coupled cluster (CC) [HPD07, HDH07] methods. Due to the high degree of computational complications, these methods cannot be applied to heavy nuclei and nuclei far from stability in the nuclear chart. For these nuclei, the method applied is the energy density functional (EDF) approach [BHR03], which is based simultaneously, on physical insights concerning fundamental nuclear properties and on the phenomenological input of the optimization by experimental data.

In the recent years, a fruitful exchange of ideas and models with other many-body physics disciplines, like condensed matter physics, has opened new horizons of research for the low-energy nuclear structure. For instance, nuclear physicists have learnt and applied with success the tools of the well-established density functional theory (DFT).

DFT is a method to calculate the physical properties of many-electrons systems and it has been originally developed for calculations in quantum chemistry and condensed matter physics [DG90, PW94, FNM03]. As a general tool for the study of many-body systems, DFT has being extended and applied also to nuclear physics; more precisely, the idea that the self-consistent mean-field (SCMF) approaches in use in nuclear structure can be understood and further developed as nuclear DFT, is emerged in the last two decades [PS89, LRV04]. In fact, nuclei are quantum many-body systems and DFT is at the present theoretical and computational state-of-art the only method that can be applied

to all nuclides of the nuclear chart. The hope to repeat in nuclear physics the spectacular achievements of the condensed-matter DFT is driving currently an intense effort of studies and projects worldwide [UNE, FID07]. The challenge is in principle well defined, namely the search of the universal energy density functional, and the quest for a spectroscopic quality in the description of nuclear properties [ZDS08]. The new functional [CDK08] studied in the present work takes a step forward in this search. In fact, the expansion in higher-order derivatives of densities provides an extension of the standard Skyrme functionals, which still require an improvement as it has been recently remarked, for instance in the context of the optimizations of the model parameters [KRB09].

Moreover, DFT is a tool of choice for the low-energy nuclear structure calculations because it is a method able to treat many-body system with a reduced computational effort, as compared to the direct solution of the Schrödinger equation, which in nuclear physics is a partial differential equation of 3N spatial variables, N spin variables and N isospin variables, with N nucleons in the nucleus. Among the many possible ways to circumvent the task of the direct solution of the Schrödinger equation, DFT is a method based on the definition of the ground-state energy of the system as value of a functional of the density. The idea of the energy as a functional of the density instead of the computationally expensive wave function is one of the key point of DFT. This implies that the variational principle used to find the ground-state energy for the system is performed by taking the density, an observable, as the variational parameter.

The path towards applications of the universal EDF in practical calculations is marked by three main stages:

I Basic derivations and studying of the theoretical features of the functional.

II Implementation of numerical codes.

III Optimization of the coupling constants of the functional by experimental data.

The present work aims at giving a contribution to the first point of the list above, for a particular approximation of the EDF, that is the functional obtained as an expansion of the nuclear energy density in higher-order derivatives of densities. For such a functional a numerical code is already available [CDT10], and adjustment of coupling constants is currently in progress [FID07].

Chapter 2

Nuclear Energy Density Functional

In the following two sections we will give a general outline of the DFT, focusing, in particular, on some issues and problems related to the applicability of DFT to nuclei. In fact, the nucleus, unlike a system of electrons bound to the lattice of nuclei, is a finite self-bound system which does not require the presence of a real external potential in order to be bound. This simple fact implies a conceptual problem also in the application of the Hohenberg-Kohn (HK) theorem to nuclear systems.

2.0.1 Basic concepts of DFT

The HK theorem [HK64] is at the heart of the DFT and traditionally introduced as the first step in any DFT primer. Because of the HK theorem, the DFT can be regarded as a stronger version of the traditional mean-field approach. In fact, if the general mean-field approach aims at calculating the energy of a many-particle system from the knowledge of the two-particle density matrix, the DFT aims at calculating the ground-state energy from the ground-state density.

The HK theorem states that there exists an energy functional of the density $\rho(\boldsymbol{r})$ that we write as,

$$E_v[\rho] = F_{HK}[\rho] + \int d\mathbf{r}\, v_{ext}(\mathbf{r})\rho(\mathbf{r}) \;, \tag{2.1}$$

which has a minimum at the ground-state energy of the system with the cor-

responding ground-state density.

The interesting feature of Eq. (2.1) is the fact that the functional is split in a part depending on $\hat{v}_{ext}$, the external potential acting on the many-particle system, and a part denoted with F_{HK}, the so called HK functional. F_{HK} depends on the kinetic energy operator $\hat{T}$ and interparticle interaction $\hat{V}$, which is the coulombic force in the electronic systems and full nucleon-nucleon interaction in nuclear case. The HK functional is defined as an expectation value over the many-body wave function,

$$F_{HK}[\rho] = \langle \Psi[\rho] | \hat{T} + \hat{V} | \Psi[\rho] \rangle, \tag{2.2}$$

and is universal in the sense that is common to all the systems sharing the same interparticle interaction, no matter how is the external potential.

Eq. (2.1), with the fact that the energy is a functional of the density and at the same time labeled by the external potential $v_{ext}(\mathbf{r})$, is in fact a direct corollary of the HK theorem. Its deep content is that the map between the set of the external potentials $v_{ext}(\mathbf{r})$ and the ground-state densities ρ_0 is a one-to-one correspondence, namely is invertible. Then of course, the existence of a link between the energy and the external potential is given by the simple fact of the Schrödinger equation.

The practical use of the HK theorem comes into play with the application of the variational principle. In fact, the ground-state density ρ_0 can be obtained by minimizing the functional E_v over all the set of densities, for a chosen external potential $\hat{v}_{ext}$. The procedure of minimization for the ground-state energy E_0 and the ground state density ρ_0 is justified by the obvious observation that,

$$E_v[\rho] = \langle \Psi[\rho] | \hat{T} + \hat{V} + \hat{v}_{ext} | \Psi[\rho] \rangle > E_0 \quad \text{if} \quad \rho \neq \rho_0. \tag{2.3}$$

Then, the minimum of the energy is obtained for the density that satisfies,

$$\frac{\delta E_{v_0}[\rho]}{\delta \rho} = 0, \tag{2.4}$$

for a fixed potential v_0.

The Kohn-Sham (KS) construction [KS65] is the second pillar of DFT, and it is based on the observation that the general result of the HK theorem does not make any assumption on the form of the interparticle potential $\hat{V}$. Then, the theorem is also valid for a non-interacting system. Despite being unrealistic, a non-interacting system can be adopted as auxiliary system, where an external potential $v_{KS}([\rho], \mathbf{r})$ leads to the same ground-state density of the interacting system with the original external potential $\hat{v}_{ext}$. Here, the fact that two different potentials produce the same density does not imply a violation of the HK

theorem, given that we are dealing with two different systems, the interacting and the non-interacting one. The non-interacting KS system is governed by the KS Hamiltonian

$$\hat{H}_{KS} = \hat{T} + \hat{v}_{KS}([\rho]), \tag{2.5}$$

while the ground-state wave function can be represented as a Slater determinant, which in turn allows to express the KS equation as single-particle equations,

$$\left(-\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + v_{KS}([\rho], \mathbf{r})\right) \phi_i(\mathbf{r}) = \varepsilon_{\mathbf{i}} \phi_{\mathbf{i}}(\mathbf{r}), \tag{2.6}$$

and the density by

$$\rho(\mathbf{r}) = \sum_{\mathbf{i=1}}^{\mathbf{A}} |\phi_{\mathbf{i}}(\mathbf{r})|^{\mathbf{2}}. \tag{2.7}$$

By simple inspection of Eq. (2.6) we see that the KS problem has a self-consistent nature, because the functional $v_{KS}([\rho], \mathbf{r})$ is implicitly defined by the KS solution of Eq. (2.6) through definition (2.7). The standard implementation to solve the equations is then by iterating until convergence is reached.

We notice here that the key point of the solution to self-consistency is to choose a good approximation of the functional $v_{KS}([\rho], \mathbf{r})$ in Eq. (2.6). In our work we are just going to give a contribution to the search of such a functional, by studying some features of one possible approximation of the EDF in nuclear physics.

2.0.2 Nuclear DFT

Our discussion about the nuclear DFT is mainly referring to one possible class of the nuclear functionals, the class of local or quasilocal functionals, whose general form can be given as

$$\begin{aligned} E[\rho_i, \tau_i, \ldots] &= \int d\mathbf{r}\, \mathcal{E}(\rho_i(\mathbf{r}), \tau_{\mathbf{i}}(\mathbf{r}), \ldots) \\ &= \int d\mathbf{r}\, \mathcal{H}_E(\mathbf{r}), \end{aligned} \tag{2.8}$$

where the energy density $\mathcal{H}_E(\mathbf{r})$ depends on local densities built with derivatives acting on nonlocal densities. The full set of definitions of such a densities for the Skyrme EDF can be found for instance in Ref. [PRD04].

This form, which is not the most general one, can be derived from a nonlocal density functional through the density matrix expansion (DME) method (see Sec. 2.1.2). It is widely used in the current nuclear EDF theories [PRD04, CDK08, CDT10] and the functional we use in our work is an extended version

of the form in Eq. (2.8). The reasons of the success of this form lie both in availability of computational codes for mean-field calculations [SDM11], which can be adapted easily to the local functionals, and in strong physical insights that we are going to discuss below.

Now we show how the form of functional (2.8) can be guessed by requiring that some physical features are included in it. The minimal requisite for an universal EDF, where universal means applicable to a system with any number of nucleons, is that it must be a scalar and real function of the local density. In view of the application of a constrained variational principle, one can fix the number of particles through the introduction of the chemical potential λ and gets,

$$E'[\rho(\mathbf{r})] = E[\rho(\mathbf{r})] - \lambda \int d\mathbf{r}\rho(\mathbf{r}). \tag{2.9}$$

In order to get the single-particle picture according to the KS scheme and be able to describe shell effects, we have to include the local kinetic density,

$$\tau(\mathbf{r}) = \left[(\boldsymbol{\nabla} \cdot \boldsymbol{\nabla}')\rho(\mathbf{r}, \mathbf{r}')\right]_{\mathbf{r}=\mathbf{r}'}, \tag{2.10}$$

and we get,

$$E[\rho(\mathbf{r}), \tau(\mathbf{r})] = \frac{\hbar^2}{2m} \int d\mathbf{r}\tau(\mathbf{r}) + \mathcal{H}[\rho(\mathbf{r})], \tag{2.11}$$

where $\mathcal{H}[\rho(\mathbf{r})]$ denotes the potential part of the energy functional $E[\rho_i, \tau_i]$ in Eq. (2.8).

To include in the description the effects due to the effective-mass, surface, spin-orbit coupling and other higher-order effects we may add dependence on the gradients of the density and spin density, namely

$$E[\rho(\mathbf{r}), \tau(\mathbf{r}), \bigtriangledown\rho(\mathbf{r}), J(\mathbf{r}), \ldots] = \frac{\hbar^2}{2m} \int d\mathbf{r}\tau(\mathbf{r}) + \mathcal{H}[\rho(\mathbf{r}), \bigtriangledown\rho(\mathbf{r}), J(\mathbf{r}), \ldots]. \tag{2.12}$$

If we decide to include time-odd densities describing the time-odds effects, we have the full-fledged quasilocal EDF of the kind in Eq. (2.8), which is a generalization of the Skyrme functional. Such a generalized functional aims to make a larger inclusion of the possible physics in a model independent picture, which is typical of the effective field theories.

The EDF's of the kind in Eq. (2.8) constructed as a functional of different local densities and currents, like for instance the extension proposed in [CDK08], can be compared with the KS scheme in many aspects, like for instance the single-particle approximation or the solution to self-consistency. But we should

not forget the presence of conceptual differences between the KS scheme and the local nuclear EDF. These differences are such that the eventual conversion of the traditional SCMF approaches into a well-established "nuclear DFT" is still an on-going process. We present here one of these conceptual differences, concerning the role of symmetries and the meaning of the HK theorem for self-bound systems like nuclei.

The problem of the broken symmetries in the nuclear EDF originates from the fact that nuclei unlike the electron system, are self-bound systems. Due to the nucleon-nucleon net attractive interaction, nuclei do not need any external potential to be bound, as the potential given by the static atomic lattice in the Born-Oppenheimer approximation of the Coulomb DFT. This means that the 'true' many-body wave function of a self-bound finite system in the ground state must obey the translational and rotational invariance. The fact that such symmetries are broken in the SCMF calculations is well-known and different techniques to restore such a symmetries beyond the mean field can be applied, like for instance the transformation to an intrinsic system and the projection techniques. But, if this works pretty well from the practical point of view, a delicate *caveat* arises for the application of the HK theorem to the nuclear systems: in fact the HK theorem states the existence of a universal functional of the laboratory density, which must be equipped with all the required symmetries, whereas in the nuclear SCMF we ended up with a intrinsic density which can be plagued by the spurious coupling with the center-of-mass motion, as it turns out in the HF case. Of course one can apply all the machinery of the restoration of the symmetries, but such an approach is working with the N-body wave function, instead of the density. The necessity of the extension of the HK theorem and KS procedure to self-bound systems in a consistent theoretical fashion has then been claimed first in [E07]. Here we refer to a recent solution to this problem, without entering in details that can be found in [MBS09].

First of all, by using the Jacobi coordinates ξ_α ($\alpha = 1, ..., N-1$) one can separate the general, translationally invariant, N-body Hamiltonian into one-body operator acting in the space of the total center of mass $\mathbf{R}$ and $(N-1)$-body operator in ξ_α space,

$$-\frac{\hbar^2}{2M}\Delta_{\mathbf{R}}\Gamma(\mathbf{R}) = E_{CM}\Gamma(\mathbf{R})\,, \tag{2.13}$$

$$\sum_{\alpha=1}^{N-1}\frac{\tau_\alpha^2}{2\mu_\alpha} + u(\{\xi_\alpha\})\psi_{int} = E_{int}\psi_{int}\,, \tag{2.14}$$

where τ_α denotes the conjugate momentum of ξ_α and the corresponding reduced mass is $\mu_\alpha = m\frac{\alpha}{\alpha+1}$.

Now, the density produced by the wave function $\Gamma(\mathbf{R})$ describing the motion of the center of mass of the system cannot be a good candidate as the density

of the HK theorem, even though is the one relative to the laboratory frame. The reason is easy to understand, being $\Gamma(\mathbf{R})$ a solution of a free Schrödinger equation and therefore delocalized in the space. On the other hand, the intrinsic density relative to the bound state ψ_{int} does not require necessarily any external one-body potential. In order to facilitate the formulation of the HK theorem, an auxiliary external potential is introduced in the center-of-mass frame as $\sum_{i=1}^{N} v_{aux}(\mathbf{r}_i - \mathbf{R})$. The contribution of this auxiliary potential to the internal energy must be taken into account in the following way,

$$\begin{aligned} E_{int} &\rightarrow E_{int} + \langle \psi_{int} | v_{aux}(\{\xi_\alpha\}) | \psi_{int} \rangle \\ &\rightarrow E_{int} + \int d\mathbf{r}\, v_{aux}(\mathbf{r}) \rho_{int}(\mathbf{r})\,. \end{aligned} \tag{2.15}$$

The internal energy E_{int} in the last equation is just the functional whose density can be mapped to the set of arbitrary v_{aux}'s according to the HK theorem. The only extra-caution one should take here is the fact that ψ_{int} must be by definition a bound state, in order to guarantee the conclusion of the theorem also when the limit $v_{aux} \rightarrow 0$ is taken. In this approach the KS scheme can be recovered in the traditional way, with the single particle KS equations depending on the Hartree and exchange-correlation potentials. The main difference with respect to the Coulomb KS scheme is given by the inclusion of the center of mass correlations besides to the other correlations which are neglected in the Hartree term.

2.1 Phenomenological approach to the nuclear EDF

The application of the effective field theories (EFTs) [L97, P02] is quite recent in the study of the properties of nuclear systems, even though the use of the phenomenological effective forces in the microscopic description of the nucleus has been a standard approach, widely used since more than fifty years and anticipating some aspects of the EFT approach.

The long-standing search for the "true" nuclear interaction is a privileged point of view to give an account of the influence of the EFT's ideas in nuclear physics [D02]. A line of research for the nuclear interaction, started by Yukawa [Y35], was devoted to the description of the nuclear force in terms of the pions degrees of freedom. The one-pion-exchange model was able to describe the attractive long-range of the nuclear force and later the larger mass mesons ρ and ω were included successfully in this picture to explain the medium-range part of the force. In this story, the further inclusion of the short-range part through the particle-exchange model was never fully accomplished and the reason of this is probably an intrinsic theoretical limit of this approach: in fact,

when two nucleons are interacting at very small distances, let us say less than 0.5 fm, many effects like strong color-polarization of the nucleons and Pauli blocking effect of the nucleons wave functions, come into play preventing the idea of two nucleons interacting *via* exchanging physical particles to be applied. The main point is that up to now, there is no a complete theoretical explanation of the behavior of the nucleons when they interact at very high-energy regime. The use of phenomenological parametrizations to mimic the unknown short-range part of the force, or also both the medium- and short-range part as in Argonne v_{18} interaction [WSS95], was seen as an acceptable compromise able to include practically the effects of the short-range physics into the description of the low-energy nucleon-nucleon scattering and structure of nuclei.

A recent "change in attitude" in considering the epistemological meaning of the Standard model (SM) in particle physics, has changed substantially among the practitioners the way to consider the so-called empirical or phenomenological approach [C02]. The SM in its infancy, during 1970s, was considered the fundamental theory of the matter and nongravitational interactions, as well as the great accomplishment of the reductionism in natural science. Afterwards, when the program of reduction of all the interactions into the SM framework was stuck for many years, new positions about what must be considered as physically fundamental have been emerged. The first one, still reductionist, claims the SM and general relativity are both effective theories of an underlying "theory of everything"; the second one is the view that scientific theories form a never-ending tower of EFTs in such a way that it does not really make sense to postulate something like the ultimate theory. In this perspective, an effective theory is qualified as emergent, namely it is not reduced to the degrees of freedom of the high-energy theory, while a different dynamics, driven by a new mechanism as the spontaneous symmetry breaking, brings novelty to the theoretical description. Aside from the epistemological issues, the concept of effective theory has become the relevant framework for low-energy theories like the nuclear SCMF theory that we are discussing.

We give a list of the main features of a general EFT. This is here understood as low-energy approximation where the effects of an arbitrary high-energy physics are included in the theory, without the need of the details of the unknown high-energy physics.

The key concepts of EFT can be listed as in the following [L97, D02]:

1. The idea of separation of scale, which is important for its theoretical meaning and its practical use as well. For instance, the local density approximation (LDA) assumed in the expansion of Eq. (2.8) or (2.16) consists in the fact that the dependence of the energy density on the one-body density matrix can be approximated by a dependence on the local density and its derivatives. Such an approximation is based on the obser-

vation that the most important part of the density matrix influencing the energy is the local part. This approximation, practically implemented in the DME approach, is possible because in the low-energy phenomena the spatial structure of the density matrix is not resolved and a local Taylor expansion can mimic the dependence to the density matrix. DME is just one possible method which works in the spirit of the EFT exploiting the separation of scale in energy, but other approaches are possible. We mention here the EFT for nuclear interactions based on the chiral perturbation theory, where an effective low-energy force is built starting from a chirally symmetric version of the QCD Lagrangian which contains pions as the basic degrees of freedom of the theory [ME11]. Also in this case the assumption of separation between the soft and hard scales is operating when the high-energy contributions to the process are "integrated out" and reabsorbed in the coupling constants of the effective Lagrangian contacts terms.

2. Strictly connected to the separation of scale, it is the choice of the relevant degrees of freedom that must be considered as building blocks for the energy density or the interaction. In particular for the DME method, the nonlocal objects like the one-body density matrix are removed from the functional and only local densities are considered as the relevant degrees of freedom. Nevertheless the nonlocal effects are taken into account in the local approximation by introducing auxiliary functions, which convey some informations relative to the nonlocal interaction, as we see in more detail in Sec. 2.1.2.

3. The effective interactions (or functionals) as expansions of contact terms mimicking the short-range physics. The operators in the contact terms of the EFT are equipped by numerical coupling constants, which are fitted to reproduce low-energy data. So, the coupling constants are theory-specific, in the sense that they carry the informations concerning the high-energy physics, while the local contact operators are model-independent. This means that the details of the high-energy physics are not only unknown but not necessary if the task is to study a low-energy behavior of a system. In this sense there is nothing like the "only true" effective interaction, but different EFT's can reproduce equally well the low-energy data set through which the coupling constants have been fitted.

4. The freedom in the choice of the effective interaction has a limit in the respect of the fundamental symmetries of the theory. One of the guiding principle of the expansion of the effective interaction that we introduce in Eqs. (3.1) and (3.2) is the restriction of all possible terms by symmetries. The symmetries assumed were of course the ones that are known to pertain globally to nuclear force, independently of the short-, medium- or long-range considered.

5. A point often misunderstood is the role of the higher-order terms in the expansion of the effective interaction. We stress the fact that by introducing higher-order terms we are not approaching at all the correct form of the true potential. More terms in the expansion means in principle a better reproduction of the experimental data of the low-energy phenomena. But these data modeling our effective interaction does contain just the short-range effects on the low-energy phenomena and not the short-range physics in general. Our effective theory cannot, by principle, converge to the exact form of the nuclear interaction.

6. A last key idea of the EFT that we wish just briefly mention is the power counting scheme. Technically the power counting is a procedure to determine the power of the expansion parameter, namely the ratio between the soft and the hard scale, for a given contribution (a Feynman diagram) to the calculation of an observable. For the effective functional in Eq. (2.16) a power counting scheme would provide a proper cut-off scale, against which the powers of derivatives could be estimated. However, such a scheme, as it has been introduced in the chiral perturbation theory, is not yet available. The use of derivatives of the regularized zero-range interactions, with the Gaussian interaction as regularized delta force, leads (through the exchange term) to non-local functionals [DG80], which involve an high degree of numerical complication. For this reason, a procedure of regularization has not yet been tried.

2.1.1 N^{3}LO nuclear EDF

As example of nuclear phenomenological EDF, we present here the functional built in terms of derivatives of densities up to N^{3}LO introduced in [CDK08]. In order to construct this EDF, the strategies proper for effective theories described in the previous section, have been applied. In particular, the choice of the appropriate degrees of freedom, the one-body density matrix, and the building of the energy density restricted by imposing the invariance with respect to selected symmetries. What has been obtained by applying such a construction, is a specific implementation and extension of the quasilocal functional we presented in Eq. (2.8).

The total energy density in this case reads (isospin degree of freedom included),

$$\mathcal{H}(\boldsymbol{r}) = \sum_{\substack{n'L'v'J',t \\ mI,nLvJ,J'}} C^{n'L'v'J',t}_{mI,nLvJ} T^{n'L'v'J',t}_{mI,nLvJ}(\boldsymbol{r}), \tag{2.16}$$

where $C^{n'L'v'J',t}_{mI,nLvJ}$ are coupling constants in front of the terms whose form is,

$$T^{n'L'v'J',t}_{mI,nLvJ} = \left[\left[\rho^t_{n'L'v'J'}(\boldsymbol{r}) \left[D_{mI} \rho^t_{nLvJ}(\boldsymbol{r}) \right]_{J'} \right]_0 \right]^0 . \tag{2.17}$$

The description of the term in Eq. (2.17) gives us the chance to start introducing the definitions of the building blocks that we are going to use in our work. The local densities $\rho^t_{nLvJ}(\boldsymbol{r})$ depends on the four indices $nLvJ$ and they are defined as,

$$\rho^t_{nLvJ}(\boldsymbol{r}) = \left\{[K_{nL}\rho^t_v(\boldsymbol{r},\boldsymbol{r}')]_J\right\}_{\boldsymbol{r}'=\boldsymbol{r}}. \tag{2.18}$$

The local densities in Eq. (2.18) are composed by the nth-order and rank-L relative derivative operator K_{nL} acting on the scalar ($v = 0$) or vector ($v = 1$) nonlocal density, and ranks L and v are then vector coupled to J. The index t specifies the isospin channel of the density, that is isoscalar for $t = 0$ and isovector for $t = 1$. The coupling of a derivatives operator with a local density is named secondary density,

$$\rho^t_{mI,nLvJ,Q}(\boldsymbol{r}) = \left[D_{mI}\rho^t_{nLvJ}(\boldsymbol{r})\right]_Q. \tag{2.19}$$

The energy density in Eq. (2.16) is expressed in the language of the spherical tensors and this implies a difference in the definition of the isovector terms when compared to the Cartesian representation. In the latter, the isovector terms depend on products of differences of neutron and proton densities, whereas in the spherical representation the isovector channel involves the coupling of two isovectors to a scalar, which brings a Clebsch-Gordan coefficient of $\left(\sqrt{3}\right)^{-1}$. For this reason, the isovector coupling constants for the spherical representation are by the factor of $\left(\sqrt{3}\right)$ *larger* than those for the Cartesian representation.

The possible terms entering in energy density (2.16) are selected according to the invariance with respect to the time-reversal symmetry and the covariance with respect to space inversion and rotation, as we are going to describe in the following. When a derivation of the functional from the interaction is not explicitly considered as in Ref. [CDK08], the functional must be explicitly built equipped with all the symmetry of the nuclear interaction. In this respect, two approaches are possible and both of them have been used in order to treat the symmetries of the higher-order in derivatives EDF. They are referred as "derivation after separation of symmetries" and "derivation before separation of symmetries" respectively.

The "derivation after separation of symmetries" is applied when there are not any symmetry-breaking terms of the local densities in the energy density, because they are previously removed through an analysis of the transformation properties of the one-body density matrix under the symmetry group; in the "derivation before the separation of symmetries" the symmetry-breaking terms of the local densities are allowed to be in the energy density, while the resulting EDF is anyway invariant for the reasons that we explain in the following. In the standard derivation of the Skyrme EDF [PRD04] the time-reversal and isospin symmetries are treated in the "derivation after separation of symmetries" approach, while the space symmetries like space inversion or rotation are treated within the "derivation before the separation of symmetries" approach.

We take the time-reversal symmetry as first illustrative example. For sake of simplicity, we do not consider here the isospin degree of freedom. However, as it is shown in Ref. [EBG75, PRD04], the rules of constructing the particle-hole energy density with proton-neutron mixing are identical to those valid in the case of no proton-neutron mixing. According to the transformation properties of the many-body wavefunction under the time-reversal transformation T, the non local densities,

$$\rho\left(\vec{r},\vec{r}'\right) = \sum_{\sigma}\rho\left(\vec{r}\sigma,\vec{r}'\sigma\right), \tag{2.20}$$

$$\vec{s}\left(\vec{r},\vec{r}'\right) = \sum_{\sigma\sigma'}\rho\left(\vec{r}\sigma,\vec{r}'\sigma'\right)\left\langle\sigma'\left|\vec{\sigma}\right|\sigma\right\rangle, \tag{2.21}$$

can be separated into the time-even and time-odd parts,

$$\rho(\vec{r},\vec{r}') = \rho_{+}(\vec{r},\vec{r}')+\rho_{-}(\vec{r},\vec{r}'), \tag{2.22}$$

$$\vec{s}(\vec{r},\vec{r}') = \vec{s}_{+}(\vec{r},\vec{r}')+\vec{s}_{-}(\vec{r},\vec{r}'), \tag{2.23}$$

where

$$\rho_{\pm}(\vec{r},\vec{r}') = \tfrac{1}{2}\left[\rho(\vec{r},\vec{r}')\pm\rho^{T}(\vec{r},\vec{r}')\right], \tag{2.24}$$

$$\vec{s}_{\pm}(\vec{r},\vec{r}') = \tfrac{1}{2}\left[\vec{s}(\vec{r},\vec{r}')\pm\vec{s}^{T}(\vec{r},\vec{r}')\right], \tag{2.25}$$

such that

$$\rho^{T}_{\pm}(\vec{r},\vec{r}') = \pm\rho_{\pm}(\vec{r},\vec{r}'), \tag{2.26}$$

$$\vec{s}^{T}_{\pm}(\vec{r},\vec{r}') = \pm\vec{s}_{\pm}(\vec{r},\vec{r}'). \tag{2.27}$$

Given that the nuclear interaction is time-reversal symmetric, the derived HF energy density will be composed only by squares of time-even and time-odd densities of Eqs. (2.24)–(2.25). Consequently, the energy density itself is time-even because there are not bilinear terms with opposite time-reversal phases. For the N^{3}LO EDF, we have in fact that

$$\begin{array}{rclcl}\rho^{T}(\vec{r},\vec{r}') & = & \rho^{*}(\vec{r},\vec{r}') & = & \rho(\vec{r}',\vec{r}),\\ \vec{s}^{T}(\vec{r},\vec{r}') & = & -\vec{s}^{*}(\vec{r},\vec{r}') & = & -\vec{s}(\vec{r}',\vec{r}).\end{array} \tag{2.28}$$

The nonlocal densities in Eqs. (2.28) must be coupled with the derivative operators K_{nL}, which are imaginary and antisymmetric with respect to exchanging variables $\vec{r}$ and $\vec{r}'$, that is the operation that performs the time inversion of the relative momentum in the coordinate representation. As consequence, the total parity of the scalar coupling of two primary densities $\rho_{nLvJ}(\vec{r})$ must fulfill,

$$(-1)^{n+v+n'+v'} = 1. \tag{2.29}$$

As example of derivation before the separation of symmetries we give the one for the space-inversion symmetry. In this case we see that the invariance of

the energy density with respect to the symmetry transformation is not a necessary condition for the invariance of the EDF, but it is enough to assume the covariance with the symmetry S of the energy density, that is,

$$\mathcal{H}^S(\vec{r}) = \mathcal{H}(S^+\vec{r}S), \tag{2.30}$$

where $S^+\vec{r}S$ denotes the space point transformed by the symmetry S.

The general covariance condition in Eq. (2.30) together with the space invariance of the integrals are together sufficient conditions to guarantee the invariance of the EDF, regardless of the symmetry properties of the many-body states of the nonlocal densities entering in the energy density. So, the covariance condition for the space-inversion symmetry is obtained from the parity $(-1)^{n+m}$ of the tensors, appearing in the definitions of the secondary density $\rho_{mI,nLvJ,Q}(\vec{r})$. The parity-covariant energy density will be then constructed by coupling together densities that fulfill the condition,

$$(-1)^{n'+n+m} = 1. \tag{2.31}$$

2.1.2 Nuclear EDF based on DME expansion

Density matrix expansion (DME) is a convenient procedure to derive quasilocal density functionals from an expansion of the nonlocal expression of the one-body density matrix, which is the key ingredients in the Hartree-Fock calculations. The DME was introduced in two seminal papers by Negele and Vautherin [NV72, NV75], who showed how to link the computationally simple results based on a phenomenological force, the Skyrme interaction, to the more fundamental mean-field calculations based on realistic nucleon-nucleon interactions. Recently, there has been a renewed interest for DME [DCK10, CD10, GDB10], also in connection with the attempts to derive EDFs from first principles [DFP10, BFS10, SKB10].

The DME gives a positive response to the question about the opportunity of approximating finite-range interactions with quasilocal density functionals. In fact, as we explained before, DFT is based on the local density but the interaction energy obtained from a local interaction, reads

$$\mathcal{E}^{int} = \frac{1}{2}\int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \hat{V}(\mathbf{r}_1,\mathbf{r}_2)(\rho(\mathbf{r}_1)\rho(\mathbf{r}_2) - \rho(\mathbf{r}_2,\mathbf{r}_1)\rho(\mathbf{r}_1,\mathbf{r}_2)), \tag{2.32}$$

where we did not consider spin and isospin indices for sake of simplicity.

The interaction energy in Eq. (2.32) is local in the first term, the direct term, whereas it is nonlocal in the second term, the exchange one, being dependent on the square of the nonlocal density $\rho(\mathbf{r}_1,\mathbf{r}_2)$. This question is strictly related

to the following one: to what extent a local contact interaction, as the Skyrme interaction or the extension in order of derivatives we proposed in paper I, can be a good approximation of a general local finite-range interaction? The expression of the energy in Eq. (2.32) is in fact the result of the averaging over the many-body wavefunction of the local interaction,

$$\hat{V}(\mathbf{r'}_1, \mathbf{r'}_2; \mathbf{r}_1, \mathbf{r}_2) = \hat{V}(\mathbf{r}_1, \mathbf{r}_2)\delta(\mathbf{r'}_1 - \mathbf{r}_1)\delta(\mathbf{r'}_2 - \mathbf{r}_2), \tag{2.33}$$

whereas the quasilocal form of the functional in Eq. (2.16) can be directly calculated by averaging over the many-body wavefunction the zero-range pseudopotential, which is introduced and study in the Chapter 3 and that has the general form,

$$\hat{V}(\mathbf{r'}_1, \mathbf{r'}_2; \mathbf{r}_1, \mathbf{r}_2) = \hat{V}(\mathbf{r}_1, \mathbf{r}_2)\hat{\delta}_{12}(\boldsymbol{r}'_1\boldsymbol{r}'_2, \boldsymbol{r}_1\boldsymbol{r}_2), \tag{2.34}$$

where we introduced the Dirac delta function,

$$\begin{aligned} \hat{\delta}_{12}(\boldsymbol{r}'_1\boldsymbol{r}'_2, \boldsymbol{r}_1\boldsymbol{r}_2) &= \delta(\boldsymbol{r}'_1-\boldsymbol{r}_1)\delta(\boldsymbol{r}'_2-\boldsymbol{r}_2)\delta(\boldsymbol{r}_1-\boldsymbol{r}_2) \\ &= \delta(\boldsymbol{r}'_1-\boldsymbol{r}_2)\delta(\boldsymbol{r}'_2-\boldsymbol{r}_1)\delta(\boldsymbol{r}_2-\boldsymbol{r}_1), \end{aligned} \tag{2.35}$$

which ensures the locality and zero-range character of the pseudopotential.

As approximation, the DME exploits two important features of the nuclear physics at low-energy scale: first, it relies on the fact that the nuclear interaction is short-range, which guarantees the possibility to map nonlocal expressions of the functional into quasilocal EDF's; second, for the low-energy nuclear physics, the separation between the energy scale of the phenomena and the energy scale of the short-range of the interaction, which allows the introduction of the LDA in dealing with the one-body density matrix. In this respect, the DME is an application of the key ideas of the EFT exposed in the previous section. In particular the content of information pertaining to the nonlocal interaction is only partially conveyed to the EDF through the calculations of the coupling constants of the functional itself.

By way of illustration, we survey the main step of the DME procedure applied to the exchange interaction energy in Ref. [DCK10], where an improved version of the Negele-Vautherin DME has been introduced and applied to the Gogny force [G75, DG80]. First of all, the one-body density matrix in the exchange term of Eq. (2.32), once expressed in the total ($\mathbf{R}$) and relative ($\mathbf{r}$) coordinates and derivatives, can be expanded with respect to the variable $\mathbf{r}$,

$$\begin{aligned} \rho(\mathbf{r}_1, \mathbf{r}_2) &= \rho(\mathbf{R}, \mathbf{r}) \\ &= \pi_0(r)\rho(\mathbf{R}) + i\pi_1(r)r_a j_a(\mathbf{R})\rho(\mathbf{R}) \\ &+ \frac{1}{2}\pi_2(r)r_a r_b \left[\frac{1}{4}\nabla_a\nabla_b\rho(\mathbf{R}) - \tau_{ab}(\mathbf{R})\right] + \dots. \end{aligned} \tag{2.36}$$

The expansion is performed in the local direction or, in other words, the relative coordinate derivatives ∂_i are always calculated at $r_i = 0$. This is enough because the density varies in the nonlocal direction at the same scale as it does in the local direction, as one could analytically check for the one-body density matrix in the infinite matter. In Eq. (2.36) the one-body density matrix is expressed through the current and kinetic densities,

$$j_a(\mathbf{R}) = \frac{1}{i}\partial_a \rho(\mathbf{R},\mathbf{r})_{r=0}, \tag{2.37}$$

$$\tau_{ab}(\mathbf{R}) = \nabla_a^{(1)}\nabla_b^{(2)}\rho(\mathbf{r}_1,\mathbf{r}_2)_{\mathbf{r}_1=\mathbf{r}_2}, \tag{2.38}$$

whereas the three auxiliary functions $\pi_0(r)$, $\pi_1(r)$ and $\pi_2(r)$ vanish at large r and are introduced to guarantee the correct asymptotic behavior of the expansion (2.36). Moreover, the auxiliary functions must be defined in such a way that expansion (2.36) be compatible with the Taylor expansion of $\rho(\mathbf{R},\mathbf{r})$, then the following condition must hold,

$$\pi_0(0) = \pi_1(0) = \pi_2(0) = 1, \quad \pi_0'(0) = \pi_1'(0) = 0, \quad \text{and} \quad \pi_0''(0) = 0. \tag{2.39}$$

In the definition of functions $\pi_i(r)$ is encoded the kind of LDA applied to the one-body density matrix: usually LDA is practically implemented through a dependence with respect to the Fermi momentum k_F, which sets the scale at which the density matrix varies. This dependence amounts to a dependence on the local density $\rho(\mathbf{R})$, when the LDA respect to the nuclear infinite matter is adopted. The explicit definitions of the $\pi_i(r)$ functions read,

$$\pi_0(r) = \frac{6j_1(k_F r) + 21 j_3(k_F r)}{2k_F r} \quad \text{and} \quad \pi_2(r) = \frac{105 j_3(k_F r)}{(k_F r)^3}, \tag{2.40}$$

where $j_n(k_F r)$ are the spherical Bessel functions. A supplementary condition, required by the local gauge invariance of the energy, defines the $\pi_1(r)$ function as,

$$\pi_1^2(r) = \pi_0(r)\pi_2(r). \tag{2.41}$$

Alternatively, the auxiliary functions can be calculated *a posteriori*, to reproduce in an approximate way the given density matrix $\rho(\boldsymbol{R},\boldsymbol{r})$.

By calculating the product of nonlocal densities $\rho(\mathbf{r}_2,\mathbf{r}_1)\rho(\mathbf{r}_1,\mathbf{r}_2)$ and plugging it into the exchange part of Eq. (2.32), one finally gets the exchange interaction energy within the quasilocal approximation (up to second order),

$$\varepsilon_{exc}^{int} = -\int d^3\mathbf{R}\frac{1}{2}\left[V_{\pi 0}^{00}\rho^2(\mathbf{R}) + \frac{1}{3}V_{\pi 2}^{02}\left(\frac{1}{4}\rho(\mathbf{R})\triangle\rho(\mathbf{R}) - (\rho(\mathbf{R}\tau(\mathbf{R}) - j^2(\mathbf{R}))\right)\right], \tag{2.42}$$

where each term of the expansion is equipped with the corresponding coupling constants, defined as moments of the interaction,

$$V_{ij}^{\pi n} = \int d^3\mathbf{r} r^n \pi_i(r)\pi_j(r)V(r) = 4\pi \int dr r^{n+2} \pi_i(r)\pi_j(r)V(r). \tag{2.43}$$

The moments of the interaction have two main features to be underlined: they are running coupling constants depending on the Fermi momentum k_F or density $\rho(\mathbf{R})$; in a few number of moments is contained all the physical information we need about the dynamic of the short-range interaction. Again, we see a strong collapse of information due to the separation of scale between the low-energy nuclear states and short-range scale of the interaction.

2.1.3 Effective pseudopotential

The study of the two-body interaction between nucleons is the starting point of the application of the techniques of many-body theory to nuclear structure. Since 1950s, the long history of the theory of nuclear interactions has been followed a twofold path: on one hand, the attempt to derive the nuclear force from first principles, namely from some more fundamental theory; on the other hand, the introduction and the use of the so-called phenomenological interactions (bare or effective).

On the side of the first-principles approach [ME11], the problem seemed to be solved in 1970s, when the "Pion Theories" program was accomplished also for the intermediate-range part of the force with the 2π-exchange theory. But all the results of the theories, which have used the mesons as ultimate degrees of freedom, became suddenly simple models with the discovery of the quantum chromodynamics (QCD) in 1980s. The latter was regarded at the beginning as the new fundamental theory, and quarks and gluons the basic degrees of freedom. Very soon it emerged the idea that the QCD-inspired derivation of the nuclear force, also plagued by the intrinsic difficulty of the nonperturbativeness of QCD at low-energy regime, was finally nothing else that another model, just like the model based on pions and heavy mesons.

With the application of chiral expansion to low-energy nucleon-nucleon interaction by Weinberg [W90], the problem of the nucleon-nucleon interaction was set on a new basis. It has been observed [ME11] that EFT applied to low-energy nuclear phenomena, with the choice of nucleons and pions as degrees of freedom, has the meaning of a return to Yukawa's meson theory, but with a crucial added ingredient, that is the broken chiral symmetry as a constraint on the pions dynamics. We are not going to give any details about the derivation of the nuclear forces from the EFT Lagrangians, because in our work we are interested in a specific version of a phenomenological effective interaction, i.e. a pseudopotential. But first, we want briefly to present the main ideas about

the phenomenological bare interactions, focusing in particular on a procedure quite recently introduced and particularly suitable for the treatment of the bare forces, the low-momentum softening techniques of RG approach [BFS10].

Bare interactions can be considered as hybrid forces, because they are built from a part derived in the framework of the meson field theory, the so called one pion exchange potential (OPEP), and by a pure phenomenological part, introduced to mimic the effects of the force in the short- and often medium-range of the force. The phenomenological part contains up to 50 parameters, fitted in order to reproduce the observed scattering phase shifts and deuteron data. At larger distance, the bare forces are dominated by the OPEP contribution, which must be common to all the different bare forces aiming at reproducing the phase shift for orbital angular momentum $L \geq 6$. The phenomenological part, driving the short- and intermediate-range of the force, can vary according to the force adopted: for instance, the central, tensor and spin-orbit parts of the original Reid soft core potential, and also the explicit account of the charge-dependence and charge-asymmetry contributions in the electromagnetic part of the Argonne v_{18}, which has been tuned to both *pp* and *np* scattering database [WSS95].

By defining the coupling strength of the pion to the nucleon as $\frac{g^2}{\hbar c} \backsimeq 0.081$ and the Compton wavelength of the pion $\frac{1}{\mu} = \frac{\hbar}{m_\pi c}$, the form of the OPEP-potential reads,

$$V^{OPEP} = \frac{g^2}{3\hbar c} m_\pi c^2 \frac{e^{-\mu r}}{\mu r} (\tau^{(1)}\tau^{(2)}) \left\{ \sigma^{(1)}\sigma^{(2)} + \left(1 + 3\frac{1}{\mu r} + 3\left(\frac{1}{\mu r}\right)^2 \right) S_{12} \right\}, \tag{2.44}$$

where S_{12} is the standard tensor term.

The main drawback of the bare interactions is not in the long-range part, but in the strong repulsion at short distances, which makes the nuclear forces very difficult to handle in the practical implementations. The problem of the hard core is indeed the problem of the coupling of low to high momenta induced by the interaction. This coupling can be seen considering the off-diagonal matrix elements of an interaction, for instance the Argonne v_{18}, calculated in the momentum space. Large regions of the off-diagonal elements are non-zero, with the consequence of a strong quenching of the probability of the relative wave function for two nucleons at short distances, the short-range repulsive correlation. An even more direct way to understand this coupling is manifested in the expression of the scattering T-matrix in perturbation theory,

$$T(k', k, E) = \langle k'|V|k\rangle + \sum_q \frac{\langle k'|V|q\rangle\langle q|V|k\rangle}{E - \varepsilon_q} + \ldots, \tag{2.45}$$

where the summation over all the intermediate states q makes evident the interplay between low- and high-momenta physics.

The modern approaches aiming at curing the problem of the hard core are the renormalization group (RG) method [BFS10], similarity renormalization group (SRG) method [BFP07] and unitary correlation operator method (UCOM). They represent different strategies to evolve nuclear N-body forces into low-momentum interactions, making in this way possible the use of the many-body perturbation theory and improving the convergence of the calculations. They are applied in order to overcome the lack of well-established *ab initio* nuclear EDFs, when compared to the situation in the study of the Coulomb systems. This is due to the fact that the *ab initio* calculations in uniform nuclear systems are not as refined as the same kind of calculations for the electron gas, which are the standard starting point for the DFT for Coulomb systems. The ultimate reason of this discrepancy is due to the non-perturbative character of the nucleon-nucleon interaction. While the Coulomb potential is derived straightforwardly from QED and its perturbative nature resulting in the dominance of the Hartree-Fock (HF) contribution to the energy, makes the DFT so suitable for electronic systems, the sources of non-perturbative physics in the nuclear interaction require methods of softening of the hard core of the potential.

For instance, the RG-based techniques, known also as "$V_{low k}$" [BFS10], decouples the high-energy modes from the soft ones by evolving the many-body Hamiltonian through unitary transformations. The unitarity of the transformation guarantees that the average values of the operators corresponding to physical observables are kept untouched, while the potential is softened and evolved to become a low-momentum interaction, practically defined as a potential that do not couple momenta $k \lesssim 2fm^{-1}$ to larger momenta. One may wonder whether this freedom in evolving the potential is allowed: the point here is that for short-range interactions between finite-mass composite particle, the potential is not an observable anymore. The strong repulsive core of the bare interactions currently used was in fact a result of the assumption, merely dictated by numerical convenience, to take a local force to be parametrized by the phase shift data.

Before the coming of the low-momentum potentials techniques, an alternative form of interactions were introduced to overcome the hard core problems of the bare potentials, the effective interactions [RS80]. Effective forces were in fact introduced as a way out of the situation of the ill-behaved bare interactions. In particular, the microscopic effective interactions as the Brückner G-matrix consist in a re-summation of the infinite series of scattering processes of two nucleons in the nuclear medium. Through this re-summation the bare interaction, which was taken as starting point or zero order of the series, is cured of the hard core problem.

Beside the microscopic effective interactions, we can consider the phenomenological effective interactions [RS80], which are more easy to handle in practical

calculations and provide a better quantitative agreement with experiment, compared to the microscopic ones. The main difference with respect to the latter is the lacking of an explicit dependence on the energy, that is always produced in a microscopic approach *via* the Lippmann-Schwinger for the scattering matrix. In the phenomenological interactions, or pseudopotential, the energy dependence is replaced by in different strength parameters adjusted to reproduce the experimental data. For the SCMF models the two widely used effective interactions are the zero-range Skyrme interaction [Sk56, Sk59] and the finite-range Gogny force [G75, DG80].

In particular, the Skyrme interaction is a contact, local pseudopotential that depends on relative momenta up to the second order. In the position-spin-isospin representation it reads [PRD04],

$$\begin{aligned}
\hat{V}(\boldsymbol{r}_1'\sigma_1'\tau_1'\boldsymbol{r}_2'\sigma_2'\tau_2', \boldsymbol{r}_1\sigma_1\tau_1\,\boldsymbol{r}_2\sigma_2\tau_2) &= \Big\{t_0(\hat{\delta}^\sigma + x_0\hat{P}^\sigma) + \tfrac{1}{6}t_3(\hat{\delta}^\sigma + x_3\hat{P}^\sigma) \\
&\quad \rho_0^\alpha\left(\tfrac{1}{2}(\boldsymbol{r}_1+\boldsymbol{r}_2)\right) \\
&+ \tfrac{1}{2}t_1(\hat{\delta}^\sigma + x_1\hat{P}^\sigma)\Big[\hat{\boldsymbol{k}}'^2 + \hat{\boldsymbol{k}}^2\Big] \\
&+ \tfrac{1}{2}t_\mathrm{e}\Big[\hat{\boldsymbol{k}}'^*\cdot\hat{\mathsf{S}}\cdot\hat{\boldsymbol{k}}'^* + \hat{\boldsymbol{k}}\cdot\hat{\mathsf{S}}\cdot\hat{\boldsymbol{k}}\Big] \\
&+ t_2(\hat{\delta}^\sigma + x_2\hat{P}^\sigma)\hat{\boldsymbol{k}}'^*\cdot\hat{\boldsymbol{k}} + t_\mathrm{o}\hat{\boldsymbol{k}}'^*\cdot\hat{\mathsf{S}}\cdot\hat{\boldsymbol{k}} \\
&+ iW_0\hat{\boldsymbol{S}}\cdot\Big[\hat{\boldsymbol{k}}'^*\times\hat{\boldsymbol{k}}\Big]\Big\} \\
&\quad \Big(\hat{\delta}^\sigma\hat{\delta}^\tau - \hat{P}^\sigma\hat{P}^\tau P^M\Big)\,\hat{\delta}_{12}, \qquad (2.46)
\end{aligned}$$

where the Kronecker delta in the spin and isospin representation, and the exchange operators read

$$\hat{\delta}^\sigma_{\sigma_1'\sigma_2'\sigma_1\sigma_2} = \delta_{\sigma_1'\sigma_1}\delta_{\sigma_2'\sigma_2}, \qquad (2.47a)$$

$$\hat{\delta}^\tau_{\tau_1'\tau_2'\tau_1\tau_2} = \delta_{\tau_1'\tau_1}\delta_{\tau_2'\tau_2}, \qquad (2.47b)$$

$$\hat{P}^\sigma_{\sigma_1'\sigma_2'\sigma_1\sigma_2} = \tfrac{1}{2}(\hat{\delta}^\sigma_{\sigma_1'\sigma_2'\sigma_1\sigma_2} + \hat{\boldsymbol{\sigma}}_{\sigma_1'\sigma_1}\cdot\hat{\boldsymbol{\sigma}}_{\sigma_2'\sigma_2}) = \delta_{\sigma_1'\sigma_2}\delta_{\sigma_2'\sigma_1}, \qquad (2.47c)$$

$$\hat{P}^\tau_{\tau_1'\tau_2'\tau_1\tau_2} = \tfrac{1}{2}(\hat{\delta}^\tau_{\tau_1'\tau_2'\tau_1\tau_2} + \hat{\vec{\tau}}_{\tau_1'\tau_1}\circ\hat{\vec{\tau}}_{\tau_2'\tau_2}) = \delta_{\tau_1'\tau_2}\delta_{\tau_2'\tau_1}. \qquad (2.47d)$$

The two-body vector and tensor spin operators are

$$\hat{\boldsymbol{S}}_{\sigma_1'\sigma_2'\sigma_1\sigma_2} = \hat{\boldsymbol{\sigma}}_{\sigma_1'\sigma_1}\delta_{\sigma_2'\sigma_2} + \hat{\boldsymbol{\sigma}}_{\sigma_2'\sigma_2}\delta_{\sigma_1'\sigma_1}, \qquad (2.48a)$$

$$\begin{aligned}
\hat{\mathsf{S}}^{ab}_{\sigma_1'\sigma_2'\sigma_1\sigma_2} &= \tfrac{3}{2}\big(\hat{\boldsymbol{\sigma}}^a_{\sigma_1'\sigma_1}\hat{\boldsymbol{\sigma}}^b_{\sigma_2'\sigma_2} + \hat{\boldsymbol{\sigma}}^b_{\sigma_1'\sigma_1}\hat{\boldsymbol{\sigma}}^a_{\sigma_2'\sigma_2}\big) \\
&- \delta_{ab}\hat{\boldsymbol{\sigma}}_{\sigma_1'\sigma_1}\cdot\hat{\boldsymbol{\sigma}}_{\sigma_2'\sigma_2}, \qquad (2.48b)
\end{aligned}$$

and the relative momentum operators,

$$\hat{\boldsymbol{k}} = \tfrac{1}{2i}\left(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2\right), \tag{2.49a}$$

$$\hat{\boldsymbol{k}}' = \tfrac{1}{2i}\left(\boldsymbol{\nabla}'_1 - \boldsymbol{\nabla}'_2\right), \tag{2.49b}$$

act on the delta functions in $\hat{\delta}_{12}$, defined in Eq. (2.35). This action has to be understood in the standard sense of derivatives of distributions.

We present in more details the Skyrme force in Sec. 3.2, in the context of the comparison with the higher-order in derivatives pseudopotential introduced in this work. Here, we are going to describe some features of the interaction by following the original version of the Skyrme interaction. First of all, in its seminal paper [Sk59], Skyrme explored the possibility of some additional terms. Beside the fourth-order term that we introduce in Eq. (3.11), a four-body zero-range term can be considered,

$$t_4\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_1 - \mathbf{r}_3)\delta(\mathbf{r}_1 - \mathbf{r}_4), \tag{2.50}$$

which Skyrme assumed as a many-body effect contribution, alternative to the eventual introduction of momentum-dependent (finite range) terms. The four-body terms was preferred because it adds just one new parameter t_4. The term in Eq. (2.50) can be expressed also as an equivalent two-body contact interaction depending on the second power of the density. Analogously, the three-body term,

$$t_3\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_1 - \mathbf{r}_3), \tag{2.51}$$

can be represented, after the averaging over the even (spin saturated) many-body wave function, as

$$t_3\delta(\mathbf{r}_1 - \mathbf{r}_2)\overline{\rho}, \tag{2.52}$$

where $\overline{\rho}$ is the nuclear density at the point of the interaction.

This term, in the analysis performed by Skyrme, turned out to be more problematic in the odd (spin not saturated) states, where it cannot be treated as two-body density-dependent term. Another problematic issue investigated by Skyrme was the capability of the two-body spin-orbit term in describing the spectroscopic properties of light nuclei. In this respect, the conclusions were that the spin-orbit term was not rich enough to be determined with sufficient accuracy by the available data of the spin-orbit splitting.

In the later HF calculations with Skyrme functionals, the density dependent term was treated with simple phenomenological arguments, and the term proportional to ρ^3 in the functional was generalized to a dependence on $\rho^{2+\alpha}$ with $\alpha \sim 0.16 - 0.3$ (see for instance parametrizations SkM [KTB80] and SkM* [BQB82]), because the original term with the power of 3 dependence was performing not very well in the description of the fission barriers and monopole oscillations.

In general, from a formal point of view, the density dependence of the Skyrme interaction prevents to correctly interpret it as interaction [EKR10]. The problems arise from the simple term,

$$\hat{V}_3(\mathbf{r}_1, \mathbf{r}_2) = \frac{t_3}{6}\delta(\mathbf{r}_1 - \mathbf{r}_2)\rho(\mathbf{r}_1) \tag{2.53}$$

that one should be able to express also in the second quantization formalism as,

$$V_3 = \sum_{\alpha_1\alpha_2\alpha_3\beta_1\beta_2\beta_3} V_{\alpha_1\alpha_2\alpha_3\beta_1\beta_2\beta_3} a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} a^\dagger_{\alpha_3} a_{\beta_3} a_{\beta_2} a_{\beta_1} \quad , \tag{2.54}$$

whose expectation value with respect to the mean-field state $|\Phi\rangle$ gives

$$\langle\Phi|V_3|\Phi\rangle = \sum_{nmk} V_{nmk,\widetilde{nmk}} \quad . \tag{2.55}$$

But if one performs the calculation of the expectation value for the density dependent term in Eq. (2.53), one finds that the result is not fully antisymmetrized as it should be, with the consequence that the term in Eq. (2.53) can be considered at most as a formal generator of the functional rather than an interaction. Moreover, the density dependence has an unpleasant consequence for the calculations beyond mean-field level. If we consider for instance the residual interaction in RPA, obtained as the second derivative of the functional with respect to the density, we cannot recover the exact form of the initial interaction. The consistency between mean-field and beyond mean-field calculations is, in this way, lost. The pseudopotential we are going to introduced in Ch. 3 is not dependent on the density, having we chosen to extend the Skyrme interaction as an expansion in order of derivatives. Anyway, in order to achieve the correct saturation property, the direct and exchange components of the two-body interaction are not enough. Then, in practical calculations using the pseudopotential, one must think to add some dependence on the density. This inclusion guarantees that the N-body components of the interaction are taking into account.

Beside the discussion about the more suitable form for the interaction or the functional, the issue of the optimization of the parameters or the coupling constants, namely the fitting to experimental data [KLM10, KRB09], is a crucial feature of the phenomenological functionals. Usually the observables selected for the fit are related to the energy and spatial distribution of the nuclear matter in the nucleus: binding energies, proton radii and surface thicknesses, along with the so called pseudo-observables obtained from various nuclear-matter properties, that can be calculated in the analytically solvable models of infinite matter. Also single-particle energies of doubly magic nuclei can be used as fitting data, in order to pin down the properties connected to the shell structure of the nuclei, even tough it turned out that recent attempts [KDM08] to improve

the prediction power of the Skyrme functional through a refit based on single-particle energies has not yet brought the spectroscopic-quality description we wished for.

The different biases in selecting the set of observables has given rise to many different parametrization in the literature for SHF. A recent parametrization performing well in reproducing experimental masses, radii and deformation is the UNEDF0 parametrization [KLM10], that we are going to present briefly here as emblematic case of the optimization procedure.

The pool of fit observables for the UNEDF database is composed by 72 nuclei, with a bias toward heavy nuclei, the ones that require necessarily a treatment with SCMF models. A large part out of this set contains 44 well-deformed ($|\beta| \gtrsim 0.25$) even-even nuclei. The consideration of deformed nuclei in the fit should improve the predictive power of the functional on the surface properties. The set of the 28 remaining nuclei is composed by spherical nuclei, whose constraints in the fit are strong due to the fact that they deviate from global mass trend. The algorithm of optimization implied is derivative-free, a feature that guarantees better performance and precision in the minimization calculation of the objective (least-squares) function. In the solution of the optimization problem is often required some trade-off decision: in the case of the UNEDF, the best parametrization in reproducing the masses was able to give a rms deviation of 0.966 MeV, but the value of the incompressibility in nuclear matter at the end of the iteration was far too large, preventing the use of the parametrization for the studies of monopole collective vibrations. The choice was then to impose hard bounds on the nuclear incompressibility, at the cost of a deteriorated rms deviation for masses equal to 1.455 MeV.

Another remarkable aspect of the modern optimization approach is the statistical analysis of the optimization results, in particular the test of eventual correlations between the parameters [RN10, DSPM10]. The experimental information carried by the data can be in fact coded into the parameters in the inter-dependent way, in the sense that one or more parameters of the interactions can be functions of the others, leading to the ill-posedness of the inverse problem. The inverse problem is the search of the best parametrization for a give set of data and technically relies on the possibility to invert the matrix of the variations of the observables with respect to a small change in the values of the parameters. The problem of the inter-dependences among some parameters can depend on the theoretical limits of the approximation used for the many-body Hamiltonian, but also on the specific choice of data for the optimization procedure.

2.1.4 Galilean and gauge invariance of the EDF

We have seen that one of the main guiding principles in building effective theories is to write Lagrangians or Hamiltonians restricted only by symmetry principles. In the framework of the SCMF methods, the restoration of the broken symmetries is the standard approach to the treatment of the symmetry of observables under transformations [RS80, BR86]. In fact, one tries to capture the relevant physics of a system by a description based on simple wave functions, but the simplicity of the single-particle basis means that the many-body wave function can break the symmetries of the nuclear Hamiltonian. For example, if we do not choose plane waves as a basis of the independent-particle states, we break the translational invariance. The standard practical method to restore the symmetries or, in other words, to include correlations in the mean field wave function, is the generator coordinate method [RS80], where a superposition of independent broken-symmetry wave functions is introduced as an ansatz that minimizes the energy and causes the many-body wave function to have the required symmetry.

In this section, we discuss the properties of the gauge and Galilean symmetries when they are applied to the functional [DD95, CDK08]. The Galilean invariance of the functional is the natural consequence of the assumption that relativistic effects are negligible, and then the dynamics of the system is driven by the Schrödinger equation instead of the Dirac equation.

The expression of the Galilean-transformed nonlocal density reads,

$$\rho'(\boldsymbol{r}\sigma\tau, \boldsymbol{r}'\sigma'\tau') = \exp\left\{\frac{i}{\hbar}\boldsymbol{p}\cdot\Big(\boldsymbol{r}-\boldsymbol{r}'\Big)\right\}\rho(\boldsymbol{r}\sigma\tau, \boldsymbol{r}'\sigma'\tau'), \tag{2.56}$$

where $\boldsymbol{p}$ is a constant linear momentum of the boost transformation. As long the interaction energy does not depend on the momentum $\boldsymbol{p}$ and on the assumption of a stationary solution (vanishing density currents), we have the following energy increase,

$$\Delta\mathcal{E}^{\text{boost}} = \frac{\boldsymbol{p}^2}{2m}A, \tag{2.57}$$

which is the translation energy of the boosted system.

Despite the fundamental character of the Galilean invariance, in many phenomenological approaches not interested in the translational motion, the Galilean symmetry is not considered. Therefore, the EDF can be in the most general case presented with the terms free from any constraints coming from this symmetry.

The Galilean transformation considered in Eq. (2.56) for the nonlocal density is in fact a special case of the general gauge transformation, whose action is,

$$\rho'(\boldsymbol{r}\sigma\tau, \boldsymbol{r}'\sigma'\tau') = e^{i\left(\gamma(\boldsymbol{r})-\gamma(\boldsymbol{r}')\right)}\rho(\boldsymbol{r}\sigma\tau, \boldsymbol{r}'\sigma'\tau'). \tag{2.58}$$

where $\gamma(\boldsymbol{r})$ in this case is an arbitrary real function of the position $\boldsymbol{r}$.

In Sec. 3.6 we show how the N^{3}LO EDF is derived from the pseudopotential. EDF is obtained by averaging the pseudopotential over a Slater determinant, which is an uncorrelated wave function, therefore we should expect to face the problem of the breaking of the symmetries in the functional. On the other hand, the results of the averaging in paper I, reviewed in Sec. 5.1.1, show that the symmetries of the pseudopotential are shared also by the derived EDF. In particular, since the pseudopotential is Galilean-invariant, the obtained EDF coupling constants obey the Galilean-invariance constraints. Similarly, when parameters of the pseudopotential are restricted to obey the gauge-invariance conditions (see Sec. 3.5), the resulting coupling constants correspond to a gauge-invariant EDF. The reason of these two invariances, with respect to Galilean and gauge transformations, is due to the fact that the pseudopotential considered in our work is local, according to expression in Eq. (2.33), that we rewrite here with spin and isospin coordinates included,

$$\begin{aligned}\hat{V}(\boldsymbol{r}'_1\sigma'_1\tau'_1\boldsymbol{r}'_2\sigma'_2\tau'_2, \boldsymbol{r}_1\sigma_1\tau_1\boldsymbol{r}_2\sigma_2\tau_2) &= \hat{V}(\boldsymbol{r}_1\sigma'_1\tau'_1\boldsymbol{r}_2\sigma'_2\tau'_2, \boldsymbol{r}_1\sigma_1\tau_1\boldsymbol{r}_2\sigma_2\tau_2)\times \\ &\quad \delta(\mathbf{r}'_1 - \mathbf{r}_1)\delta(\mathbf{r}'_2 - \mathbf{r}_2).\end{aligned} \tag{2.59}$$

In fact, one can see that expression of the interaction energy,

$$\begin{aligned}\mathcal{E} &= \frac{1}{4}\int \mathrm{d}\,\boldsymbol{r}_1\boldsymbol{r}_2\boldsymbol{r}'_1\boldsymbol{r}'_2 \sum_{\substack{\sigma_1\sigma_2\\ \sigma'_1\sigma'_2}}\sum_{\substack{\tau_1\tau_2\\ \tau'_1\tau'_2}} \hat{V}(\boldsymbol{r}'_1\sigma'_1\tau'_1\boldsymbol{r}'_2\sigma'_2\tau'_2, \boldsymbol{r}_1\sigma_1\tau_1\boldsymbol{r}_2\sigma_2\tau_2) \\ &\quad (\rho(\boldsymbol{r}_1\sigma_1\tau_1, \boldsymbol{r}'_1\sigma'_1\tau'_1)\rho(\boldsymbol{r}_2\sigma_2\tau_2, \boldsymbol{r}'_2\sigma'_2\tau'_2) \\ &\quad -\rho(\boldsymbol{r}_2\sigma_2\tau_2, \boldsymbol{r}'_1\sigma'_1\tau'_1)\rho(\boldsymbol{r}_1\sigma_1\tau_1, \boldsymbol{r}'_2\sigma'_2\tau'_2)),\end{aligned} \tag{2.60}$$

becomes invariant with respect to the local gauge, when the locality of the interaction is assumed (Eq. (2.59)), and it acquires the form of Eq. (2.32),namely,

$$\begin{aligned}\mathcal{E} &= \frac{1}{4}\int \mathrm{d}\,\boldsymbol{r}_1\boldsymbol{r}_2 \sum_{\substack{\sigma_1\sigma_2\\ \sigma'_1\sigma'_2}}\sum_{\substack{\tau_1\tau_2\\ \tau'_1\tau'_2}} \hat{V}(\boldsymbol{r}_1\sigma'_1\tau'_1\boldsymbol{r}_2\sigma'_2\tau'_2, \boldsymbol{r}_1\sigma_1\tau_1\boldsymbol{r}_2\sigma_2\tau_2) \\ &\quad (\rho(\boldsymbol{r}_1\sigma_1\tau_1, \boldsymbol{r}_1\sigma'_1\tau'_1)\rho(\boldsymbol{r}_2\sigma_2\tau_2, \boldsymbol{r}_2\sigma'_2\tau'_2) \\ &\quad -\rho(\boldsymbol{r}_2\sigma_2\tau_2, \boldsymbol{r}_1\sigma'_1\tau'_1)\rho(\boldsymbol{r}_1\sigma_1\tau_1, \boldsymbol{r}_2\sigma'_2\tau'_2)).\end{aligned} \tag{2.61}$$

as it is explicitly showed in the following.

A general finite-range interaction energy is not invariant with respect to the gauge symmetry, but when the interaction is assumed to be local as in Eq. (2.59), then the corresponding interaction energy Eq. (2.60) turns out to be invariant under the local gauge transformation. In fact, the direct term is invariant because it depends only local densities depending on only one position coordinate. On the other hand, in the exchange term the gauge factors coming from two density matrices cancel one another, because the position coordinates appear in opposite order in the two densities, that is, $\rho(\mathbf{r}_2, \mathbf{r}_1)\rho(\mathbf{r}_1, \mathbf{r}_2)$.

The transformations in Eq. (2.58) is generated by the identity operator and corresponds to the standard abelian group U(1). This is just one case of a class of different local gauge groups acting on the spin and isospin spaces,

$$U_v^t(\boldsymbol{r}) \quad = \quad \exp\left(i\left[\left[\gamma_v^t(\boldsymbol{r})\sigma_v\right]_0\tau^t\right]^0\right). \tag{2.62}$$

The U(1) group corresponds to $\gamma(\boldsymbol{r}) \equiv \gamma_0^0(\boldsymbol{r})$ and is an abelian group, because the only generator of the transformations, which is the identity operator, commutes trivially with itself. $U_1^0(\boldsymbol{r})$ and $U_0^1(\boldsymbol{r})$ form the non-abelian gauge groups SU(2). The generators of these two groups of transformations are the Pauli spin and isospin matrices respectively, which do not commute because of the well-known relation of commutation for angular momentum operators. They represent the rotations in the spin and isospin spaces. $U_1^1(\boldsymbol{r})$ corresponds to the non-abelian gauge group SU(2)×SU(2) in both spin and isospin spaces.

Chapter 3

Pseudopotential for N^{3}LO nuclear EDF

3.1 Overview of the paper I

In this section we are going to recall the main contents exposed in paper I and to list topics of the following sections, which have been left out from the paper I for sake of brevity, or because they are related to the technical implementation of the calculations, but are nevertheless helpful for a thorough understanding of our results.

In paper I, we have derived a zero-range pseudopotential including all possible terms up to sixth order in derivatives, and within the HF approximation we have calculated the quasilocal EDF built of derivatives of the one-body density matrix up to sixth order. The EDF derived from the pseudopotential turns out to be constrained in such a way that the number of independent coupling constants of the functional is reduced by a factor of two. These constraints have been explicitly calculated for different symmetries imposed on the functional and on the pseudopotential.

The detailed description of the general form of the pseudopotential was presented in Sec. II of paper I and the complete list of all the terms order by order was given in Sec. IIB therein. In Sec. 3.2 of the present chapter we discuss in more detail the consequence of the locality and zero-range character of the pseudopotential, showing explicitly how the number of free parameters of the pseudopotential reduces by half when the zero-range character is assumed. We stress this point because it is at the basis of the constraints we can impose on the

functional by the direct reference to the pseudopotential. In the same section we are going to present also the correspondence between the pseudopotential at NLO and Skyrme interaction, making in this way more transparent the connection given in Sec. IIB of paper I by the relations of conversion between the parameters of the pseudopotential and those of the Skyrme interaction.

Also the discussion of symmetries will be extended in Sec. 3.3 and, in particular, derivation of the condition for the gauge invariance of the pseudopotential is presented in details (Sec. 3.5). This gives the details of the practical implementation required to obtain the results listed in Appendix B of paper I, concerning the set of the gauge-invariant combinations of the parameters and terms of the pseudopotential. Since the hermiticity is a requirement that plays an important role in defining the form of the pseudopotential, we decided to complete the calculation of the adjoint pseudopotential given in Appendix A of paper I, with an alternative derivation that can be found in Sec. 3.4.

Sec. III of paper I is mainly devoted to the presentation of the results concerning the reference of the EDF to the pseudopotential. For assumed gauge invariance of the EDF and pseudopotential, the constraints on the EDF that are derived by averaging the pseudopotential up to N^{3}LO are given as expressions of a set of isovector coupling constants written as functions of the isoscalar ones. These expressions have been obtained by means of the relations between the coupling constants in a given isospin channel and parameters of the pseudopotential, along with the inverse relations, namely the relations in which the parameters are expressed as linear combinations of the coupling constants. The same analysis has been repeated also for the imposed Galilean invariance and the results collected in supplemental material of paper I.

The calculation of the averaging of the pseudopotential is lengthy and in paper I we have just given the general idea about how it proceeds. In Sec. 3.7 we fill all the steps of this calculation. First of all, the recoupling of the relative momentum tensors in the pseudopotential is performed and results of the recoupling for the second order are listed and compared with the corresponding Cartesian expressions, which are required to derive the Skyrme functional. Such a comparison completes the one made between the pseudopotential at second order and Skyrme interaction, and it has been practically used as a test to double check our derivation of the recoupling of the momentum tensors, which is a formula valid also for the higher orders.

Other derivations that we think are worth presenting here in detail are the ones concerning the recoupling of the tensors composed by derivatives to the density matrices, in order to get the secondary densities of the EDF, and to attain the recoupling to the specific form of the functional used in Ref. [CDK08]. Both recouplings are presented in Sec. 3.7.2.

A more specific overview concerning the numerical results obtained in paper

I is given in Secs. 5.1.1- 5.1.2, where we treat, in particular, the case of the EDF with conserved spherical, space-inversion, and time-reversal symmetries, discussed in Sec. IV of paper I as simple case applicable to the spherical even-even nuclei.

3.2 Zero-range pseudopotential and Skyrme force

We introduce the N^{3}LO pseudopotential as a phenomenological interaction represented in the spherical-tensor formalism, which extends the standard Skyrme interaction to higher-order derivatives,

$$\hat{V} = \sum_{\substack{\tilde{n}'\tilde{L}',\\ \tilde{n}\tilde{L},v_{12}S}} C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S} \hat{V}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S}, \tag{3.1}$$

where the sum runs over the allowed indices of the tensors according to the symmetries discussed in Sec. 3.3. The terms are accompanied by the corresponding strength parameter $C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S}$, and explicitly read,

$$\begin{aligned}\hat{V}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S} = \quad & \frac{1}{2} i^{v_{12}} \Big(\Big[\big[K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}} \big]_S \hat{S}_{v_{12}S} \Big]_0 \\ & + (-1)^{v_{12}+S} \Big[\big[K'_{\tilde{n}\tilde{L}} K_{\tilde{n}'\tilde{L}'} \big]_S \hat{S}_{v_{12}S} \Big]_0 \Big) \\ & \times \Big(1 - \hat{P}^M \hat{P}^\sigma \hat{P}^\tau \Big) \hat{\delta}_{12}(\boldsymbol{r}'_1 \boldsymbol{r}'_2; \boldsymbol{r}_1 \boldsymbol{r}_2). \end{aligned} \tag{3.2}$$

In Eq. (3.2), $K_{\tilde{n}\tilde{L}}$ and $K'_{\tilde{n}\tilde{L}}$ are the spherical tensor derivatives of order $\tilde{n}$ and rank $\tilde{L}$ built of the spherical representations of the relative momenta,

$$\boldsymbol{k} = \frac{1}{2i}(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2), \tag{3.3}$$

$$\boldsymbol{k}' = \frac{1}{2i}(\boldsymbol{\nabla}'_1 - \boldsymbol{\nabla}'_2), \tag{3.4}$$

while the symmetrized two-body spin operators $\hat{S}_{v_{12}S}$ are defined as,

$$\hat{S}_{v_{12}S} = \big(1 - \tfrac{1}{2}\delta_{v_1,v_2}\big) \Big([\sigma^{(1)}_{v_1} \sigma^{(2)}_{v_2}]_S + [\sigma^{(1)}_{v_2} \sigma^{(2)}_{v_1}]_S \Big). \tag{3.5}$$

The definitions of the building blocks in the previous equations can be found in Sec. IIA of paper I, defining also the exchange operator in spherical tensor formalism as,

$$\begin{aligned}\hat{P}^M\hat{P}^\sigma\hat{P}^\tau &= (-1)^{\tilde{n}'}\frac{1}{4}\Big(1+\sqrt{3}\left[\sigma_1^{(1)}\sigma_1^{(2)}\right]_0 \\ &+\sqrt{3}\left[\tau_1^{(1)}\tau_1^{(2)}\right]^0+3\left[\sigma_1^{(1)}\sigma_1^{(2)}\right]_0\left[\tau_1^{(1)}\tau_1^{(2)}\right]^0\Big).\end{aligned} \tag{3.6}$$

The main feature of the Skyrme interaction is its zero-range form (contact force) and this feature is of course shared by our pseudopotential. We stress here an important consequence concerning the number of terms of a contact force: it is easy to realize that a general zero-range nucleon-nucleon interaction has half the number of terms compared to the general finite-range nucleon-nucleon interaction. The argument goes in the following way. The general form of a central force is [RS80],

$$\begin{aligned}V_C(1,2) &= \Big(V_0(r)+V_\sigma(r)\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}+V_\tau(r)\boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)} \\ &+V_{\sigma\tau}(r)\boldsymbol{\sigma}^{(1)}\boldsymbol{\sigma}^{(2)}\boldsymbol{\tau}^{(1)}\boldsymbol{\tau}^{(2)}\Big)\left(1-P^MP^\sigma P^\tau\right),\end{aligned} \tag{3.7}$$

where the operators $P^MP^\sigma P^\tau$ are the Cartesian version of the exchange operators in Eq. (3.6) expressing the Pauli principle. The action of the exchange operators onto the antisymmetrized wave function is specified by the relation, valid when the coordinate representation of the interaction is assumed,

$$P^MP^\sigma P^\tau\Psi(x_1,x_2)=-\Psi(x_2,x_1), \tag{3.8}$$

where we have used the collective coordinates $x_i\equiv(\boldsymbol{r}_i,\sigma_i,\tau_i)$.

By using the relation of Eq. (3.8), Eq. (3.7) can be recast in such a way that it contains just exchange operators,

$$V_C(1,2)=\left(V_W(r)+V_M(r)P^M+V_B(r)P^\sigma+V_H(r)P^MP^\sigma\right)\left(1-P^MP^\sigma P^\tau\right), \tag{3.9}$$

where the suffix relative to the different components of the force denote linear combinations of the former components of Eq. (3.7) and are named after Wigner, Majorana, Bartlett and Heisenberg,

$$\begin{aligned}V_W(r) &= V_0(r)-V_\sigma(r)-V_\tau(r)+V_{\sigma\tau}(r),\\ V_M(r) &= -4V_{\sigma\tau}(r),\\ V_B(r) &= 2V_\sigma(r)-2V_{\sigma\tau}(r),\\ V_H(r) &= -2V_\tau(r)+2V_{\sigma\tau}(r).\end{aligned} \tag{3.10}$$

	Terms	Cartesian representation (Skyrme force)
1	$\hat{V}^{20}_{00,00}$	$\frac{1}{\sqrt{3}}(\boldsymbol{k'}^2\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)+\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\boldsymbol{k}^2)$
2	$\hat{V}^{20}_{00,20}$	$\frac{1}{3}(\boldsymbol{k'}^2\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)+\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\boldsymbol{k}^2)(\boldsymbol{\sigma^{(1)}}\cdot\boldsymbol{\sigma^{(2)}})$
3	$\hat{V}^{22}_{00,22}$	$\frac{1}{\sqrt{5}}((\boldsymbol{k'}\cdot\boldsymbol{\sigma^{(1)}})(\boldsymbol{k'}\cdot\boldsymbol{\sigma^{(2)}})\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)+\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)(\boldsymbol{k}\cdot\boldsymbol{\sigma^{(1)}})(\boldsymbol{k}\cdot\boldsymbol{\sigma^{(2)}}))$ $-\frac{1}{3\sqrt{5}}((\boldsymbol{k'}^2\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)+\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\boldsymbol{k}^2)(\boldsymbol{\sigma^{(1)}}\cdot\boldsymbol{\sigma^{(2)}}))$
4	$\hat{V}^{11}_{11,00}$	$\frac{1}{\sqrt{3}}(\boldsymbol{k'}\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\cdot\boldsymbol{k})$
5	$\hat{V}^{11}_{11,20}$	$\frac{1}{3}(\boldsymbol{k'}\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\cdot\boldsymbol{k})(\boldsymbol{\sigma^{(1)}}\cdot\boldsymbol{\sigma^{(2)}})$
6	$\hat{V}^{11}_{11,11}$	$\frac{1}{\sqrt{6}}i(\boldsymbol{k'}\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\times\boldsymbol{k})(\boldsymbol{\sigma^{(1)}}+\boldsymbol{\sigma^{(2)}})$
7	$\hat{V}^{11}_{11,22}$	$\frac{1}{\sqrt{5}}(\boldsymbol{k'}\cdot\boldsymbol{\sigma^{(1)}})\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)(\boldsymbol{k}\cdot\boldsymbol{\sigma^{(2)}})-\frac{1}{3\sqrt{5}}(\boldsymbol{k'}\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\cdot\boldsymbol{k})(\boldsymbol{\sigma^{(1)}}\cdot\boldsymbol{\sigma^{(2)}})$

Table 3.1: Cartesian representation of the pseudopotential.

Now, if we consider a zero-range interaction the exchange operator P^M for the spatial coordinates turns into a simple phase and the first two component of the interaction (3.9) are in fact the same operator and they can be grouped together. The same stands for the last two components of the interaction (3.9) and in all the zero-range interaction is formed by the half of number of independent terms compared to the general central finite-range interaction. This observation is crucial for the discussion in Sec. III of paper I, and reviewed in Sec. 5.1.1, about the relations between the coupling constants of the EDF and parameters of the pseudopotential.

Indeed the pseudopotential of Eq. (3.1), considered up to second order, is strictly equivalent to the Skyrme interaction, which is instead traditionally written in Cartesian representation. The equivalence between these two forms of interaction can be seen explicitly by using Eqs. (9) of paper I, that give a vocabulary of translation between the parameters of zero- and second-order pseudopotential in spherical-tensor representation and those of the Skyrme interaction. In Table (3.1) we show the Cartesian representation term by term up to second order and in Eq. (3.11) we include also the fourth-order term corresponding to the one originally considered by Skyrme,

$$\hat{V}^{20}_{20,00}=\frac{1}{2}\left(\boldsymbol{k'}^2\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\boldsymbol{k}^2-\boldsymbol{k'}(\boldsymbol{k'}\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\cdot\boldsymbol{k})\cdot\boldsymbol{k}\right), \tag{3.11}$$

where in the last term of Eq. (3.11) both scalar products mix the primed and non-primed coordinates.

3.3 Symmetry properties of the pseudopotential

The form and number of terms of the pseudopotential are restricted by imposing a certain number of symmetries, which pertain to a general two-body force [RS80]. In the following we discuss the main symmetries applied to the pseudopotential, leaving the derivations of the hermiticity for the next section.

- The invariance under an exchange of the coordinates. This symmetry is ultimately connected to the fact that the particles in quantum mechanics are indistinguishable and is equivalent to the invariance of the tensor with respect to the interchange of the labels of the particle 1 and 2. The spin operator of Eq. (3.5) was built to preserve the invariance under discussion, whereas the coupling at higher orders of the relative momentum operators $\boldsymbol{k}$ and $\boldsymbol{k}'$ can be invariant only when the following condition is respected,

$$(-1)^{\tilde{n}+\tilde{n}'} = 1, \tag{3.12}$$

  that is, only for terms which are even in the order of derivatives. This explains why the pseudopotential at N^{3}LO in Eq. (3.1) is composed only by the second-, fourth-, and sixth-order terms.

- Translational invariance. It is a very basic symmetry of physical systems, whose energy must not depend on the system of reference adopted to make measurements. In the case of the quasilocal potential, the translational invariance is guaranteed by the fact that the building blocks of the spatial part of the pseudopotential are relative momentum operators $\boldsymbol{k}$.

- Galilean invariance. As before, the simple dependence on the relative momentum $\boldsymbol{k}$ is enough to ensure the invariance of the pseudopotential with respect to a transformation to a system moving with a constant velocity.

- Parity invariance. The invariance of the phenomenological potential under the space inversion reflects the more fundamental parity invariance of the strong interaction. In the case of the N^{3}LO pseudopotential, the parity transformation brings a minus sign for each relative momentum operator $\boldsymbol{k}$: then to get the invariance we should require the same condition of Eq. (3.12) already found for the exchange of coordinates transformation.

- Time-reversal invariance. The pseudopotential is required to be time-reversal invariant because the Schrödinger equation of the system must not depend on the direction of the time evolution. In Appendix A of paper I, we give a detailed justification of the phase factor $i^{v_{12}}$ in the definition

of the pseudopotential in Eq. (3.2), which guarantees the invariance under the time-reversal transformation.

- Rotational invariance. The rotational invariance can be implemented naturally on the pseudopotential written in the spherical tensor formalism. In fact we required that all the terms of the pseudopotential be scalars, namely tensors of rank zero. A special attention is needed here for the spin operator of Eq. (3.5) when $v_{12} = 1$,

$$\hat{\boldsymbol{S}}_{11} = \tfrac{1}{2}\left(\boldsymbol{\sigma}^{(1)} + \boldsymbol{\sigma}^{(2)}\right). \tag{3.13}$$

  Since $\hat{\boldsymbol{S}}_{11}$ is a vector, it must be coupled with another vector built from relative-momentum operators. At second order one then finds the well-known spin-orbit term, whereas at fourth and sixth orders one finds higher-order spin-orbit terms (terms 6 and 14 in Table (IV) of paper I and terms 6, 15, 20 and 25 in Table V of paper I).

- Rotational invariance in the isospin space. It is equivalent to the request that the total isospin operator $T = t_1^{(1)} + t_1^{(2)}$ commutes with the effective interaction. Given that the isospin operators, living in their proper isospin space, do not couple with the operators momentum and spin, the only isospin invariant coupling allowed is the one appearing is the isospin exchange operator,

$$\hat{P}^{\tau} = \frac{1}{2}\left(1 + \sqrt{3}\left[\tau_1^{(1)}\tau_1^{(2)}\right]^0\right). \tag{3.14}$$

3.4 Hermiticity of the pseudopotential

In this section we show an alternative derivation of the hermiticity of the pseudopotential in Eq. (3.2) and we complete in this way the discussion about the symmetries of the pseudopotential made in the previous section. A derivation has already been presented in Appendix A of paper I. The following derivation considers explicitly the fact that the pseudopotential has the Dirac deltas and derivatives acting onto them. Therefore, the formal way to calculate the adjoint of the pseudopotential must take into account the fact that the Dirac deltas are distributions.

In order to do this, we consider the most simple term built with the spin and relative-momentum tensors and respecting the symmetries of Sec. 3.3,

$$(i)^{v_{12}}\left[\left[K'_{\tilde{n}'\tilde{L}'}K_{\tilde{n}\tilde{L}}\right]_S \hat{S}_{v_{12}S}\right]_0 \hat{\delta}_{12}(\boldsymbol{r}'_1\boldsymbol{r}'_2;\boldsymbol{r}_1\boldsymbol{r}_2). \tag{3.15}$$

For the following calculation, we denote the term (3.15) expressed in second quantization form through the field operators, in this way,

$$\begin{aligned} T_{\hat{V}} \equiv & \sum_{\substack{s_1 s_1', \\ s_2 s_2'}} \int d\boldsymbol{r}_1' d\boldsymbol{r}_2' d\boldsymbol{r}_1 d\boldsymbol{r}_2 (i)^{v_{12}} \left[\left[K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}} \right]_S \hat{S}_{v_{12}S} \right]_0 \\ & \times \hat{\delta}_{12}(\boldsymbol{r}_1'\boldsymbol{r}_2'; \boldsymbol{r}_1\boldsymbol{r}_2) \hat{\Psi}^\dagger(\boldsymbol{r}_1') \hat{\Psi}^\dagger(\boldsymbol{r}_2') \hat{\Psi}(\boldsymbol{r}_2) \hat{\Psi}(\boldsymbol{r}_1). \end{aligned} \tag{3.16}$$

Then, the Hermitian conjugate of the term $T_{\hat{V}}$ is

$$\begin{aligned} \left(T_{\hat{V}}\right)^\dagger = & \sum_{\substack{s_1 s_1', \\ s_2 s_2'}} \int d\boldsymbol{r}_1' d\boldsymbol{r}_2' d\boldsymbol{r}_1 d\boldsymbol{r}_2 (-i)^{v_{12}} \left(\sum_\mu \frac{(-1)^{S-\mu}}{\sqrt{2S+1}} \left(\left(K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}} \right)_{S,-\mu} \hat{S}_{v_{12}S,\mu} \right) \right. \\ & \left. \hat{\delta}_{12}(\boldsymbol{r}_1'\boldsymbol{r}_2'; \boldsymbol{r}_1\boldsymbol{r}_2) \right)^\dagger \hat{\Psi}^\dagger(\boldsymbol{r}_1) \hat{\Psi}^\dagger(\boldsymbol{r}_2) \hat{\Psi}(\boldsymbol{r}_2') \hat{\Psi}(\boldsymbol{r}_1') \\ = & \sum_{\substack{s_1 s_1', \\ s_2 s_2'}} \int d\boldsymbol{r}_1' d\boldsymbol{r}_2' d\boldsymbol{r}_1 d\boldsymbol{r}_2 (-i)^{v_{12}} \sum_\mu \frac{(-1)^{S-\mu}}{\sqrt{2S+1}} \hat{\delta}_{12}(\boldsymbol{r}_1'\boldsymbol{r}_2'; \boldsymbol{r}_1\boldsymbol{r}_2) (-1)^{S-\mu} \\ & \hat{S}_{v_{12}S,-\mu} (-1)^{S+\mu} \left(K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}} \right)_{S,\mu} \hat{\Psi}^\dagger(\boldsymbol{r}_1) \hat{\Psi}^\dagger(\boldsymbol{r}_2) \hat{\Psi}(\boldsymbol{r}_2') \hat{\Psi}(\boldsymbol{r}_1'), \\ = & \sum_{\substack{s_1 s_1', \\ s_2 s_2'}} \int d\boldsymbol{r}_1' d\boldsymbol{r}_2' d\boldsymbol{r}_1 d\boldsymbol{r}_2 (-i)^{v_{12}} \sum_\mu \frac{(-1)^{S-\mu}}{\sqrt{2S+1}} \hat{\delta}_{12}(\boldsymbol{r}_1'\boldsymbol{r}_2'; \boldsymbol{r}_1\boldsymbol{r}_2) \\ & \left(K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}} \right)_{S,\mu} \hat{S}_{v_{12}S,-\mu} \hat{\Psi}^\dagger(\boldsymbol{r}_1) \hat{\Psi}^\dagger(\boldsymbol{r}_2) \hat{\Psi}(\boldsymbol{r}_2') \hat{\Psi}(\boldsymbol{r}_1'). \end{aligned} \tag{3.17}$$

where we applied the Hermitian conjugation to the fields operators in the first step and to tensors in the second step, whereas in the last equality we used the fact that the relative-momentum operators and spin operator $\hat{S}_{v_{12}S}$ commute.

The relative momentum operators and Dirac delta $\hat{\delta}_{12}(\boldsymbol{r}_1'\boldsymbol{r}_2'; \boldsymbol{r}_1\boldsymbol{r}_2)$ in the last line do not commute. So, we use the fact that the pseudopotential is inserted into integrals, when the coordinate representation is adopted. We can use the trick of the integration by parts to move the Dirac deltas to the right-hand side of the momentum operators. Each momentum transferred operator brings a minus sign in the expression.

So, the Hermitian conjugate of the term $T_{\hat{V}}$ reads now,

$$
\begin{aligned}
\left(T_{\hat{V}}\right)^{\dagger} &= \sum_{\substack{s_1 s_1', \\ s_2 s_2'}} \int d\boldsymbol{r}_1' d\boldsymbol{r}_2' d\boldsymbol{r}_1 d\boldsymbol{r}_2 (-i)^{v_{12}} \sum_{\mu} \frac{(-1)^{S-\mu}}{\sqrt{2S+1}} (-1)^{n+n'} \left(K_{\tilde{n}\tilde{L}} K'_{\tilde{n}'\tilde{L}'}\right)_{S,\mu} \\
&\quad \hat{S}_{v_{12}S,-\mu} \hat{\delta}_{12}(\boldsymbol{r}_1'\boldsymbol{r}_2'; \boldsymbol{r}_1\boldsymbol{r}_2) \hat{\Psi}^{\dagger}(\boldsymbol{r}_1) \hat{\Psi}^{\dagger}(\boldsymbol{r}_2) \hat{\Psi}(\boldsymbol{r}_2') \hat{\Psi}(\boldsymbol{r}_1') \\
&= \sum_{\substack{s_1 s_1', \\ s_2 s_2'}} \int d\boldsymbol{r}_1' d\boldsymbol{r}_2' d\boldsymbol{r}_1 d\boldsymbol{r}_2 (-i)^{v_{12}} \sum_{\mu} \frac{(-1)^{S-\mu}}{\sqrt{2S+1}} (-1)^{S} \left(K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}}\right)_{S,\mu} \\
&\quad \hat{S}_{v_{12}S,-\mu} \hat{\delta}_{12}(\boldsymbol{r}_1'\boldsymbol{r}_2'; \boldsymbol{r}_1\boldsymbol{r}_2) \hat{\Psi}^{\dagger}(\boldsymbol{r}_1) \hat{\Psi}^{\dagger}(\boldsymbol{r}_2) \hat{\Psi}(\boldsymbol{r}_2') \hat{\Psi}(\boldsymbol{r}_1'), \qquad (3.18)
\end{aligned}
$$

and the factor $(-1)^S$ in the last equality of Eq. (3.18) comes from exchanging the order of the operators $K_{\tilde{n}\tilde{L}}$ and $K'_{\tilde{n}'\tilde{L}'}$ coupled to rank S. The tensor is not self-adjoint but we can hermitize it using the following expression, valid for an operator $\hat{A}$ depending on the indices n, L, n', L' and S, and defined as $\hat{A} = (i)^{v_{12}} \tilde{A}(n, L, n', L', S)$, that is

$$
\frac{1}{2}(i)^{v_{12}} \left(\tilde{A}(n, L, n', L', S) + (-1)^{v_{12}+S} \tilde{A}(n', L', n, L, S) \right), \qquad (3.19)
$$

where the flip in the indices $(n, L \longleftrightarrow n', L')$ is equivalent to the change of the coordinates,

$$
\begin{aligned}
\boldsymbol{r}_1' &\longleftrightarrow \boldsymbol{r}_1 \qquad (3.20) \\
\boldsymbol{r}_2' &\longleftrightarrow \boldsymbol{r}_2,
\end{aligned}
$$

which is required to guarantee the full hermiticity of the expression in the first line of Eq. (3.17). Formula (3.19) applied to the tensor,

$$
(i)^{v_{12}} \left[\left[K'_{\tilde{n}'\tilde{L}'} K_{\tilde{n}\tilde{L}} \right]_S \hat{S}_{v_{12}S} \right]_0 \hat{\delta}_{12}(\boldsymbol{r}_1'\boldsymbol{r}_2'; \boldsymbol{r}_1\boldsymbol{r}_2), \qquad (3.21)
$$

gives the expression in Eq. (3.2).

3.5 Gauge invariance of the pseudopotential

In Sec. (3.3) we did not treat the gauge invariance as a general symmetry of the pseudopotential, but we can impose it as further symmetry on the terms of the higher-order pseudopotential. As matter of fact, the zero-range Skyrme interaction is locally gauge-invariant and the Skyrme EDF is gauge-invariant as well [EBG75, DD95]. This circumstance, which is highly non trivial due to the presence of the momentum operators in the interaction, has been explained from the fact that its velocity dependence has been introduced in order to mimic

the finite-range effects of a local interaction. One can see that by going further in the expansion on the relative momentum operators, the higher-order terms of the pseudopotential are not anymore all stand-alone gauge invariant. By imposing the invariance under the gauge transformation, we force the parameters $C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S}$ to occur in certain linear combinations, which are gauge invariant.

These linear combination can be derived from a condition of invariance of the pseudopotential under the gauge transformation, after having transferred the action of the gauge transformation from the many-body wavefunction to the pseudopotential,

$$\hat{V}\prime = e^{-i\phi(r'_2)}e^{-i\phi(r'_1)}\hat{V}e^{i\phi(r_1)}e^{i\phi(r_2)}. \tag{3.22}$$

In the following we fill the gap in the derivation of Eq. 13 of paper I from Eq. (3.22) and we show how the gauge-invariant condition has been effectively implemented. The results of this analysis can be read from Sec. IIC and from Appendix B of paper I.

By using twice the Baker-Hausdorff lemma we can work out Eq. (3.22),

$$\begin{aligned}
\hat{V}\prime &= e^{-i\phi(r'_2)}\left(\hat{V} + [\phi(r_1),\hat{V}] + \frac{1}{2}[\phi(r_1),[\phi(r_1),\hat{V}]] + ...\right)e^{i\phi(r_2)} \\
&= \left(\hat{V} + [\phi(r_1),\hat{V}] + \frac{1}{2}[\phi(r_1),[\phi(r_1),\hat{V}]] + ...\right) \\
&+ \left[\phi(r_2),\left(\hat{V} + [\phi(r_1),\hat{V}] + \frac{1}{2}[\phi(r_1),[\phi(r_1),\hat{V}]] + ...\right)\right] \\
&+ \frac{1}{2}\left[\phi(r_2),\left[\phi(r_2),\left(\hat{V} + [\phi(r_1),\hat{V}] + \frac{1}{2}[\phi(r_1),[\phi(r_1),\hat{V}]] + ...\right)\right]\right] \\
&+ \ldots,
\end{aligned} \tag{3.23}$$

where the commutators must be interpreted according to the following definition ($i = 1, 2$),

$$[\phi(r_i),\hat{V}] \equiv \phi(r'_i)\hat{V} - \hat{V}\phi(r_i). \tag{3.24}$$

Then the condition for the gauge invariance of the pseudopotential is,

$$\begin{aligned}
&[\phi(r_1),\hat{V}]+\frac{1}{2}[\phi(r_1),[\phi(r_1),\hat{V}]]+\dots\\
&+[\phi(r_2),\hat{V}]+[\phi(r_2),[\phi(r_1),\hat{V}]]+\frac{1}{2}[\phi(r_2),[\phi(r_1),[\phi(r_1),\hat{V}]]]+\dots\\
&+\frac{1}{2}[\phi(r_2),[\phi(r_2),\hat{V}]]+\frac{1}{2}[\phi(r_2),[\phi(r_2),[\phi(r_1),\hat{V}]]]\\
&+\frac{1}{4}[\phi(r_2),[\phi(r_1),[\phi(r_1),\hat{V}]]]+...=0.
\end{aligned} \tag{3.25}$$

In Eq. (3.25) there are commutators, double commutators, and so on in a sum composed by an infinite number of terms. At first order, we see that the condition for the gauge invariance of the pseudopotential is

$$[\phi(r_1),\hat{V}]+[\phi(r_2),\hat{V}]=0, \tag{3.26}$$

which is in fact the condition of Eq. 13 of paper I.

This condition is sufficient to guarantee that all other high-order commutators are null, provided that it is verified when two generic test functions $F(r_1',r_2')$ and $G(r_1,r_2)$ are applied on it. The function $F(r_1',r_2')$ represents a generic function obtained as a product of the functions $\phi(r_1')$ and $\phi(r_2')$, that is,

$$F(r_1',r_2')\equiv\phi^m(r_1')\phi^n(r_2'), \tag{3.27}$$

for two integers m and n, and analogously for the other function $G(r_1,r_2)$. Both functions appears respectively on the left-hand side and on right-hand side of the terms $[\phi(r_i),\hat{V}]$ in the expansion of Eq. (3.25).

Therefore the condition for the gauge invariance of the pseudopotential in Eq. (3.26) is now,

$$F(r_1',r_2')\left([\phi(r_1),\hat{V}]+[\phi(r_2),\hat{V}]\right)G(r_1,r_2)=0, \tag{3.28}$$

and it has been explicitly implemented as

$$\begin{aligned}
&F(r_1',r_2')\phi(r_1')\hat{V}G(r_1,r_2)-F(r_1',r_2')\hat{V}\phi(r_1)G(r_1,r_2)\\
&+F(r_1',r_2')\phi(r_2')\hat{V}G(r_1,r_2)-F(r_1',r_2')\hat{V}\phi(r_2)G(r_1,r_2)=0.
\end{aligned} \tag{3.29}$$

In this section, we have applied the gauge transformation to the pseudopotential and we have calculated the condition (3.29) that gives the constraints among the parameters of the gauge-invariant pseudopotential. With the aid of symbolic programming, we have obtained the specific set of constraints on the parameters and terms of the pseudopotentials, which are collected in Appendix B of paper I.

3.6 The averaging of the pseudopotential

In the mean-field approximation, for instance in the HF theory, the ground-state energy is obtained as the expectation value of the Hamiltonian over a product state $|\Phi\rangle$ and it turns out to be a functional of the single-particle density matrix ρ,

$$E^{HF} = \langle\Phi|H|\Phi\rangle = \mathrm{Tr}(\hat{T}\rho) + \frac{1}{2}\mathrm{Tr}(\hat{\Gamma}\rho), \tag{3.30}$$

where the shorthand notation Tr denotes integration over spatial coordinates and sum over spin and isospin indices. In Eq. (3.30), we find the one-body kinetic energy $\hat{T}$, while the two-body interaction $\hat{V}$ is contained in the single-particle (p-h) self-consistent potential,

$$\hat{\Gamma}(\boldsymbol{r}_1' s_1' t_1', \boldsymbol{r}_1 s_1 t_1) = \int \mathrm{d}\,\boldsymbol{r}_2 d\boldsymbol{r}_2' \sum_{\substack{s_2 t_2 \\ s_2' t_2'}} \hat{V}(\boldsymbol{r}_1' s_1' t_1' \boldsymbol{r}_2' s_2' t_2', \boldsymbol{r}_1 s_1 t_1 \boldsymbol{r}_2 s_2 t_2)\rho(\boldsymbol{r}_2 s_2 t_2, \boldsymbol{r}_2' s_2' t_2'). \tag{3.31}$$

By inserting our zero-range pseudopotential of Eq. (3.2) in the expression of Eq. (3.31) and by inserting in turn the expression obtained in the HF-energy (3.30), we can write the energy functional as a three-dimensional spatial integral of a quasilocal energy density. This lengthy calculation yields a relation between the parameters of the pseudopotential and coupling constants of the functional, according to the schematic expression in Eq. 21 of paper I, that we report here for sake of clarity,

$$\langle C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S} \hat{V}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S} \rangle = \sum C^{n'L'v'J',t}_{mI,nLvJ} T^{n'L'v'J',t}_{mI,nLvJ}. \tag{3.32}$$

As important consequence of having derived the N^{3}LO functional from a pseudopotential is the fact that the energy functional is free from the self-interaction problem [PZ81]. The self-interaction problem in DFT is due to the fact that the exchange-correlation potential is given in an approximate way. The approximation may not take into account correctly the Pauli exclusion principle, leading in this way to a nonphysical interaction of the particles with themselves. The derivation from an interaction is a sufficient condition to guarantee that the internal energy in the one-particle limit vanishes exactly. The averaging is in fact performed within an HF approximation, where the self-interaction is removed by the exact cancellation between direct and exchange terms. Of course, the presence of an interaction is not a necessary condition and the removal of spurious self-interactions in nuclear functionals can be also achieved directly

on the functional, by imposing the constraints among the coupling constants which lead to a vanishing functional in the one-particle limit [Ch10].

3.7 Technical details of the averaging procedure

In this section we discuss some technicalities concerning the calculation of the averaging of the pseudopotential over the uncorrelated wave function, the Slater determinant, that we have discussed in the previous section.

3.7.1 Recoupling of the relative-momentum operators

If we compare the tensorial forms of the pseudopotential and functional, we see that both are composed by the same building blocks, differential and spin operators. As a matter of fact, both pseudopotential and EDF have relative-momentum tensors but, as manifested by different indices denoting the order and rank of the K operators, they are built in different ways. In the pseudopotential, the relative-momentum tensors are built as differences of differential operators acting on two distinct particles, whereas in the EDF the relative-momentum tensors only act on one particle at the time: the reason of this is that the relative-momentum tensors in the interaction are interpreted as the finite range component of the two-body interaction, while in the functional these operators are used to build the higher-order densities of the single particle. Therefore, the averaging calculation has required a recoupling of spherical tensors inside the integral in the averaging formula,

$$\begin{aligned}\mathcal{E} &= \frac{1}{4}\int \mathrm{d}\,\boldsymbol{r}_1\boldsymbol{r}_2\boldsymbol{r}'_1\boldsymbol{r}'_2 \sum_{\substack{\sigma_1\sigma_2\\ \sigma'_1\sigma'_2}}\sum_{\substack{\tau_1\tau_2\\ \tau'_1\tau'_2}} \hat{V}(\boldsymbol{r}'_1\sigma'_1\tau'_1\boldsymbol{r}'_2\sigma'_2\tau'_2, \boldsymbol{r}_1\sigma_1\tau_1\boldsymbol{r}_2\sigma_2\tau_2)\\ &\quad \rho(\boldsymbol{r}_1\sigma_1\tau_1, \boldsymbol{r}'_1\sigma'_1\tau'_1)\rho(\boldsymbol{r}_2\sigma_2\tau_2, \boldsymbol{r}'_2\sigma'_2\tau'_2),\end{aligned} \tag{3.33}$$

and it has been performed with the aid of symbolic programming. We have considered at each order of the expansion in derivatives, all the possible different couplings of the spherical tensor derivatives entering in the pseudopotential, whose general form can be read from Eq. (3.2) as,

$$\left[K'_{\tilde{n}'\tilde{L}'}K_{\tilde{n}\tilde{L}}\right]_S + (-1)^{v_{12}+S}\left[K'_{\tilde{n}\tilde{L}}K_{\tilde{n}'\tilde{L}'}\right]_S. \tag{3.34}$$

Considering all the possible values of the rank S, they are 5 at second order (see Table III of paper I), 11 at fourth order (see Table IV of paper I) and 20 at sixth order (see Table V of paper I). Each different spherical tensor (3.34) is

explicitly built as a coupling of the building block component, i.e. the vector (rank 1) operator ∇ according to definitions given in Eqs. (3.3) and (3.4), and it was applied on a generic test function. Then, from the resulting expression was subtracted an ansatz given by a combination of all possible recoupled forms suitable for the functional, that is,

$$\sum_{\substack{m'I',n'L',R' \\ mI,nL,R}} C^{m'I',n'L',R'}_{mI,nL,RS} \left[\left[D^{(1)}_{m'I'} K^{(1)}_{n'L'} \right]_{R'} \left[D^{(2)}_{mI} K^{(2)}_{nL} \right]_{R} \right]_{S}, \tag{3.35}$$

where $C^{m'I',n'L',R'}_{mI,nL,RS}$ are the numerical coefficients of the combination of terms, and the relative-momentum tensors $K^{(1)}_{n'L'}$ and $K^{(2)}_{nL}$ are built from the spherical representation of the relative-momenta operators acting on one particle at the time,

$$\boldsymbol{k}_1 = \frac{1}{2i}(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}'_1), \tag{3.36}$$

$$\boldsymbol{k}_2 = \frac{1}{2i}(\boldsymbol{\nabla}_2 - \boldsymbol{\nabla}'_2), \tag{3.37}$$

whereas the differential operators $D^{(1)}_{m'I'}$ and $D^{(2)}_{mI}$ are built from the spherical representation of the derivatives operators acting on one particle at the time,

$$\boldsymbol{D}_1 = -i(\boldsymbol{\nabla}_1 + \boldsymbol{\nabla}'_1), \tag{3.38}$$

$$\boldsymbol{D}_2 = -i(\boldsymbol{\nabla}_2 + \boldsymbol{\nabla}'_2). \tag{3.39}$$

We see that combination (3.35) preserves the total rank of the tensor in Eq. (3.34) and also the total order must be preserved, namely, we require that

$$2(\tilde{n}' + \tilde{n}) = m' + n' + m + n. \tag{3.40}$$

Also the spherical tensor (3.35) was applied previously on a generic test function. What we finally obtained by subtracting equations (3.35) and (3.34), was required to be identically equal to zero, giving in such a way a set of equations for coefficients $C^{m'I',n'L',R'}_{mI,nL,RS}$ in Eq. (3.35). The analytic solution of this system of equations was again calculated by using symbolic programming. In the following we give the results of the recoupling for the 5 second-order tensors. These expressions can be compared with the corresponding ones calculated in Cartesian representation[PRD04],

$$
\begin{aligned}
K'_{20}+K_{20} &= \frac{1}{4}\left(K^{(1)}_{20}+K^{(2)}_{20}\right)-\frac{1}{16}\left(D^{(1)}_{20}+D^{(2)}_{20}\right) \\
&\quad -\frac{1}{2}\left[K^{(1)}_{11}K^{(2)}_{11}\right]_0+\frac{1}{8}\left[D^{(1)}_{11}D^{(2)}_{11}\right]_0, && \text{(3.41a)}\\
K'_{22}+K_{22} &= \frac{1}{4}\left(K^{(1)}_{22}+K^{(2)}_{22}\right)-\frac{1}{16}\left(D^{(1)}_{22}+D^{(2)}_{22}\right) \\
&\quad -\frac{1}{2}\left[K^{(1)}_{11}K^{(2)}_{11}\right]_2+\frac{1}{8}\left[D^{(1)}_{11}D^{(2)}_{11}\right]_2, && \text{(3.41b)}\\
[K'_{11}K_{11}]_0 &= \frac{1}{4}\left(K^{(1)}_{20}+K^{(2)}_{20}\right)+\frac{1}{16}\left(D^{(1)}_{20}+D^{(2)}_{20}\right) \\
&\quad -\frac{1}{2}\left[K^{(1)}_{11}K^{(2)}_{11}\right]_0-\frac{1}{8}\left[D^{(1)}_{11}D^{(2)}_{11}\right]_0, && \text{(3.41c)}\\
[K'_{11}K_{11}]_1 &= \frac{i}{4}\left(\left[D^{(1)}_{11}K^{(1)}_{11}\right]_1+\left[D^{(2)}_{11}K^{(2)}_{11}\right]_1+\left[K^{(1)}_{11}D^{(2)}_{11}\right]_1\right) \\
&\quad -\frac{i}{4}\left[D^{(1)}_{11}K^{(2)}_{11}\right]_1, && \text{(3.41d)}\\
[K'_{11}K_{11}]_2 &= \frac{1}{4}\left(K^{(1)}_{22}+K^{(2)}_{22}\right)+\frac{1}{16}\left(D^{(1)}_{22}+D^{(2)}_{22}\right) \\
&\quad -\frac{1}{2}\left[K^{(1)}_{11}K^{(2)}_{11}\right]_2-\frac{1}{8}\left[D^{(1)}_{11}D^{(2)}_{11}\right]_2. && \text{(3.41e)}
\end{aligned}
$$

3.7.2 Recouplings on the functional

When the recoupling of the relative-momentum operators described in Sec. (3.7.1) and summations over spin and isospin are performed, we are left with a functional whose general form is now,

$$
\begin{aligned}
\mathcal{T} \;\equiv\; & \frac{1}{4}\int \mathrm{d}\,\boldsymbol{r}_1\boldsymbol{r}_2\boldsymbol{r}'_1\boldsymbol{r}'_2\left[\left[\left[\left[D^{(1)}_{m'I'}K^{(1)}_{n'L'}\right]_{R'}\left[D^{(2)}_{mI}K^{(2)}_{nL}\right]_R\right]_S\hat{\mathcal{R}}_{v_{12}S}\right]_0\right]^0 \\
& \hat{\delta}_{12}(\boldsymbol{r}'_1\boldsymbol{r}'_2;\boldsymbol{r}_1\boldsymbol{r}_2), \qquad \text{(3.42)}
\end{aligned}
$$

where a summation over all the indices of the tensor is implicit and we kept the notation adopted in Eqs. (3.41) with superscript (1) and (2). We decided to use the symbol $\mathcal{T}$ instead of $\mathcal{E}$ to denote the term in Eq. (3.42) because it does not coincide exactly with the EDF, having we dropped in the integrand the coupling constants and numerical coefficients coming from the traces and the relative-momenta recouplings.

The tensor $\hat{\mathcal{R}}_{v_{12}S}$ is defined similarly to the symmetrized two-body spin operator in Eq. (3.5) as,

$$\hat{\mathcal{R}}_{v_{12}S} = \left(1 - \frac{1}{2}\delta_{v,v'}\right)\left(\left[\left[\rho^{t(1)}_{v'}\rho^{t(2)}_{v}\right]_S\right]^0 + \left[\left[\rho^{t(1)}_{v}\rho^{t'(2)}_{v'}\right]_S\right]^0\right), \tag{3.43}$$

with $v_{12} = v + v'$, through the different channels of the density matrix,

$$\rho^{t(1)}_{v'} \equiv \rho^{t}_{v'}(\boldsymbol{r}_1, \boldsymbol{r}'_1), \tag{3.44a}$$
$$\rho^{t(2)}_{v} \equiv \rho^{t}_{v}(\boldsymbol{r}_2, \boldsymbol{r}'_2), \tag{3.44b}$$

and analogously for t'.

The expression of the tensors in Eq. (3.42) formally matches the structure of the EDF, but we may notice that the form of the tensor in the integrand does not match with the one on the r.h.s of Eq. (3.32), explicitly shown in Eq. (2.17).

In the following we show explicitly all the recouplings needed to get the form $T^{n'L'v'J',t}_{mI,nLvJ}$ of the functional. The starting point is the spherical tensor,

$$\hat{\mathcal{T}} \equiv \left[\left[\left[\left[D^{(1)}_{m'I'}K^{(1)}_{n'L'}\right]_{R'}\left[D^{(2)}_{mI}K^{(2)}_{nL}\right]_R\right]_S\left[\rho^{t(1)}_{v'}\rho^{t(2)}_{v}\right]_S\right]_0\right]^0, \tag{3.45}$$

which is a term in the integrand in Eq. (3.42).

Then we can proceed with the recoupling, in which the two tensors composed by derivatives operators with index (1) and (2) are coupled with the two corresponding densities,

$$\begin{aligned}
\hat{\mathcal{T}} &= \left[\left[\left[\left[\left[D^{(1)}_{m'I'}K^{(1)}_{n'L'}\right]_{R'}\left[D^{(2)}_{mI}K^{(2)}_{nL}\right]_R\right]_S\rho^{t(2)}_{v}\right]_{v'}\rho^{t(1)}_{v'}\right]_0\right]^0 \\
&= \sum_{Q=|R-v|}^{R+v}(-1)^{R+R'+v+v'}\sqrt{2S+1}\sqrt{2Q+1}\begin{Bmatrix} R' & R & S \\ v & v' & Q\end{Bmatrix} \\
&\quad \left[\left[\left[\left[D^{(1)}_{m'I'}K^{(1)}_{n'L'}\right]_{R'}\left[\left[D^{(2)}_{mI}K^{(2)}_{nL}\right]_R\rho^{t(2)}_{v}\right]_Q\right]_{v'}\rho^{t(1)}_{v'}\right]_0\right]^0 \\
&= \sum_{Q=|R-v|}^{R+v}(-1)^{R+v-Q}\sqrt{2S+1}\sqrt{2Q+1}\begin{Bmatrix} R' & R & S \\ v & v' & Q\end{Bmatrix} \\
&\quad \left[\left[\left[\left[D^{(1)}_{m'I'}K^{(1)}_{n'L'}\right]_{R'}\rho^{t(1)}_{v'}\right]_Q\left[\left[D^{(2)}_{mI}K^{(2)}_{nL}\right]_R\rho^{t(2)}_{v}\right]_Q\right]_0\right]^0.
\end{aligned} \tag{3.46}$$

The two tensors of rank Q in the last step of Eq. (3.46) require to be separately recoupled in order to obtain a secondary density according to the definition (2.19). The first one becomes (we write explicitly here the limit $\boldsymbol{r}_1 = \boldsymbol{r}'_1$ given by the Dirac delta in the pseudopotential),

$$\left\{\left[\left[D^{(1)}_{m'I'}K^{(1)}_{n'L'}\right]_{R'}\rho^{t(1)}_{v'}\right]_{Q}\right\}_{\boldsymbol{r}_1=\boldsymbol{r}'_1} = \sum_{J'=|L'-v'|}^{L'+v'}(-1)^{I'+L'+v'+Q}\sqrt{2R'+1}\sqrt{2J'+1}\begin{Bmatrix} I' & L' & R' \\ v' & Q & J' \end{Bmatrix}\rho^{t}_{m'I',n'L'v'J',Q}(\boldsymbol{r}_1), \tag{3.47}$$

and analogously the second one is,

$$\left\{\left[\left[D^{(2)}_{mI}K^{(2)}_{nL}\right]_{R}\rho^{t(2)}_{v}\right]_{Q}\right\}_{\boldsymbol{r}_2=\boldsymbol{r}'_2} = \sum_{J=|L-v|}^{L+v}(-1)^{I+L+v+Q}\sqrt{2R+1}\sqrt{2J+1}\begin{Bmatrix} I & L & R \\ v & Q & J \end{Bmatrix}\rho^{t}_{mI,nLvJ,Q}(\boldsymbol{r}_2). \tag{3.48}$$

By inserting Eqs. (3.47) and (3.48) into the coupling to a scalar in Eq. (3.46), we can write the term in (3.42) as,

$$\begin{aligned}\mathcal{T} = \int \mathrm{d}\,\boldsymbol{r} \sum_{Q=|R-v|}^{R+v}(-1)^{R+v-Q}\sqrt{2S+1}\sqrt{2Q+1}\begin{Bmatrix} R' & R & S \\ v & v' & Q \end{Bmatrix} \\ \times \sum_{J'=|L'-v'|}^{L'+v'}\sum_{J=|L-v|}^{L+v}(-1)^{I'+L'+v'+I+L+v}\sqrt{2R'+1}\sqrt{2J'+1} \\ \times\sqrt{2R+1}\sqrt{2J+1}\begin{Bmatrix} I' & L' & R' \\ v' & Q & J' \end{Bmatrix}\begin{Bmatrix} I & L & R \\ v & Q & J \end{Bmatrix}T^{mI,nLvJ,t}_{mI,nLvJ,Q}(\boldsymbol{r}).\end{aligned} \tag{3.49}$$

The recoupled form in the last line of Eq. (3.49) corresponds to the first form of the nuclear EDF introduced in [CDK08] (see Eq. (28) therein). This is the most general form which is suitable for the case of density-dependent coupling constants. In our study, we do not consider density-dependent parameters in the pseudopotential, therefore we are in the case of density-independent coupling constants of the functional. Then, by performing integration by parts, we are allowed to transfer tensor $D_{m'I'}$ from the first density to the second and our averaging calculation will produce a functional whose terms have the form showed in Eq. (2.17). In the following we present the explicit recoupling needed in order to perform the integration by parts.

So we have,

$$\begin{aligned}
&\left[\left[\left[D^{(1)}_{m'I'}\rho^t_{m'I',n'L'v'J'}(\boldsymbol{r}_1)\right]_Q\left[D^{(2)}_{mI}\rho^t_{mI,nLvJ}(\boldsymbol{r}_2)\right]_Q\right]_0\right]^0 \qquad (3.50)\\
&= (-1)^{m'}\sum_{I_{12}=|I-I'|}^{I+I'}(2I_{12}+1)(2Q+1)\begin{Bmatrix} I' & I & I_{12}\\ J' & J & I_{12}\\ Q & Q & 0\end{Bmatrix}\\
&\left[\left[\left[D^{(1)}_{m'I'}D^{(2)}_{mI}\right]_{I_{12}}\left[\rho^t_{m'I',n'L'v'J'}(\boldsymbol{r}_1)\rho^t_{mI,nLvJ}(\boldsymbol{r}_2)\right]_{I_{12}}\right]_0\right]^0\\
&= (-1)^{m'}\sum_{I_{12}=|I-I'|}^{I+I'}\sqrt{2I_{12}+1}\sqrt{2Q+1}(-1)^{I_{12}+Q+I+J'}\begin{Bmatrix} I' & I & I_{12}\\ J & J' & Q\end{Bmatrix}\\
&(-1)^{J'+J-I_{12}}\left[\left[\rho^t_{m'I',n'L'v'J'}(\boldsymbol{r}_1)\left[\left[D^{(2)}_{m'I'}D^{(2)}_{mI}\right]_{I_{12}}\rho^t_{mI,nLvJ}(\boldsymbol{r}_2)\right]_{J'}\right]_0\right]^0,
\end{aligned}$$

where we see that both differential operators are now acting on the same coordinate. Now, the two differential operators acting on the same density need to be transformed into one differential operator with the same order $m+m'$ and rank I_{12}. The coefficients of the transformation can be obtained through the following derivation, made on the coupling of simple functions of the space coordinate, and applied to the more complicated case of the differential operators. By using the expansion of the functions $r^{(2)}_{mI}$ and $r^{(2)}_{m'I'}$ in solid harmonics, we get[C10]

$$\begin{aligned}
\left[r^{(2)}_{mI}r^{(2)}_{m'I'}\right]_{I_{12}M} &= \left[\sum_{M_IM'_I}\frac{4\pi}{\sqrt{2I+1}\sqrt{2I'+1}}C^r_{mI}C^r_{m'I'}r_2^{I+I'}Y_{IM_I}Y_{I'M'_I}\right]_{I_{12}M_I}\\
&= \frac{4\pi}{\sqrt{2I+1}\sqrt{2I'+1}}C^r_{mI}C^r_{m'I'}r_2^{m+m'}\left[Y_{IM_I}Y_{I'M'_I}\right]_{I_{12}M_I}\\
&= \sqrt{\frac{4\pi}{(2I_{12}+1)}}C^r_{mI}C^r_{m'I'}r_2^{m+m'}C^{I_{12}0}_{I0,I'0}Y_{I_{12}M}(\vartheta,\varphi)\\
&= \sqrt{\frac{4\pi}{(2I_{12}+1)}}C^r_{mI}C^r_{m'I'}C^{I_{12}0}_{I0,I'0}\sqrt{\frac{2I_{12}+1}{4\pi}}\frac{r_{(m+m')I_{12}M}}{C^r_{(m+m')I_{12}}}\\
&= \frac{C^r_{mI}C^r_{m'I'}}{C^r_{(m+m')I_{12}}}C^{I_{12}0}_{I0,I'0}r_{(m+m')I_{12}M}, \qquad (3.51)
\end{aligned}$$

where in the first step we used the condition $I+I'=m+m'$, which is valid because the function expanded was in fact a power of r and the total order must be conserved in the expansion, whereas in the second step we used a relation involving a direct product of two spherical harmonics of the same argument (see Eq. (10) of Ch. 5.6 in [VMK88]).

With the use of the coefficients from Eq. (3.51), we can write the relation between the two alternative forms of the EDF,

$$
\begin{aligned}
T^{mI,nLvJ,t}_{mI,nLvJ,Q}(\boldsymbol{r}) &= (-1)^{m'}\sqrt{2Q+1}\sum_{I_{12}=|I-I'|}^{I+I'}\sqrt{2I_{12}+1}(-1)^{Q+I+J} \\
&\times \begin{Bmatrix} I' & I & I_{12} \\ J & J' & Q \end{Bmatrix} \frac{C^r_{mI}C^r_{m'I'}}{C^r_{(m+m')I_{12}}} C^{I_{12}0}_{I0,I'0} T^{nLvJ,t}_{(m+m')I_{12},nLvJ,Q}(\boldsymbol{r}),
\end{aligned} \tag{3.52}
$$

and by inserting back this relation in Eq. (3.49) we have obtained the fully recoupled form of the term $\mathcal{T}$ as it is calculated through the averaging of the pseudopotential in Eq. (3.42), namely,

$$
\begin{aligned}
\mathcal{T} &= \int \mathrm{d}\,\boldsymbol{r} \sum_{Q=|R-v|}^{R+v} (-1)^{R+v-Q}\sqrt{2S+1}\sqrt{2Q+1}\begin{Bmatrix} R' & R & S \\ v & v' & Q \end{Bmatrix} \\
&\times \sum_{J'=|L'-v'|}^{L'+v'} \sum_{J=|L-v|}^{L+v} (-1)^{I'+L'+v'+I+L+v}\sqrt{2R'+1}\sqrt{2J'+1} \\
&\times \sqrt{2R+1}\sqrt{2J+1}\begin{Bmatrix} I' & L' & R' \\ v' & Q & J' \end{Bmatrix}\begin{Bmatrix} I & L & R \\ v & Q & J \end{Bmatrix}(-1)^{m'} \\
&\times \sqrt{2Q+1}\sum_{I_{12}=|I-I'|}^{I+I'}\sqrt{2I_{12}+1}(-1)^{Q+I+J} \\
&\times \begin{Bmatrix} I' & I & I_{12} \\ J & J' & Q \end{Bmatrix} \frac{C^r_{mI}C^r_{m'I'}}{C^r_{(m+m')I_{12}}} C^{I_{12}0}_{I0,I'0} T^{nLvJ,t}_{(m+m')I_{12},nLvJ,Q}(\boldsymbol{r}).
\end{aligned} \tag{3.53}
$$

In this section, we have worked out two technical results concerning the averaging of the pseudopotential over the uncorrelated many-body wave function. We list them briefly:

- The recoupling of the relative-momentum operators in the pseudopotential. Such a recoupling was needed in order to obtain the relative momentum tensors, entering in the definition of the higher-order densities of the functional (Sec. (3.7.1)).
- The recoupling relating two alternative forms to write the functional, that is the two forms denoted respectively by $T^{m'I',n'L'v'J',t}_{mI,nLvJ}$ and $T^{n'L'v'J',t}_{mI,nLvJ}$ (Sec. (3.7.2)).

Chapter 4

Continuity Equation for N^{3}LO Nuclear EDF

4.1 Overview of the paper II

As we did in Sec. 3.1 for the paper on the pseudopotential, in this section we review the main contents exposed in paper II and we introduce topics that were not included in paper II. These topics are treated extensively in the following sections in order to complete our study of the continuity equation for N^{3}LO EDFs.

In paper II, we analyzed conditions under which the continuity equation (CE) is valid for the N^{3}LO EDFs or pseudopotentials built of higher-order derivatives. We derived constraints on the coupling constant of the functional that guarantee the validity of the CE in all spin-isospin channels. We also linked these constraints to local gauge symmetries for abelian and non-abelian transformation groups.

In Sec. IIA of paper II, we recalled the CE for a single particle moving in a scalar and vector local potentials. The CE can describe the conservative transport of the probability scalar density [Me62], as in the case of the equation

$$\frac{\partial}{\partial t}\rho(\boldsymbol{r},t) = -\frac{\hbar}{m}\boldsymbol{\nabla}\cdot\boldsymbol{j}(\boldsymbol{r},t), \tag{4.1}$$

where the density and current are defined respectively as,

$$\rho(\boldsymbol{r},t) = \sum_{\sigma} |\psi(\boldsymbol{r}\sigma,t)|^2, \tag{4.2a}$$

$$\boldsymbol{j}(\boldsymbol{r},t) = \sum_{\sigma} \mathrm{Im}\Big(\psi^*(\boldsymbol{r}\sigma,t)\boldsymbol{\nabla}\psi(\boldsymbol{r}\sigma,t)\Big). \tag{4.2b}$$

We can be interested also in the conservative transport of the spin orientation of the particle, then we end up with a CE relating the spin density $s_\nu(\boldsymbol{r},t)$ to the spin current $\boldsymbol{J_\nu}(\boldsymbol{r},t)$,

$$\frac{\partial}{\partial t}s_\nu(\boldsymbol{r},t) = -\frac{\hbar}{m}\boldsymbol{\nabla}\cdot\boldsymbol{J}_\nu(\boldsymbol{r},t) + \frac{1}{\hbar}\Big(\boldsymbol{V}_1(\boldsymbol{r},t)\times\boldsymbol{s}(\boldsymbol{r},t)\Big)_\nu, \tag{4.3}$$

where

$$s_\nu(\boldsymbol{r},t) = \sum_{\sigma'\sigma} \psi^*(\boldsymbol{r}\sigma',t)\langle\sigma'|\sigma_\nu|\sigma\rangle\psi(\boldsymbol{r}\sigma,t), \tag{4.4a}$$

$$\boldsymbol{J_\nu}(\boldsymbol{r},t) = \sum_{\sigma'\sigma} \mathrm{Im}\Big(\psi^*(\boldsymbol{r}\sigma',t)\langle\sigma'|\sigma_\nu|\sigma\rangle\boldsymbol{\nabla}\psi(\boldsymbol{r}\sigma,t)\Big), \tag{4.4b}$$

and $\boldsymbol{V}_1(\boldsymbol{r},t)$ is a vector real time-dependent potential.

In Sec. IIB of paper II, we put ourselves in the framework of the time-dependent density functional theory (TDDFT) in order to generalize the CE to the case of the many-body systems. The equation of motion for the one-body density matrix $\rho_{\alpha\beta}$ is the starting point for the CE in the many-body theory,

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\rho = [h,\rho], \tag{4.5}$$

where the mean-field Hamiltonian $h_{\alpha\beta}$ is defined as the derivative of the total energy $E\{\rho\}$ with respect to the density matrix [RS80],

$$h_{\alpha\beta} = \frac{\partial E\{\rho\}}{\partial\rho_{\beta\alpha}}, \tag{4.6}$$

and total energy is the sum of the kinetic and potential-energy terms,

$$E\{\rho\} = E_k\{\rho\} + E_p\{\rho\}. \tag{4.7}$$

We have presented the argument [BR86] stating that the potential energy density, that is,

$$\Gamma_{\alpha\beta} = \frac{\partial E_p\{\rho\}}{\partial\rho_{\beta\alpha}}, \tag{4.8}$$

which is gauge-invariant, produces the CE for the scalar-isoscalar density,

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_0^0(\boldsymbol{r},t) = -\frac{\hbar}{m}\boldsymbol{\nabla}\cdot\boldsymbol{j}_0^0(\boldsymbol{r},t). \tag{4.9}$$

In particular, we showed that the gauge invariance of the potential energy is a necessary and sufficient condition for the validity of the CE.

The argument was explicitly performed for abelian local gauge transformation, defined as,

$$\psi'_\alpha(\boldsymbol{r}\sigma\tau) \equiv (U\psi_\alpha)(\boldsymbol{r}\sigma\tau) = e^{i\gamma(\boldsymbol{r})}\psi_\alpha(\boldsymbol{r}\sigma\tau), \tag{4.10}$$

whose action on the nonlocal density was specified in Eq. (2.58). The local gauge transformation in Eq. (4.10) can be generalized to the four local spin-isospin groups according to Eq. (2.62). In fact, the invariance of the potential energy under the transformations induced by the groups in Eq. (2.62), leads to the corresponding CEs for densities in the scalar-isoscalar ($v = 0$, $t = 0$), scalar-isovector ($v = 0$, $t = 1$), vector-isoscalar ($v = 1$, $t = 0$), and vector-isovector ($v = 1$, $t = 1$) channels,

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho^t_v(\boldsymbol{r}) = -\frac{\hbar}{m}\boldsymbol{\nabla}\cdot\boldsymbol{J}^t_v(\boldsymbol{r}), \tag{4.11}$$

where the spin-isospin densities can be expressed as traces of the density matrix,

$$\rho^t_v(\boldsymbol{r},\boldsymbol{r}') \;=\; \sum_{\sigma\tau,\sigma'\tau'} \sigma^{\sigma'\sigma}_v \tau^t_{\tau'\tau}\rho(\boldsymbol{r}\sigma\tau,\boldsymbol{r}'\sigma'\tau'). \tag{4.12}$$

The argument presented in Sec. IIB of paper II was confirmed by considering, as potential energy, the one-body pseudopotential, which is obtained as variation of the N^{3}LO EDF (2.16) with respect to the density matrix. For this purpose, the strategy used in Sec. IIC was to start from the Schrödinger equation with the one-body pseudopotential for the time evolution of the single-particle wave function, and then derive a condition for the validity of the CE. The definition and the main features of the one-body pseudopotential are reviewed in Secs. 4.2.2- 4.3, whereas the general condition for the validity of the CEs in all spin-isospin channel can be found in Sec. 4.2 and its complete derivation in Appendix A. In particular, the contributions from the kinetic and pseudopotential operators in the Schrödinger equation are treated separately in Sec. 4.2: the former gives rise to the current density term in the CE and can be found in Sec. 4.2.1, the latter produces the condition that sets the constraints between the coupling constants of the EDF compatible with the CE and is presented in Sec. 4.2.2.

As main result, we have obtained four different sets of constraints on the coupling constants of the N^{3}LO EDF that guarantee the validity of the CE in the corresponding spin-isospin channels. All these results are displayed in Sec. III and Appendix A of paper II. In general, we found that the validity of the CE for a channel of the density matrix is equivalent to the invariance of the N^{3}LO EDF under a local gauge transformation. A more detailed overview of the results obtained in paper II is given in Sec 5.2.1.

4.2 Derivation of the CE's for the four channels of the density matrix

The Schrödinger equation for a non-relativistic spin-$\frac{1}{2}$ particle with isospin degree of freedom included, is

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\phi_l(\boldsymbol{r}\sigma\tau,t) &= -\frac{\hbar^2}{2m}\triangle\phi_l(\boldsymbol{r}\sigma\tau,t) \\ &+ \sum_{\sigma''\tau''} <\sigma\tau|\hat{\Gamma}(\boldsymbol{r})|\sigma''\tau''>\phi_l(\boldsymbol{r}\sigma''\tau'',t), \end{aligned} \tag{4.13}$$

where $\hat{\Gamma}(\boldsymbol{r})$ can be in general interpreted as one-body pseudopotential, namely, a local or quasilocal interaction which can depend on density. In our study, we discuss the quasilocal one-body pseudopotential corresponding to the N^{3}LO functional [CDT10], which is presented in detail in Sec. 4.2.2.

The corresponding complex-conjugated equation of motion is

$$\begin{aligned} -i\hbar\frac{\partial}{\partial t}\phi_l^*(\boldsymbol{r}'\sigma'\tau',t) &= -\frac{\hbar^2}{2m}\triangle'\phi_l^*(\boldsymbol{r}'\sigma'\tau',t) \\ &+ \sum_{\sigma''\tau''}\Big(<\sigma'\tau'|\hat{\Gamma}(\boldsymbol{r}')|\sigma''\tau''>\Big)^*\phi_l^*(\boldsymbol{r}'\sigma''\tau'',t). \end{aligned} \tag{4.14}$$

Now we multiply Eq. (4.13) by the complex-conjugated wavefunction and sum over the single-particle index l,

$$\begin{aligned} \sum_l i\hbar(\frac{\partial}{\partial t}\phi_l(\boldsymbol{r}\sigma\tau,t))\phi_l^*(\boldsymbol{r}'\sigma'\tau',t) &= \sum_l -\frac{\hbar^2}{2m}(\triangle\phi_l(\boldsymbol{r}\sigma\tau,t))\phi_l^*(\boldsymbol{r}'\sigma'\tau',t) \\ &+ \sum_l\sum_{\sigma''\tau''}\Big(\hat{\Gamma}^{\sigma\sigma''}_{\tau\tau''}(\boldsymbol{r}) \\ &\phi_l(\boldsymbol{r}\sigma''\tau'',t)\phi_l^*(\boldsymbol{r}'\sigma'\tau',t)\Big), \end{aligned} \tag{4.15}$$

and analogously for the complex-conjugated Eq. (4.15),

$$
\begin{aligned}
-\sum_l i\hbar(\frac{\partial}{\partial t}\phi_l^*(\boldsymbol{r}'\sigma'\tau',t))\phi_l(\boldsymbol{r}\sigma\tau,t) &= \sum_l -\frac{\hbar^2}{2m}(\triangle'\phi_l^*(\boldsymbol{r}'\sigma'\tau',t))\phi_l(\boldsymbol{r}\sigma\tau,t) \\
&+ \sum_l \sum_{\sigma''\tau''}\Big(\Big(\hat{\Gamma}^{\sigma'\sigma''}_{\tau'\tau''}{}^*(\boldsymbol{r}') \\
&\quad \phi_l^*(\boldsymbol{r}'\sigma''\tau'',t)\Big)\phi_l(\boldsymbol{r}\sigma\tau,t)\Big), \qquad (4.16)
\end{aligned}
$$

where we have introduced the notation,

$$
< \sigma\tau|\hat{\Gamma}(\boldsymbol{r})|\sigma''\tau'' > \equiv \hat{\Gamma}^{\sigma\sigma''}_{\tau\tau''}(\boldsymbol{r}). \qquad (4.17)
$$

Now we proceed by subtracting member by member the last two equations and we use the definition of the one-body density matrix in the mean-field approximation (Slater determinants), namely

$$
\rho(\boldsymbol{r}\sigma\tau,\boldsymbol{r}'\sigma'\tau') = \sum_l \phi_l^*(\boldsymbol{r}'\sigma'\tau',t)\phi_l(\boldsymbol{r}\sigma\tau,t). \qquad (4.18)
$$

What we get, using the fact that the complex-conjugated density matrix is

$$
\rho^*(\boldsymbol{r}\sigma\tau,\boldsymbol{r}'\sigma'\tau') = \rho(\boldsymbol{r}'\sigma'\tau',\boldsymbol{r}\sigma\tau), \qquad (4.19)
$$

is finally

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\sum_{\sigma\sigma'\tau\tau'}\rho(\boldsymbol{r}\sigma\tau,\boldsymbol{r}'\sigma'\tau') &= \sum_l -\frac{\hbar^2}{2m}\big((\triangle\phi_l(\boldsymbol{r}\sigma\tau,t))\phi_l^*(\boldsymbol{r}'\sigma'\tau',t) \\
&- (\triangle'\phi_l^*(\boldsymbol{r}'\sigma'\tau',t))\phi_l(\boldsymbol{r}\sigma\tau,t)\big) \\
&+ \sum_l\sum_{\sigma''\tau''}(\hat{\Gamma}^{\sigma\sigma''}_{\tau\tau''}(\boldsymbol{r})\phi_l(\boldsymbol{r}\sigma''\tau'',t)\phi_l^*(\boldsymbol{r}'\sigma'\tau',t) \\
&- (\hat{\Gamma}^{\sigma'\sigma''}_{\tau'\tau''}{}^*(\boldsymbol{r}')\phi_l^*(\boldsymbol{r}'\sigma''\tau'',t))\phi_l(\boldsymbol{r}\sigma\tau,t)). \qquad (4.20)
\end{aligned}
$$

With Eq. (4.20) we have obtained a general equation which describes the transport of the four channels included in the one-body density matrix. On the r.h.s. two different terms appear, the first coming from the kinetic term of the Schrödinger equation and the second depending on the one-body pseudopotential. These two contribution will be separately treated in the next sections.

4.2.1 Contribution to the CE from the kinetic term

In this section we use the Cartesian notation in order to obtain the term of the CE depending on the current density in the traditional form, leaving the spherical tensor notation for the part depending on the pseudopotential. To see the contribution of the kinetic part we multiply the first term in the r.h.s. of Eq. (4.20) by the spin and isospin operators,

$$\sigma_v^{\sigma\sigma'}\tau^t_{\tau\tau'} \equiv \langle\sigma|\sigma_v|\sigma'\rangle\langle\tau|\tau^t|\tau'\rangle, \tag{4.21}$$

and we sum up over spin and isospin coordinates. In this way, what we get is

$$\begin{aligned}
&\sum_{\sigma\sigma'\tau\tau'}\sum_{l} -\frac{\hbar^2}{2m}\big((\triangle\phi_l(\boldsymbol{r}\sigma\tau,t))\phi_l^*(\boldsymbol{r}'\sigma'\tau',t)\\
&-(\triangle'\phi_l^*(\boldsymbol{r}'\sigma'\tau',t))\phi_l(\boldsymbol{r}\sigma\tau,t)\big)\sigma_v^{\sigma\sigma'}\tau^t_{\tau\tau'}\\
&= -\frac{\hbar^2}{2m}(2i)\sum_{\sigma\sigma'\tau\tau'}\boldsymbol{\nabla}\cdot\left\{\frac{1}{2i}\left(\boldsymbol{\nabla}-\boldsymbol{\nabla}'\right)\rho(\boldsymbol{r}\sigma\tau,\boldsymbol{r}'\sigma'\tau')\right\}_{r'=r}\sigma_v^{\sigma\sigma'}\tau^t_{\tau\tau'}\\
&= (-\frac{\hbar^2}{2m})(2i)\boldsymbol{\nabla}\cdot\left\{\frac{1}{2i}\left(\boldsymbol{\nabla}-\boldsymbol{\nabla}'\right)\rho^t_v(\boldsymbol{r},\boldsymbol{r}')\right\}_{r'=r}\\
&= (-\frac{\hbar^2}{m})(i)\boldsymbol{\nabla}\cdot J^t_v(\boldsymbol{r}),
\end{aligned} \tag{4.22}$$

where we introduced the definition of the current density,

$$J^t_v(\boldsymbol{r}) \equiv \left\{\frac{1}{2i}\left(\boldsymbol{\nabla}-\boldsymbol{\nabla}'\right)\rho^t_v(\boldsymbol{r},\boldsymbol{r}')\right\}_{r'=r}. \tag{4.23}$$

Therefore, combining Eq. (4.20) with Eq. (4.22), we get a generalized CE,

$$\frac{d}{dt}\rho^t_v(\boldsymbol{r}) = -\frac{\hbar}{m}\nabla\cdot J^t_v(\boldsymbol{r}), \tag{4.24}$$

only if the potential part in Eq. (4.20) does not contribute, namely when the following condition is satisfied,

$$\begin{aligned}
&\sum_{l\sigma''\tau''}(\hat{\Gamma}^{\sigma\sigma''}_{\tau\tau''}(\boldsymbol{r})\phi_l(\boldsymbol{r}\sigma''\tau'',t)\phi_l^*(\boldsymbol{r}'\sigma'\tau',t) - (\hat{\Gamma}^{\sigma'\sigma''*}_{\tau'\tau''}(\boldsymbol{r}')\phi_l^*(\boldsymbol{r}'\sigma''\tau'',t))\phi_l(\boldsymbol{r}\sigma\tau,t))\\
&= \sum_{\sigma''\tau''}\left(\hat{\Gamma}^{\sigma\sigma''}_{\tau\tau''}(\boldsymbol{r})\rho(\boldsymbol{r}\sigma''\tau'',\boldsymbol{r}'\sigma'\tau') - \hat{\Gamma}^{\sigma'\sigma''*}_{\tau'\tau''}(\boldsymbol{r}')\rho(\boldsymbol{r}\sigma\tau,\boldsymbol{r}'\sigma''\tau'')\right) = 0.
\end{aligned} \tag{4.25}$$

In the next section we introduce the explicit form of the N^{3}LO one-body pseudopotential and we examine condition (4.25) for such a pseudopotential.

4.2.2 Contribution to the CE from the one-body pseudopotential

The one-body pseudopotential has the following form in the spherical tensor formalism [CDT10],

$$\hat{\Gamma}(\boldsymbol{r}) = \sum_{\gamma,t} \left[\left[U^t_\gamma(\boldsymbol{r}) \left[D_{n_\gamma L_\gamma} \sigma_{v_\gamma} \right]_{J_\gamma} \right]_0 \tau^t \right]^0 . \tag{4.26}$$

where the potentials

$$U^t_\gamma(\boldsymbol{r}) = \sum_{a\alpha\beta;d\delta} C^{\beta,t}_{a,\alpha} \chi^{\beta;d\delta}_{a,\alpha;\gamma} \left[D_d \rho^t_\delta(\boldsymbol{r}) \right]_{J_\gamma} , \tag{4.27}$$

are linear combinations of the secondary densities, here denoted as $\left[D_d\rho^t_\delta(\boldsymbol{r})\right]_{J_\gamma} \equiv \rho^t_{m_d I_d, n_\delta L_\delta v_\delta J_\delta, J_\gamma}(\boldsymbol{r})$ (see Eq. (2.19)) and $\chi^{\beta;d\delta}_{a,\alpha;\gamma}$ are numerical coefficients. We remark here the use of a grouped notation for the indices, such as the Greek indices $\gamma = \{n_\gamma L_\gamma v_\gamma J_\gamma\}$ and roman indices $a = \{m_a I_a\}$. The precise definitions of all the building blocks constituting the pseudopotential can be found in paper II.

The following recoupling within a scalar is useful for the explicit calculation of condition (4.25),

$$\hat{\Gamma}(\boldsymbol{r}) = \sum_{\gamma,t} \left[\left[U^t_\gamma(\boldsymbol{r}) \left[D_{n_\gamma L_\gamma} \sigma_{v_\gamma} \right]_{J_\gamma} \right]_0 \tau^t \right]^0 = \sum_{\gamma,t} \left[\left[\left[U^t_\gamma(\boldsymbol{r}) D_{n_\gamma L_\gamma} \right]_{v_\gamma} \sigma_{v_\gamma} \right]_0 \tau^t \right]^0 . \tag{4.28}$$

Then the matrix element of the one-body pseudopotential in spin and isospin space can be written as,

$$\hat{\Gamma}^{\sigma\sigma'}_{\tau\tau'}(\boldsymbol{r}) = < \sigma\tau | \hat{\Gamma}(\boldsymbol{r}) | \sigma'\tau' > = \sum_{\gamma,t} \left[\left[\left[U^t_\gamma(\boldsymbol{r}) D_{n_\gamma L_\gamma} \right]_{v_\gamma} \sigma^{\sigma\sigma'}_{v_\gamma} \right]_0 \tau^t_{\tau\tau'} \right]^0 . \tag{4.29}$$

After having inserted Eq. (4.29) in Eq. (4.25) and performed the entire derivation, one ends up with the following condition that implies the CE of the

Eq. (4.24). This condition reads,

$$\sum_{\gamma}\frac{1}{4}\frac{1}{\sqrt{2t''+1}}\sum_{v_\varphi t}(-1)^{-v}(-1)^{-t}\mathcal{A}(v_\gamma,v_\varphi,v;t'',t',t)$$
$$\sum_{J=|L_\gamma-v_\varphi|}^{L_\gamma+v_\varphi}(-1)^{J_\gamma+L_\gamma+v_\varphi+v}\sqrt{2J+1}\left\{\begin{array}{ccc} J_\gamma & L_\gamma & v_\gamma \\ v_\varphi & v & J\end{array}\right\}$$
$$\sum_{n_\varphi L_\varphi m_f I_f}K^{n_\gamma L_\gamma}_{n_\varphi L_\varphi m_f I_f}(i)^{n_\varphi}(\frac{1}{2})^{m_f}\sum_{J_\varphi}(-1)^{I_f+n_\varphi+v_\varphi+J}\sqrt{2L_\gamma+1}\sqrt{2J_\varphi+1}$$
$$\left\{\begin{array}{ccc} I_f & L_\varphi & L_\gamma \\ v_\varphi & J & J_\varphi\end{array}\right\}\sum_{a\alpha\beta;d\delta}\Big(1-(-1)^{v_\gamma-v_\varphi+v}(-1)^{t''-t'+t}(-1)^{n_\varphi+n_\gamma+m_a+m_d}\Big)$$
$$C^{\beta,t''}_{a,\alpha}\,\chi^{\beta;d\delta}_{a,\alpha;\gamma}\left[\Big[\Big[D_d\rho^{t''}_{\delta}(\boldsymbol{r})\Big]_{J_\gamma}\Big[D_f\rho^{t'}_{\varphi}(\boldsymbol{r})\Big]_{J}\Big]_{v\lambda}\right]^{tr}=0, \tag{4.30}$$

where we introduced the following shorthand expression to denote the result of the traces over the spin and isospin indices,

$$\begin{aligned}\mathcal{A}(v_\gamma,v_\varphi,v;t'',t',t) \;=\; &\Big(2(\delta_{(v_\gamma+v_\varphi+v),0}+\frac{1}{2}(1-\delta_{(v_\gamma+v_\varphi+v),0})\\ &(\frac{\sqrt{2}}{i})^{(v_\gamma+v_\varphi+v)}\sqrt{3}(-1)^{\delta_{(v_\gamma+v_\varphi+v),2}}(-1)^{v_\gamma-v_\varphi}\frac{1}{\sqrt{2v+1}})\\ &2(\delta_{(t''+t'+t),0}+\frac{1}{2}(1-\delta_{(t''+t'+t),0})(\frac{\sqrt{2}}{i})^{(t''+t'+t)}\\ &\sqrt{3}(-1)^{\delta_{(t''+t'+t),2}}(-1)^{t''-t'}\frac{1}{\sqrt{2t+1}}\Big).\end{aligned} \tag{4.31}$$

For sake of clarity, we give the link between the expression $\mathcal{A}(v_\gamma,v_\varphi,v;t'',t',t)$ and analogous shorthand symbols $A(v_\gamma,v_\varphi,v)$ and $A(t'',t',t)$ appearing in the CE condition of Eq. (46) in paper II,

$$\begin{aligned}\mathcal{A}(v_\gamma,v_\varphi,v;t'',t',t) \;=\; &A(v_\gamma,v_\varphi,v)(-1)^{v_\gamma-v_\varphi}\frac{1}{\sqrt{2v+1}}\times\\ &A(t'',t',t)(-1)^{t''-t'}\frac{1}{\sqrt{2t+1}}.\end{aligned} \tag{4.32}$$

Expression (4.30) must be considered as condition on the coupling constants $C^{\beta,t''}_{a,\alpha}$ of the N^{3}LO EDF, producing a set of constraints among these coupling constants. The full set of constraints showed in paper II have been derived from formula (4.30) implemented with a symbolic programming. The complete derivation of condition (4.30) can be found in Appendix A.

4.3 Complex conjugation of the one-body pseudopotential

A simple inspection of Eq. (4.25) shows that the complex conjugation of the one-body potential-energy term plays an important role in the assessment of the correct relations among the coupling constants, which allow the CE to be valid. The correct phase of the complex conjugated one-body pseudopotential must then be carefully derived.

In the following we determine this phase by explicitly calculating the complex conjugated field, that is,

$$\hat{\Gamma}^{\sigma\sigma'*}_{\tau\tau'}(\boldsymbol{r}). \tag{4.33}$$

Before we have to define the phase convention for the isospin degree of freedom. The assumption we make is that the phases of isoscalars and the zero-components of isovectors are the same, that is,

$$\begin{aligned} \tau^{t=0,0} &= \tau^0, & (4.34)\\ \tau^{t=1,\lambda=\{-1,0,1\}} &= \left\{ \tfrac{1}{\sqrt{2}} \left(\tau^x - i\tau^y\right), \tau^z, \tfrac{-1}{\sqrt{2}} \left(\tau^x + i\tau^y\right) \right\}, & (4.35) \end{aligned}$$

which is different from the definition we assumed, of the Pauli matrices in the spin space,

$$\begin{aligned} \sigma_{v=0,0} &= \sigma_0, & (4.36)\\ \sigma_{v=1,\mu=\{-1,0,1\}} &= -i \left\{ \tfrac{1}{\sqrt{2}} \left(\sigma_x - i\sigma_y\right), \sigma_z, \tfrac{-1}{\sqrt{2}} \left(\sigma_x + i\sigma_y\right) \right\}. & (4.37) \end{aligned}$$

On the other hand, we start from the Biedenharn-Rose phase convention for the isospin Pauli matrices as we did for the spin ones. In order to keep our assumptions valid, we have to fix in the following way the phases for the adjoint and the complex conjugation of the Pauli matrices,

$$\begin{aligned} \tau^{t\lambda+} &= P_t(-1)^{t-\lambda} \left(\tau^{t,-\lambda}\right), & (4.38)\\ \tau^{t\lambda*} &= P_t(-1)^{t-\lambda} \left(\tau^{t,-\lambda}\right)^T, & (4.39) \end{aligned}$$

for $P_t = (-1)^t$, and

$$\begin{aligned} \sigma^+_{v\mu} &= (-1)^{v-\mu}\sigma_{v,-\mu}, & (4.40)\\ \sigma^*_{v\mu} &= (-1)^{v-\mu}\sigma^T_{v,-\mu}. & (4.41) \end{aligned}$$

Now we can proceed by assuming the form of the one-body pseudopotential in the space coordinates of Eq. (4.29) along with the form of the potentials $U^t_\gamma(\boldsymbol{r})$ in Eq. (4.27), then we get,

$$\begin{aligned}
\hat{\Gamma}^{\sigma\sigma'*}_{\tau\tau'}(\boldsymbol{r}) &\equiv \sum_{\gamma,t}\left(\left[\left[U^t_\gamma(\boldsymbol{r})\left[D_{n_\gamma L_\gamma}\sigma^{\sigma\sigma'}_{v_\gamma}\right]_{J_\gamma}\right]_0\tau^t_{\tau\tau'}\right]^0\right)^* \\
&= \sum_{\gamma,t}\sum_{a\alpha\beta;d\delta}\left(C^{\beta,t}_{a,\alpha}\chi^{\beta;d\delta}_{a,\alpha;\gamma}\left[\left[\left[D_d\rho^t_\delta(\boldsymbol{r})\right]_{J_\gamma}\left[D_{n_\gamma L_\gamma}\sigma^{\sigma\sigma'}_{v_\gamma}\right]_{J_\gamma}\right]_0\tau^t_{\tau\tau'}\right]^0\right)^* \\
&= \sum_{\gamma,t}\sum_{a\alpha\beta;d\delta}(-1)^{n_\gamma+m_a+m_d}C^{\beta,t}_{a,\alpha}\chi^{\beta;d\delta}_{a,\alpha;\gamma} \\
&\quad\left(\left[\left[\left[D_d\rho^t_\delta(\boldsymbol{r})\right]_{J_\gamma}\left[D_{n_\gamma L_\gamma}\sigma^{\sigma\sigma'}_{v_\gamma}\right]_{J_\gamma}\right]_0\tau^t_{\tau\tau'}\right]^0\right)^*, \qquad (4.42)
\end{aligned}$$

where we have used the fact that the coupling constants $C^{\beta,t}_{a,\alpha}$ are pure real coefficients, whereas the coefficients $\chi^{\beta;d\delta}_{a,\alpha;\gamma}$ of the potentials can have a pure imaginary phase which yields the factor $(-1)^{n_\gamma+m_a+m_d}$. Next, we calculate the complex-conjugated tensor in the last line of Eq. (4.42), namely,

$$\begin{aligned}
&\left(\left[\left[\left[D_d\rho^t_\delta(\boldsymbol{r})\right]_{J_\gamma}\left[D_{n_\gamma L_\gamma}\sigma^{\sigma\sigma'}_{v_\gamma}\right]_{J_\gamma}\right]_0\tau^t_{\tau\tau'}\right]^0\right)^* \\
&= \sum_{M_{J_\gamma}m_t}C^{00}_{mtm-t}C^{00}_{J_\gamma M_{J_\gamma}J_\gamma-M_{J_\gamma}}P_t(-1)^{J_\gamma-M_{J_\gamma}}(-1)^{t-m_t} \\
&\left(D_d\rho^{t,-m_t}_\delta(\boldsymbol{r})\right)_{J_\gamma,-M_{J_\gamma}}\sum_{M_{L_\gamma}\mu_\gamma}C^{J_\gamma-M_{J_\gamma}}_{L_\gamma M_{L_\gamma}v_\gamma\mu_\gamma}P_{D_{n_\gamma L_\gamma}}(-1)^{L_\gamma-M_{L_\gamma}} \\
&D_{n_\gamma L_\gamma,-M_{L_\gamma}}P_s(-1)^{v_\gamma-\mu_\gamma}\sigma^{\sigma\sigma'}_{v_\gamma,-\mu_\gamma}P_t(-1)^{t-m_t}\tau^{tm_t}_{\tau\tau'}, \qquad (4.43)
\end{aligned}$$

where we have used the Biedenharn-Rose convention for the secondary densities,

$$\begin{aligned}
\left[D_d\rho^{t\lambda}_\delta(\boldsymbol{r})\right]^*_{J_\gamma M_\gamma} &\equiv \rho^{t\lambda*}_{m_dI_d,n_\delta L_\delta v_\delta J_\delta,J_\gamma M_\gamma}(\boldsymbol{r}) \qquad (4.44)\\
&= P_t(-1)^{t-\lambda}(-1)^{J_\gamma-M_\gamma}\rho^{t,-\lambda}_{m_dI_d,n_\delta L_\delta v_\delta J_\delta,J_\gamma,-M_{J_\gamma}}(\boldsymbol{r}).
\end{aligned}$$

In Eq. (4.43) we applied the standard transformation rules for spherical tensors under complex conjugation [VMK88],

$$A^*_{\lambda\mu} = P_A(-1)^{\lambda-\mu}A_{\lambda,-\mu}. \qquad (4.45)$$

The phase conventions for the factors P_A for the building blocks of the N^{3}LO

operators can be read from Eqs. (4.39) and (4.41), that give for the expression (4.43),

$$
\begin{aligned}
&\sum_{M_{J_\gamma} m_t} C^{00}_{tm_t t-m_t} C^{00}_{J_\gamma M_{J_\gamma} J_\gamma -M_{J_\gamma}} (-1)^{J_\gamma - M_{J_\gamma} + L_\gamma - M_{L_\gamma} + v_\gamma - \mu_\gamma} \qquad (4.46)\\
&\left(D_d \rho^{t,-m_t}_{\delta}(\boldsymbol{r})\right)_{J_\gamma,-M_{J_\gamma}} \sum_{M_{L_\gamma}\mu_\gamma} C^{J_\gamma - M_{J_\gamma}}_{L_\gamma M_{L_\gamma} v_\gamma \mu_\gamma} D_{n_\gamma L_\gamma,-M_{L_\gamma}} \sigma^{\sigma\sigma'}_{v_\gamma,-\mu_\gamma} \tau^{tm_t}_{\tau\tau'}\\
&= \sum_{M_{J_\gamma} m_t} C^{00}_{tm_t t-m_t} C^{00}_{J_\gamma M_{J_\gamma} J_\gamma -M_{J_\gamma}} (-1)^{J_\gamma - M_{J_\gamma} + L_\gamma + v_\gamma + M_{J_\gamma}}\\
&\left(D_d \rho^{t,-m_t}_{\delta}(\boldsymbol{r})\right)_{J_\gamma,-M_{J_\gamma}} \sum_{M_{L_\gamma}\mu_\gamma} (-1)^{L_\gamma + v_\gamma - J_\gamma} C^{J_\gamma M_{J_\gamma}}_{L_\gamma - M_{L_\gamma} v_\gamma - \mu_\gamma}\\
&D_{n_\gamma L_\gamma,-M_{L_\gamma}} \sigma^{\sigma\sigma'}_{v_\gamma,-\mu_\gamma} \tau^{tm_t}_{\tau\tau'}\\
&= \sum_{M_{J_\gamma} m_t} C^{00}_{tm_t t-m_t} C^{00}_{J_\gamma M_{J_\gamma} J_\gamma -M_{J_\gamma}}\\
&\left(D_d \rho^{t,-m_t}_{\delta}(\boldsymbol{r})\right)_{J_\gamma,-M_{J_\gamma}} \left(D_{n_\gamma L_\gamma} \sigma^{\sigma\sigma'}_{v_\gamma}\right)_{J_\gamma M_{J_\gamma}} \tau^{tm_t}_{\tau\tau'}\\
&= \left[\left[\left[D_d \rho^{t}_{\delta}(\boldsymbol{r})\right]_{J_\gamma} \left[D_{n_\gamma L_\gamma} \sigma^{\sigma\sigma'}_{v_\gamma}\right]_{J_\gamma}\right]_0 \tau^{t}_{\tau\tau'}\right]^0,
\end{aligned}
$$

where in the first step we used the Clebsch-Gordan identity $C^{J_\gamma - M_{J_\gamma}}_{L_\gamma M_{L_\gamma} v_\gamma \mu_\gamma} = (-1)^{L_\gamma + v_\gamma - J_\gamma} C^{J_\gamma M_{J_\gamma}}_{L_\gamma - M_{L_\gamma} v_\gamma - \mu_\gamma}$, and in the next steps we recoupled the tensors to a scalar in the spin and isospin space.

So, the global phase for each terms of the one-body pseudopotential is due entirely to the $\chi^{\beta;d\delta}_{a,\alpha;\gamma}$ coefficients and we obtain the expressions,

$$\hat{\Gamma}^{\sigma'\sigma''*}_{\tau'\tau''}(\boldsymbol{r}') = \hat{\Gamma}^{'\sigma'\sigma''}_{\tau'\tau''}(\boldsymbol{r}'), \qquad (4.47)$$

for

$$\hat{\Gamma}^{'\sigma\sigma'}_{\tau\tau'}(\boldsymbol{r}') = \sum_{\gamma,t} \left[\left[\left[U^{'t}_{\gamma}(\boldsymbol{r}) D'_{n_\gamma L_\gamma}\right]_{v_\gamma} \sigma^{\sigma\sigma'}_{v_\gamma}\right]_0 \tau^{t}_{\tau\tau'}\right]^0 \qquad (4.48)$$

and

$$U^{'t}_{\gamma}(\boldsymbol{r}') = \sum_{a\alpha\beta;d\delta} (-1)^{n_\gamma + m_a + m_d} C^{\beta,t}_{a,\alpha} \chi^{\beta;d\delta}_{a,\alpha;\gamma} \left[D_d \rho^{t}_{\delta}(\boldsymbol{r}')\right]_{J_\gamma}. \qquad (4.49)$$

Chapter 5

Results

5.1 Results for the pseudopotential

5.1.1 General overview of the results concerning the pseudopotential

For sake of clarity, we start this part of the thesis with a general review of the main results achieved in our study on the pseudopotential.

The first result, exposed in Sec. II of paper I, was to have listed all possible terms of the pseudopotential in Eq. (3.2), according to the symmetries discussed in Sec. 3.3. We found the total number of 50 terms up to N^3LO: at zero, second, fourth, and sixth order, the terms are respectively 2, 7, 15, and 26 (see second column of Table (5.1)). We could then notice that these numbers of terms are exactly equal to those corresponding to the Galilean-invariant EDF in each isospin channel. The same correspondence was found between the numbers of terms of the gauge-invariant EDF and gauge-invariant pseudopotential, whose analysis was performed in Sec. IIC of paper I, by imposing condition (3.29) on the pseudopotential. The numbers of independent terms of the gauge-invariant pseudopotential are of 2 at zero order, 7 at second order, 6 at fourth order, and 6 at sixth order, as it is showed in the third column of Table (5.1).

In Fig. 5.1 we show the comparison between the numbers of terms of the Galilean-invariant pseudopotential, namely the full pseudopotential not restricted by any symmetry but the ones already encoded in the definition of an effective interaction as expansion in relative momenta, and gauge-invariant pseudopotential. The total number of terms for the Galilean-invariant pseu-

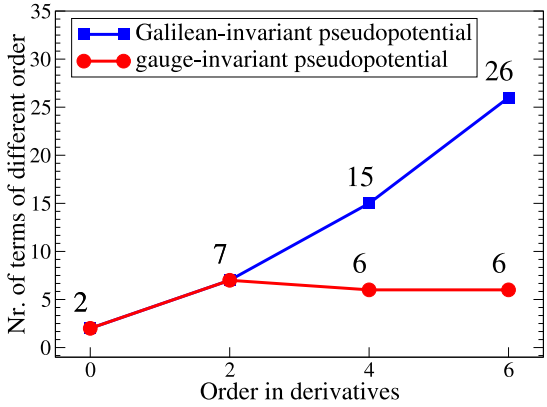

Figure 5.1: Number of terms of the pseudopotential (3.1) , plotted as a function of the order in derivatives.

dopotential is 50, whereas the gauge symmetry brings a reduction of terms to 21. We stress again the fact that in both cases the numbers of terms is exactly the same as the numbers of the free coupling constants of the EDF constrained by the same symmetries.

The discussion of the gauge invariance allowed us to group the terms of the pseudopotential in four different classes, composed by independent, dependent, stand-alone gauge-invariant, and stand-alone gauge-noninvariant terms. The last group is composed by terms whose parameters are forced to be equal to zero by condition (3.29), therefore the corresponding parameters are called vanishing parameters. The last but one group is composed by terms that verify alone condition (3.29), and we refer to the corresponding parameters as unrestricted parameters. The first two groups are defined by the fact that it may happen that the pseudopotential can respect the gauge symmetry only if its terms occur in certain linear combinations, each of them verifying condition (3.29). One of the parameters of terms in each linear combination can be selected (arbitrarily) as the independent parameter, and the others ones become the dependent parameters expressed through the independent ones, as it is showed in Appendix B of paper I. We stressed the fact that the choice of the independent parameters is not unique, but the number of independent terms at each order is a property of the gauge-invariant pseudopotential.

The distinction made above in four different classes of terms can be generalized to any symmetry. We have then the distinction between independent, depen-

dent, unrestricted, and vanishing terms. This grouping of terms can be found for different symmetries applied on both coupling constants of the EDF and parameters of the pseudopotential. Moreover, we can use the expression 'free parameters' (free coupling constants) to refer to the group of terms composed either by the independent or unrestricted parameters (coupling constants). The general trend valid for all the symmetries studied, is a reduction of the number of the free terms as the result of the application of a certain symmetry, because the symmetry can rule out terms of the pseudopotential (EDF), or force a subset of terms to be dependent on another ones. It is easy to understand that the reduction of the number of the free terms due to the symmetries imposed, is crucial when we are dealing with effective interactions and EDF based on expansions, as it is the case for our higher-order pseudopotential.

In Sec. IID of paper I, we presented the tensorlike form of the pseudopotential,

$$\hat{V} = \sum_{\substack{\tilde{n}'\tilde{L}',\\ \tilde{n}\tilde{L},v_{12}J}} \tilde{C}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}J} \hat{\tilde{V}}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}J}, \tag{5.1}$$

where

$$\begin{aligned}
\hat{\tilde{V}}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}J} = \quad & \frac{1}{2} i^{v_{12}} \left(1 - \tfrac{1}{2}\delta_{v_1,v_2}\right) \times \\
& \Bigg(\Big[\Big[K'_{\tilde{n}'\tilde{L}'} \sigma^{(1)}_{v_1} \Big]_J \Big[K_{\tilde{n}\tilde{L}} \sigma^{(2)}_{v_2} \Big]_J \Big]_0 \\
& + \Big[\Big[K'_{\tilde{n}'\tilde{L}'} \sigma^{(2)}_{v_1} \Big]_J \Big[K_{\tilde{n}\tilde{L}} \sigma^{(1)}_{v_2} \Big]_J \Big]_0 \\
& + \Big[\Big[K'_{\tilde{n}\tilde{L}} \sigma^{(1)}_{v_1} \Big]_J \Big[K_{\tilde{n}'\tilde{L}'} \sigma^{(2)}_{v_2} \Big]_J \Big]_0 \\
& + \Big[\Big[K'_{\tilde{n}\tilde{L}} \sigma^{(2)}_{v_1} \Big]_J \Big[K_{\tilde{n}'\tilde{L}'} \sigma^{(1)}_{v_2} \Big]_J \Big]_0 \Bigg) \times \\
& \left(1 - \hat{P}^M \hat{P}^\sigma \hat{P}^\tau\right) \hat{\delta}_{12}(\boldsymbol{r}'_1 \boldsymbol{r}'_2; \boldsymbol{r}_1 \boldsymbol{r}_2),
\end{aligned} \tag{5.2}$$

which is built from the same building blocks of the form in Eq. (3.2). The tensorlike pseudopotential is built from a different form of coupling of the relative-momentum operators with spin operators. We determined the relations between the two different coupling scheme of the pseudopotential, central-like and tensorlike, by using the recoupling technique (see Appendix C of paper I). At each order, the tensorlike form of the pseudopotential has more terms than the central-like form, which means that not all the possible terms of the tensorlike pseudopotential are linearly independent. At the end of Sec. II of paper I we listed the linear combinations expressing the relations between the dependent and independent parameters.

In Sec. III of paper I, the results concerning the averaging of the pseudopotential over the uncorrelated many-body wave function, are showed. The result of

the averaging generates the N^{3}LO EDF, and can be written as,

$$\langle C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S} \hat{V}^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S} \rangle = \sum C^{n'L'v'J',t}_{mI,nLvJ} T^{n'L'v'J',t}_{mI,nLvJ}, \tag{5.3}$$

where the l.h.s. denotes the averaging of the pseudopotential (3.1) and r.h.s. denotes instead the resulting EDF (2.16) with added superscripts t, which denote the isoscalar ($t = 0$) and isovector ($t = 1$) channels.

The evaluation of the relations (5.3) produces a set of linear combinations in which the coupling constants $C^{n'L'v'J',t}_{mI,nLvJ}$ are expressed through the pseudopotential strength parameters $C^{\tilde{n}'\tilde{L}'}_{\tilde{n}\tilde{L},v_{12}S}$. With these relations we could see directly that the symmetries of the pseudopotential are transferred on the EDF: the EDF coupling constants obtained from Eq. (5.3) in fact obey the Galilean-invariance constraints [CDK08], whereas the coupling constants obtained from the gauge-restricted pseudopotential correspond to the gauge-invariant EDF. In Sec. III of paper I we showed only the 12 second-order isoscalar and isovector coupling constants expressed by the 7 second-order pseudopotential parameters. In the supplemental material of the paper I, we included the analogous relations expressing at fourth (sixth) order 45 (129) isoscalar and isovector coupling constants to 15 (26) pseudopotential parameters.

We proceeded then in calculating the inverse relations, namely, we expressed the parameters of the pseudopotential through both isoscalar and isovector coupling constants of the EDF. This was possible because of the fact that once either the Galilean or gauge invariance is imposed, the numbers of parameters of the pseudopotential are the same, at each order, as the numbers of coupling constants of the EDF for *each* isospin. The inverse relations, collected in Sec. IIIA of paper I for the gauge invariance and in supplemental material for Galilean invariance, were in fact a preliminary result for the analysis performed in Sec. IIIB. There, by eliminating the pseudopotential parameters from pairs of relationships connecting the parameters to isoscalar and isovector coupling constants respectively, we derived a set of constraints expressing, at each order, the isovector coupling constants through the isoscalar ones. Again, we listed these relations in paper I (Sec. IIIB) for the case of gauge invariance, while the similar expressions for the case of Galilean invariance were collected in the supplemental material.

In Sec. IV of paper I we applied our results to the case of spherical even-even nuclei; in other words, we assumed the spherical, space-inversion, and time-reversal symmetries of the EDF and then we investigated the constraints on the EDF coupling constants in this restricted case. At the NLO, when the gauge symmetry is imposed on the EDF with the isospin degree of freedom included, we have 8 independent spherical EDF terms at second order, 6 at fourth order, and 6 at sixth order (see seventh column of Table (5.1)). Also for the case of spherical symmetry it was possible to repeat the analysis producing

the relations between parameters and coupling constants, and also the corresponding inverse relations were found. In particular, at second order, where we have one more independent coupling constant than independent pseudopotential parameters, we used the fact that the isoscalar and isovector spin-orbit coupling constants depend both on one spin-orbit pseudopotential parameter. This fact allowed us to write the relation,

$$C^{0000,1}_{11,1111} = \frac{1}{\sqrt{3}} C^{0000,0}_{11,1111}, \tag{5.4}$$

and we were left in this way with seven second order coupling constants related to the remaining seven parameters of the pseudopotential.

Since at second order the Galilean-invariant and gauge-invariant functionals are equivalent, when the Galilean invariance is imposed on the spherical EDF, we have to discuss just the fourth and sixth orders. At fourth (sixth) order, we have 16 (28) independent terms, of which 4 (8) are of the spin-orbit character, as it listed in sixth column of Table (5.1). Analogously to what we have just see for the second order functional in the case of gauge symmetry, the higher-order spin-orbit coupling constants are related only to the spin-orbit pseudopotential parameters. Because of this, we could find the following constraints on the spin-orbit coupling constants.

At fourth order,

$$C^{0000,1}_{31,1111} = -\frac{1}{\sqrt{3}} C^{0000,0}_{31,1111} - \frac{2}{\sqrt{3}} C^{0000,0}_{11,3111}, \tag{5.5a}$$

$$C^{0000,1}_{11,3111} = -\frac{2}{\sqrt{3}} C^{0000,0}_{31,1111} - \frac{1}{\sqrt{3}} C^{0000,0}_{11,3111}, \tag{5.5b}$$

and at sixth order the constraints,

$$C^{0000,1}_{51,1111} = -\frac{1}{\sqrt{3}} C^{0000,0}_{51,1111} + \frac{2}{\sqrt{3}} C^{0000,0}_{11,5111}, \tag{5.6a}$$

$$C^{0000,1}_{11,5111} = \frac{2}{\sqrt{3}} C^{0000,0}_{51,1111} - \frac{1}{\sqrt{3}} C^{0000,0}_{11,5111}, \tag{5.6b}$$

$$C^{0000,1}_{31,3111} = \frac{1}{\sqrt{3}} C^{0000,0}_{31,3111}, \tag{5.6c}$$

$$C^{0000,1}_{33,3313} = \frac{1}{\sqrt{3}} C^{0000,0}_{33,3313}. \tag{5.6d}$$

If now we consider Galilean-invariant and spherical EDF without spin-orbit terms, we are left with 12 (20) fourth-order (sixth-order) coupling constants related to the remaining 13 (22) parameters of the pseudopotential, that means 1 (2) possible relation(s) involving the remaining parameters. By considering now also the spin-orbit ones, the number of independent coupling constants at

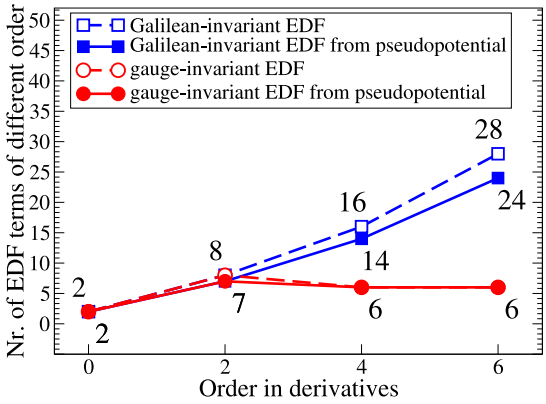

Figure 5.2: Number of terms of the spherical EDF that is related to a pseudopotential (solid lines), compared to the EDF not related to a pseudopotential (dashed lines). Full squares and circles show results for the Galilean and gauge invariance, respectively.

fourth order is 14, whereas the number of independent coupling constants at sixth order is 24, as it can be read from tenth column of Table (5.1).

In Fig. 5.2 we summarize the discussion on the EDF with conserved spherical symmetry in both cases when the reference to the pseudopotential is either assumed or released. Also both Galilean and gauge symmetries are considered.

The principal result of our study can be grasped by comparing the four columns of the EDF not related to pseudopotential with the correspective four columns of EDF related to pseudopotential, in Table (5.1). We can see, in general, that the reference of the EDF to the pseudopotential yields a reduction of the number of the free coupling constants of the functional, with the lower limit given by the number of the terms of the pseudopotential restricted by the symmetry under consideration. In particular, we get a reduction by half for the case of the general EDF, namely not restricted by any further symmetry but the ones (typically the Galilean and gauge symmetries) imposed also on the pseudopotential. The reduction is instead less important for the case of the spherical symmetric EDF, because the spherical symmetry, defined as self-consistent symmetry of the density matrix, can be just imposed on the functional and it is not defined for a force.

It is worth remarking once again the importance of the reduction of the free

	Pseudopotential		EDF							
			Not related to pseudopotential				Related to pseudopotential			
			General		Spherical		General		Spherical	
Order	Galilean	Gauge	Galilean	Gauge	Galilean	Gauge	Galilean	Gauge	Galilean	Gauge
0	2	2	4	4	2	2	2	2	2	2
2	7	7	14	14	8	8	7	7	7	7
4	15	6	30	12	16	6	15	6	14	6
6	26	6	52	12	28	6	26	6	24	6
N^3LO	50	21	100	42	54	22	50	21	47	21

Table 5.1: Number of terms of different orders in the pseudopotential (3.1) and in the EDF up to N^3LO (2.16), evaluated for the conserved Galilean and gauge symmetries. The last four columns show the number of terms in the EDF evaluated by taking into account the additional constraints coming from the relation of the EDF to pseudopotential.

coupling constants in the functional, by means of either imposed symmetries or other physical features as the reference of the EDF to an interaction. This result may be appreciated in connection with the adjustment of model parameters and the problems usually tackled by the practitioners of the optimization. In fact the non-uniqueness of the sample of fitting data, the estimation of the uncertainties in the extrapolations to other observables and of theoretical errors associated to them, with the consequent arbitrariness in the weight attributed in the global quality measure, are all hints of the insufficiency of the present-day density functionals. An extension of these functionals is then in order, but the increase of free coupling constants must be moderated on the basis of some justified restriction imposed on the functional.

As we claimed before, the reduction by half of the terms of the general EDF is due to the zero-range character of the pseudopotential, as it has been shown also in Ref. [DCK10] in the framework of the density matrix expansion, by a comparison between the Skyrme force and a general finite-range effective interaction up to NLO. As we showed in Sec. 3.2 of the present work, the ultimate reason is that the general zero-range effective interaction has half of the terms compared to the general form of the finite-range effective interaction.

The review of the results has given to us the chance to correct two mistakes contained in Sec. IV of paper I, namely the one devoted to the relations between the pseudopotential and EDF with conserved spherical symmetry. The analysis required to amend these mistakes will be discussed in next Sec. 5.1.2.

5.1.2 Relations between the pseudopotential and EDF with conserved spherical symmetry. Erratum of Sec. IV of paper I.

In this section, we repeat the analysis performed in Sec. IV of paper I and we correct the mistakes made there, due to the miscount of the number of the fourth and sixth order terms in the Galilean-invariant and spherical symmetric EDF.

The number of terms at higher orders when the Galilean invariance is imposed on the spherical EDF, which was given before the set of Eqs. 24 of paper I, should read as follows: we have at fourth (sixth) order 16 (28) independent terms, of which 4 (8) are of the spin-orbit character. Let us note that the number of the spin-orbit terms of the functional was correct for both the higher orders. Therefore the relations expressing the spin-orbit EDF coupling constants through the spin-orbit pseudopotential parameters and the resulting relations between the isovector and isoscalar spin-orbit EDF coupling constants were not affected at all by the miscount (see Eqs. (5.5a)–(5.6d)). The latter has instead affected the analysis, carried out in the last paragraph of the Sec. IV and in the supplemental material of the paper I, concerning the Galilean-invariant and spherical EDF without spin-orbit-terms.

When we consider the fourth (sixth) Galilean-invariant and spherical EDF without spin-orbit terms, we are left with 12 (20) coupling constants related to the remaining 13 (22) parameters of the pseudopotential, that means 1 (2) possible relation(s) involving the remaining parameters. Such relations can be imposed in many different ways; in fact we have checked that not any of the 1 (2) parameters of the fourth- (sixth-) pseudopotential can be taken as expressed through all the other parameters. Here we present one possible selection of the dependent parameters.

At fourth order we can have

$$C^{42}_{00,22} = \frac{7}{3}C^{22}_{20,22} - \frac{2}{3}\sqrt{7}C^{22}_{22,22}, \tag{5.7}$$

and at sixth order we can have

$$C^{62}_{00,22} = -4C^{42}_{20,22} + \frac{49}{5}C^{40}_{22,22} - \frac{20}{\sqrt{7}}C^{42}_{22,22} + \frac{8}{3\sqrt{5}}C^{44}_{22,22}, \tag{5.8a}$$

$$C^{51}_{11,22} = \frac{11}{18}\sqrt{\frac{35}{3}}C^{53}_{11,22} + \frac{7}{5}C^{31}_{31,22} - \frac{11}{2}\sqrt{\frac{7}{15}}C^{33}_{31,22} + \frac{4}{9}\sqrt{14}C^{33}_{33,22}. \tag{5.8b}$$

		$v=0,\ t=0$				$v=0,\ t=1$				$v=1,\ t=0$				$v=1,\ t=1$			
Order	Total	U	V	I	D	U	V	I	D	U	V	I	D	U	V	I	D
0	4	4	0	0	0	4	0	0	0	4	0	0	0	1	0	1	2
2	24	6	0	8	10	3	7	6	8	2	10	4	8	1	11	1	11
4	90	6	54	6	24	3	57	6	24	2	64	4	20	1	65	1	23
6	258	6	200	6	46	3	203	6	46	2	216	4	36	1	217	1	39
N^3LO	376	22	254	20	80	13	267	18	78	10	290	12	64	4	293	4	75

Table 5.2: Number of unrestricted (U), vanishing (V), independent (I), and dependent (D) coupling constants of different orders in the EDF up to N^3LO, shown for the four spin-isospin channels.

The Eqs. (5.7)–(5.8) show how the parameters of the pseudopotential can be constrained by means of the relation to the EDF, when this one is restricted by a symmetry, in this case the spherical one. In other words, the independent parameters of the pseudopotential that produces the spherical symmetric functional, are 14 at fourth order and 24 at sixth order.

The corrections presented in this section will soon be submitted to Physical Review C in form of the erratum of paper I.

5.2 Results for the continuity equation

5.2.1 General overview of the results concerning the continuity equation

In the same way we did in Sec. 5.1.1 for the pseudopotential, we give in this section a general review of the results obtained in paper II concerning the CE for N^3LO EDFs.

Table (5.2) summarizes the results for the CEs in the four spin-isospin channels, as presented in Sec. III of paper II. For each choice of the indices (v,t), the condition (4.30) sets constraints on the coupling constants $C_{a,\alpha}^{\beta,t}$ of the EDF. The constraints are obtained as solutions of a system of linear equations, where each equation is obtained considering the coefficients standing at a given pair of secondary densities in the last line of Eq. (4.30). The coupling constants not appearing in any constraints are unrestricted (U), the other ones can be involved in the constraints in different ways, namely, they can be vanishing (V), independent (I), and dependent (D) coupling constants, according to the same classification given in Sec. 5.1.1 for the parameters of the gauge-invariant pseudopotential.

The numbers of all the categories of coupling constants for all four channels of CE is displayed in Table (5.2). The first row in the table displays the numbers of the zero-order coupling constants, that are discussed in Sec. IIIA of paper II. In particular, we pointed out the analogy between the CE in the vector channel treated in Sec. IIA of paper II and the results for the zero-order EDF in both vector-isoscalar and scalar-isovector channel. This analogy is manifest when we consider the contribution coming from the vector potential to the CE for the spin-$\frac{1}{2}$ particle in Eq. (4.3). In Sec. 5.2.2, by calculating explicitly the constraints on the zero-order coupling constants, we make clear that algebraic rule of the vector product in Eq. (4.3) is equivalent to the coupling of pairs of identical commuting rank 1 tensors to rank 1, which is identically null. This explains why the coupling to rank $v = 1$ ($t = 1$) in the spin (isospin) space for the vector-isoscalar (scalar-isovector) channel of the CE, in which the identically null tensors formed by the pairs of densities at zero order leave the corresponding coupling constants unrestricted. When instead in both spin and isospin we have the coupling to rank 1, the selection rule above does not apply anymore, because the two negative sign in the commutation of identical densities cancel each other. Then we find the the constraints,

$$C^{0000,1}_{00,0000} = \frac{1}{\sqrt{3}} C^{0011,1}_{00,0011}, \tag{5.9a}$$

$$C^{0011,0}_{00,0011} = \frac{1}{\sqrt{3}} C^{0011,1}_{00,0011}. \tag{5.9b}$$

The results in Table (5.2) are divided in four groups of four columns, each group for a spin-isospin channel. The first group gives the numbers of the standard scalar-isoscalar ($v = 0$ $t = 0$) CE, which are discussed in Sec. IIIB of paper II. The constraints found for this case are exactly the same as those defining the gauge-invariant EDF up to N^{3}LO [CDK08], showing in this way the equivalence between the validity of the CE and invariance under the abelian gauge transformation.

The second group of results in Table (5.2) pertains to the scalar-isovector ($v = 0$ $t = 1$) CE and it is discussed in Sec. IIIC of paper II. Unlike the scalar-isoscalar CE which keeps the isospin channels disconnected, the scalar-isovector constraints connect the isovector and isoscalar coupling constants. We also notice that the number of vanishing coupling constants is bigger than the previous case, because the selection rule concerning the identical pairs couple to rank 1 comes into play in the isospin space.

The numbers of coupling constants of the vector-isoscalar ($v = 1$ $t = 0$) CE is discussed in Sec. IIID of paper II and summarized in the third group of four columns in Table (5.2). The coupling to rank $v = 1$ of the pair of densities in condition (4.30) gives rise to constraints that now connect scalar and vector coupling constants.

The rightmost columns in Table (5.2) show the numbers of the coupling constants of the vector-isovector ($v = 1$ $t = 1$) CE. These results are discussed in Sec. IIIE of paper II, where the listed constraints contain coupling constants which are related in both spin and isospin spaces. In fact, at all the orders, all the dependent coupling constants can be expressed through only one vector coupling constant, and this one can be chosen to be either vector-isoscalar or vector-isovector.

In general, the relations among the coupling constants, in the four spin-isospin channels, can be seen as the constraints on the EDF forced to be invariant under the four local spin-isospin groups of Eq. (2.62). In particular, $U_0^0(\boldsymbol{r})$ gives the standard abelian gauge group U(1), $U_1^0(\boldsymbol{r})$ and $U_0^1(\boldsymbol{r})$ form the non-abelian gauge groups SU(2), whereas $U_1^1(\boldsymbol{r})$ corresponds to the non-abelian gauge group SU(2)×SU(2).

5.2.2 Illustrative example of the zero-order one-body pseudopotential contributions to CE

Because of its simplicity and the fact that it involves a small number of coupling constants, the zero order is the only one in which the calculations can be performed in a simple way without the help of the symbolic programming. To perform such calculations is useful for understanding how the constraints on the coupling constants appear from the derivation.

At zero order, the EDF has only four terms that we write down explicitly,

$$\begin{aligned}
\varepsilon_{LO}(\boldsymbol{r}) &= C^{0000,0}_{00,0000}\left[\left[\rho^0_{0000}(\boldsymbol{r})\rho^0_{00,0000,0}(\boldsymbol{r})\right]_0\right]^0 \\
&+ C^{0000,1}_{00,0000}\left[\left[\rho^1_{0000}(\boldsymbol{r})\rho^1_{00,0000,0}(\boldsymbol{r})\right]_0\right]^0 \\
&+ C^{0011,0}_{00,0011}\left[\left[\rho^0_{0011}(\boldsymbol{r})\rho^0_{00,0011,1}(\boldsymbol{r})\right]_0\right]^0 \\
&+ C^{0011,1}_{00,0011}\left[\left[\rho^1_{0011}(\boldsymbol{r})\rho^1_{00,0011,1}(\boldsymbol{r})\right]_0\right]^0 . \qquad (5.10)
\end{aligned}$$

For comparison, we also give the Cartesian representation of the leading order EDF, which reads [PRD04],

$$\varepsilon_{LO}(\boldsymbol{r}) = C_0^\rho \rho_0^2 + C_1^\rho \vec{\rho}^{\,2} + C_0^s \boldsymbol{s}_0^2 + C_1^s \vec{\boldsymbol{s}}^{\,2}, \qquad (5.11)$$

with the relations between the coupling constants in spherical and Cartesian

representations, that is,

$$
\begin{aligned}
C^{0000,0}_{00,0000} &= C^{\rho}_{0}, && (5.12a)\\
C^{0000,1}_{00,0000} &= \sqrt{3}C^{\rho}_{1}, && (5.12b)\\
C^{0011,0}_{00,0011} &= \sqrt{3}C^{s}_{0}, && (5.12c)\\
C^{0011,1}_{00,0011} &= 3C^{s}_{1}. && (5.12d)\\
& && (5.12e)
\end{aligned}
$$

The one-body pseudopotential corresponding to the functional in Eq. (5.10) reads,

$$
\begin{aligned}
\hat{\Gamma}^{\sigma\sigma'}_{\tau\tau'}(\boldsymbol{r})_{LO} &= 2C^{0000,0}_{00,0000}\rho^{0}_{0000}(\boldsymbol{r}) + 2C^{0000,1}_{00,0000}\left[\rho^{1}_{0000}(\boldsymbol{r})\tau^{1}_{\tau\tau'}\right]^{0} && (5.13)\\
&+ 2C^{0011,0}_{00,0011}\left[\rho^{0}_{0011}(\boldsymbol{r})\sigma^{\sigma\sigma'}_{1}\right]_{0} + 2C^{0011,1}_{00,0011}\left[\left[\rho^{1}_{0011}(\boldsymbol{r})\sigma^{\sigma\sigma'}_{1}\right]_{0}\tau^{1}_{\tau\tau'}\right]^{0}.
\end{aligned}
$$

Condition (4.25) for the CE can be written at the leading order as,

$$
\begin{aligned}
&\sum_{\sigma''\tau''}\left(\hat{\Gamma}^{\sigma\sigma''}_{\tau\tau''}(\boldsymbol{r})_{LO}\rho(\boldsymbol{r}\sigma''\tau'',\boldsymbol{r}'\sigma'\tau') - \hat{\Gamma}^{\sigma'\sigma''*}_{\tau'\tau''}(\boldsymbol{r}')_{LO}\rho(\boldsymbol{r}\sigma\tau,\boldsymbol{r}'\sigma''\tau'')\right) =\\
&2\sum_{\sigma''\tau''}\sum_{v_\gamma t''} C^{00v_\gamma v_\gamma,t''}_{00,00v_\gamma v_\gamma}\Big(\left[\left[\rho^{t''}_{00v_\gamma v_\gamma}(\boldsymbol{r})\sigma^{\sigma\sigma''}_{v_\gamma}\right]_{0}\tau^{t''}_{\tau\tau''}\right]^{0}\\
&\frac{1}{4}\sum_{v't'}(\sqrt{3})^{v'+t'}\left[\sigma^{\sigma''\sigma'}_{v'},\left[\tau^{t'}_{\tau''\tau'},\rho^{t'}_{v'}(\boldsymbol{r},\boldsymbol{r}')\right]^{0}\right]_{0}\\
&-\left[\left[\rho^{t''}_{00v_\gamma v_\gamma}(\boldsymbol{r}')\sigma^{\sigma''\sigma'}_{v_\gamma}\right]_{0}\tau^{t''}_{\tau''\tau'}\right]^{0}\\
&\frac{1}{4}\sum_{v't'}(\sqrt{3})^{v'+t'}\left[\sigma^{\sigma\sigma''}_{v'},\left[\tau^{t'}_{\tau\tau''},\rho^{t'}_{v'}(\boldsymbol{r},\boldsymbol{r}')\right]^{0}\right]_{0}\Big) = 0. \qquad (5.14)
\end{aligned}
$$

As it is explained in the derivation of Appendix A, we can select a specific spin and isospin channel by multiplying on the right by the opportune spin and isospin operators and by taking the traces after. We obtain then,

$$
\begin{aligned}
&\sum_{\sigma\sigma'\tau\tau'} 2 \sum_{\sigma''\tau''} \sum_{v_\gamma t''} C^{00 v_\gamma v_\gamma, t''}_{00,00 v_\gamma v_\gamma} \Big(\Big[\Big[\rho^{t''}_{00 v_\gamma v_\gamma}(\boldsymbol{r}) \sigma^{\sigma\sigma''}_{v_\gamma} \Big]_0 \tau^{t''}_{\tau\tau''} \Big]^0 \qquad (5.15)\\
&\frac{1}{4} \sum_{v' t'} (\sqrt{3})^{v'+t'} \Big[\sigma^{\sigma''\sigma'}_{v'}, \Big[\tau^{t'}_{\tau''\tau'}, \rho^{t'}_{v'}(\boldsymbol{r},\boldsymbol{r}') \Big]^0 \Big]_0 \\
&- \Big[\Big[\rho^{t''}_{00 v_\gamma v_\gamma}(\boldsymbol{r}') \sigma^{\sigma''\sigma'}_{v_\gamma} \Big]_0 \tau^{t''}_{\tau''\tau'} \Big]^0 \\
&\frac{1}{4} \sum_{v' t'} (\sqrt{3})^{v'+t'} \Big[\sigma^{\sigma\sigma''}_{v'}, \Big[\tau^{t'}_{\tau\tau''}, \rho^{t'}_{v'}(\boldsymbol{r},\boldsymbol{r}') \Big]^0 \Big]_0 \Big) \sigma^{\sigma'\sigma}_{v\lambda} \tau^{tr}_{\tau' \tau} \\
&= \frac{1}{2} \sum_{v_\gamma t''} \sum_{v' t'} \sum_{m_{v_\gamma} m_{t''}} \sum_{m_{v'} m_{t'}} C^{00 v_\gamma v_\gamma, t''}_{00,00 v_\gamma v_\gamma} \frac{(-1)^{v_\gamma - m_{v_\gamma}}}{(\sqrt{3})^{v_\gamma}} \frac{(-1)^{t''-m_{t''}}}{(\sqrt{3})^{t''}} \frac{(-1)^{v'-m_{v'}}}{(\sqrt{3})^{v'}} \\
&\frac{(-1)^{t'-m_{t'}}}{(\sqrt{3})^{t'}} A(v_\gamma + v' + v) A(t'' + t' + t) (-1)^{v_\gamma + m_{v_\gamma}} (-1)^{t''+m_{t''}} \\
&\Big(C^{v_\gamma m_{v_\gamma}}_{v' m_{v'} v\lambda} C^{t'' m_{t''}}_{t' m_{t'} tr} \rho^{t'' m_{t''}}_{00 v_\gamma v_\gamma m_{v_\gamma}}(\boldsymbol{r}) \rho^{t', -m_{t'}}_{v', -m_{v'}}(\boldsymbol{r},\boldsymbol{r}') \\
&- C^{v_\gamma m_{v_\gamma}}_{v\lambda v' m_{v'}} C^{t'' m_{t''}}_{tr t' m_{t'}} \rho^{t'' m_{t''}}_{00 v_\gamma v_\gamma m_{v_\gamma}}(\boldsymbol{r}') \rho^{t', -m_{t'}}_{v', -m_{v'}}(\boldsymbol{r},\boldsymbol{r}') \Big) = 0,
\end{aligned}
$$

where the values needed for symbols $A(v_\gamma + v' + v)$ and $A(t'' + t' + t)$ are $A(0) = 2$, $A(2) = 2\sqrt{3}$, $A(3) = 2\sqrt{2}\, i$ (see Eq. (4.32)).

Now we consider the constraints among the EDF coupling constants deriving from Eq. (5.15), when different spin-isospin channels are selected according to the choice of the indices v and t.

Scalar-isoscalar channel ($v = 0$, $t = 0$)

For this selected channel we have,

$$
\sigma^{\sigma'\sigma}_0 \tau^0_{\tau'\tau} \equiv \delta_{\sigma'\sigma} \delta_{\tau'\tau}, \qquad (5.16)
$$

and the condition in Eq. (5.15) becomes,

$$
\begin{aligned}
&\frac{1}{2} \sum_{v_\gamma t''} \sum_{v' t'} \sum_{m_{v_\gamma} m_{t''}} \sum_{m_{v'} m_{t'}} C^{00 v_\gamma v_\gamma, t''}_{00,00 v_\gamma v_\gamma} \qquad (5.17)\\
&\frac{1}{(\sqrt{3})^{v_\gamma}} \frac{1}{(\sqrt{3})^{t''}} \frac{(-1)^{v'-m_{v'}}}{(\sqrt{3})^{v'}} \frac{(-1)^{t'-m_{t'}}}{(\sqrt{3})^{t'}} A(v_\gamma + v') A(t'' + t') \\
&\Big(C^{v_\gamma m_{v_\gamma}}_{v' m_{v'} 00} C^{t'' m_{t''}}_{t' m_{t'} 00} \rho^{t'' m_{t''}}_{00 v_\gamma v_\gamma m_{v_\gamma}}(\boldsymbol{r}) \rho^{t', -m_{t'}}_{v', -m_{v'}}(\boldsymbol{r},\boldsymbol{r}') \\
&- C^{v_\gamma m_{v_\gamma}}_{00 v' m_{v'}} C^{t'' m_{t''}}_{00 t' m_{t'}} \rho^{t'' m_{t''}}_{00 v_\gamma v_\gamma m_{v_\gamma}}(\boldsymbol{r}') \rho^{t', -m_{t'}}_{v', -m_{v'}}(\boldsymbol{r},\boldsymbol{r}') \Big) = 0.
\end{aligned}
$$

Because of the simple properties of the Clebsch-Gordan coefficients, the two terms in parentheses are equivalent and cancel each other exactly. Therefore the condition in Eq. (5.17) cannot constrain any of the coupling constants in the zero-order EDF of Eq. (5.10).

Scalar-isovector channel ($v = 0$, $t = 1$)

For this selected channel we have,

$$\sigma_0^{\sigma'\sigma}\tau^1_{\tau'\tau} \equiv \delta_{\sigma'\sigma}\tau^1_{\tau'\tau}, \tag{5.18}$$

and the condition in Eq. (5.15) becomes now,

$$\begin{aligned}
&\frac{1}{2}\sum_{v_\gamma t''}\sum_{v' t'}\sum_{m_{v_\gamma} m_{t''}}\sum_{m_{v'} m_{t'}} C^{00 v_\gamma v_\gamma, t''}_{00,00 v_\gamma v_\gamma} \qquad (5.19)\\
&\frac{1}{(\sqrt{3})^{v_\gamma}}\frac{1}{(\sqrt{3})^{t''}}\frac{(-1)^{v'-m_{v'}}}{(\sqrt{3})^{v'}}\frac{(-1)^{t'-m_{t'}}}{(\sqrt{3})^{t'}} A(v_\gamma + v') A(t'' + t' + 1)\\
&\Big(C^{v_\gamma m_{v_\gamma}}_{v' m_{v'} 00} C^{t'' m_{t''}}_{t' m_{t'} 10} \rho^{t'' m_{t''}}_{00 v_\gamma v_\gamma m_{v_\gamma}}(\boldsymbol{r}) \rho^{t', -m_{t'}}_{v', -m_{v'}}(\boldsymbol{r}, \boldsymbol{r}')\\
&- C^{v_\gamma m_{v_\gamma}}_{00 v' m_{v'}} C^{t'' m_{t''}}_{10 t' m_{t'}} \rho^{t'' m_{t''}}_{00 v_\gamma v_\gamma m_{v_\gamma}}(\boldsymbol{r}') \rho^{t', -m_{t'}}_{v', -m_{v'}}(\boldsymbol{r}, \boldsymbol{r}')\Big) = 0.
\end{aligned}$$

We can simplify the calculation of the constraints resulting from Eq. (5.19) by distinguishing three cases corresponding to different values assumed by the isospin indices t'' and t':

1. both are null ($t'' = 0$ and $t' = 0$), then the condition is identically null because we are left with the trace of the single Pauli matrix $\tau^1_{\tau'\tau}$ which is null;

2. only one index is null ($t'' = 1$, $t' = 0$ or $t'' = 0$, $t' = 1$), then the two terms in parentheses of Eq. (5.19) are identical and opposite in sign, in an analogous way to what we saw for the scalar-isoscalar channel, and again the condition is identically null;

3. both indices are not null ($t'' = 1$, $t' = 1$), then the coupling of the tensors in the isospin space will give in all the cases, where the two spin indices v_γ and v' must take the same value, two identical tensors coupled to the odd rank $t = 1$. But such a coupling is ruled out by the selection rule stating that an irreducible tensor of odd rank, obtained by the coupling of two identical commuting tensors, is identically null [VMK88].

So, in all three cases taken into account, there are no any constraints among the zero-order coupling constants, which are left unrestricted by the scalar-isovector channel.

Vector-isoscalar channel ($v = 1$, $t = 0$)

For this selected channel we have,

$$\sigma_1^{\sigma'\sigma}\tau^0_{\tau'\tau} \equiv \delta_{\tau'\tau}\sigma^1_{\sigma'\sigma}, \tag{5.20}$$

and condition in Eq. (5.15) becomes,

$$\begin{aligned}
&\frac{1}{2}\sum_{v_\gamma t''}\sum_{v't'}\sum_{m_{v_\gamma}m_{t''}}\sum_{m_{v'}m_{t'}} C^{00v_\gamma v_\gamma,t''}_{00,00v_\gamma v_\gamma} \qquad (5.21)\\
&\frac{1}{(\sqrt{3})^{v_\gamma}}\frac{1}{(\sqrt{3})^{t''}}\frac{(-1)^{v'-m_{v'}}}{(\sqrt{3})^{v'}}\frac{(-1)^{t'-m_{t'}}}{(\sqrt{3})^{t'}}A(v_\gamma+v'+1)A(t''+t')\\
&\big(C^{v_\gamma m_{v_\gamma}}_{v'm_{v'}10}C^{t''m_{t''}}_{t'm_{t'}00}\rho^{t''m_{t''}}_{00v_\gamma v_\gamma m_{v_\gamma}}(\boldsymbol{r})\rho^{t',-m_{t'}}_{v',-m_{v'}}(\boldsymbol{r},\boldsymbol{r}')\\
&-C^{v_\gamma m_{v_\gamma}}_{10v'm_{v'}}C^{t''m_{t''}}_{00t'm_{t'}}\rho^{t''m_{t''}}_{00v_\gamma v_\gamma m_{v_\gamma}}(\boldsymbol{r}')\rho^{t',-m_{t'}}_{v',-m_{v'}}(\boldsymbol{r},\boldsymbol{r}')\big)=0.
\end{aligned}$$

In the case of the zero-order functional, where we do not have momentum operators coupled with the spins, the treatment of the spin operators is specular to the one of the isospin that we have previously considered in the case of the scalar-isovector channel. We can then distinguish in Eq. (5.21) three cases of different values assumed by the spin indices v_γ and v' as we did before for the isospin. The three possible cases are, *mutatis mutandis*, the same ones found for the scalar-isovector channel.

So, there are no any constraints among the zero-order coupling constants, which are left unrestricted also by the vector-isoscalar channel.

Vector-isovector channel ($v = 1$, $t = 1$)

In this case we have

$$\sigma_1^{\sigma'\sigma}\tau^1_{\tau'\tau}, \tag{5.22}$$

as the operators selecting the channel of the vector-isovector CE. It is clear that now the possible cases we examined before in the spin and isospin spaces are somehow mixed together. We then are going to solve explicitly the condition in Eq. (5.15), by following the derivation we did in Sec. II-A of paper II.

Once again, the starting point is given by the Schrödinger equation of a single particle with spin and isospin degrees of freedom included,

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r}\sigma\tau,t) &= -\frac{\hbar^2}{2m}\triangle\psi(\boldsymbol{r}\sigma\tau,t)+\sum_{\sigma''\tau''}\Gamma^{\sigma\sigma''}_{\tau\tau''}(\boldsymbol{r})_{LO}\psi(\boldsymbol{r}\sigma''\tau'',t)\\
&= -\frac{\hbar^2}{2m}\triangle\psi(\boldsymbol{r}\sigma\tau,t)+2\sum_{\sigma''\tau''}C^{0000,0}_{00,0000}\rho^0_{0000}(\boldsymbol{r})\delta_{\sigma\sigma''}\delta_{\tau\tau''}\psi(\boldsymbol{r}\sigma''\tau'',t)\\
&+ 2\sum_{\sigma''\tau''}C^{0000,1}_{00,0000}\left[\rho^1_{0000}(\boldsymbol{r})\tau^1_{\tau\tau''}\right]^0\delta_{\sigma\sigma''}\psi(\boldsymbol{r}\sigma''\tau'',t)\\
&+ 2\sum_{\sigma''\tau''}C^{0011,0}_{00,0011}\left[\rho^0_{0011}(\boldsymbol{r})\sigma^{\sigma\sigma''}_1\right]_0\delta_{\tau\tau''}\psi(\boldsymbol{r}\sigma''\tau'',t)\\
&+ 2\sum_{\sigma''\tau''}C^{0011,1}_{00,0011}\left[\left[\rho^1_{0011}(\boldsymbol{r})\sigma^{\sigma\sigma''}_1\right]_0\tau^1_{\tau\tau''}\right]^0\psi(\boldsymbol{r}\sigma''\tau'',t). \qquad (5.23)
\end{aligned}
$$

By multiplying Eq. (5.23) with $\psi^*(\boldsymbol{r}\sigma'\tau',t)\sigma^{\sigma'\sigma}_\nu\tau^r_{\tau'\tau}$, summing up over σ',σ,τ' and τ, and taking the imaginary part, we obtain the CE for the isovector spin density $\rho^1_1(\boldsymbol{r},t)$ in term of the isovector spin current $\boldsymbol{J}^1_1(\boldsymbol{r},t)$.

Let us treat separately the imaginary part relative to the potential in Eq. (5.23), that reads

$$
\begin{aligned}
&2\sum_{\tau\tau'\tau''}\sum_{\sigma\sigma'\sigma''}C^{0000,1}_{00,0000}\sum_{pq}\sum_{\mu}\frac{(-1)^{1-p}}{\sqrt{3}}\frac{(-1)^{1-q}}{\sqrt{3}}\frac{(-1)^{1-\mu}}{\sqrt{3}}\\
&\rho^{1p}_0(\boldsymbol{r})\tau^{1-p}_{\tau\tau''}\delta_{\sigma\sigma''}\frac{3}{4}\rho^{1q}_{1\mu}(\boldsymbol{r})\sigma^{\sigma''\sigma'}_{1-\mu}\tau^{1-q}_{\tau''\tau'}\sigma^{\sigma'\sigma}_\nu\tau^r_{\tau'\tau}\\
+\;&2\sum_{\tau\tau'\tau''}\sum_{\sigma\sigma'\sigma''}C^{0011,0}_{00,0011}\sum_{q}\sum_{\mu\lambda}\frac{(-1)^{1-\lambda}}{\sqrt{3}}\frac{(-1)^{1-q}}{\sqrt{3}}\frac{(-1)^{1-\mu}}{\sqrt{3}}\\
&\rho^0_{1\lambda}(\boldsymbol{r})\sigma^{\sigma\sigma''}_{1-\lambda}\delta_{\tau\tau''}\frac{3}{4}\rho^{1q}_{1\mu}(\boldsymbol{r})\sigma^{\sigma''\sigma'}_{1-\mu}\tau^{1-q}_{\tau''\tau'}\sigma^{\sigma'\sigma}_\nu\tau^r_{\tau'\tau}\\
+\;&2\sum_{\tau\tau'\tau''}\sum_{\sigma\sigma'\sigma''}C^{0011,1}_{00,0011}(\sum_{pq}\sum_{\lambda}\frac{(-1)^{1-p}}{\sqrt{3}}\frac{(-1)^{1-\lambda}}{\sqrt{3}}\frac{(-1)^{1-q}}{\sqrt{3}}\\
&\rho^{1p}_{1\lambda}(\boldsymbol{r})\sigma^{\sigma\sigma''}_{1-\lambda}\tau^{1-p}_{\tau\tau''}\frac{\sqrt{3}}{4}\rho^{1q}_0(\boldsymbol{r})\tau^{1-q}_{\tau''\tau'}\delta_{\sigma''\sigma'}\sigma^{\sigma'\sigma}_\nu\tau^r_{\tau'\tau}\\
+\;&\sum_{p}\sum_{\mu\lambda}\frac{(-1)^{1-p}}{\sqrt{3}}\frac{(-1)^{1-\lambda}}{\sqrt{3}}\frac{(-1)^{1-\mu}}{\sqrt{3}}\\
&\rho^{1p}_{1\lambda}(\boldsymbol{r})\sigma^{\sigma\sigma''}_{1-\lambda}\tau^{1-p}_{\tau\tau''}\frac{\sqrt{3}}{4}\rho^0_{1\mu}(\boldsymbol{r})\sigma^{\sigma''\sigma'}_{1-\mu}\delta_{\tau''\tau'}\sigma^{\sigma'\sigma}_\nu\tau^r_{\tau'\tau}). \qquad (5.24)
\end{aligned}
$$

We compute the trace over the spin and isospin indices in Eq. (5.24) and we obtain,

$$
\begin{aligned}
&= 2C^{0000,1}_{00,0000}\sum_{pq}\sum_{\mu}\frac{(-1)^{1-p}}{\sqrt{3}}(-1)^{1-q}(-1)^{1-\mu}\frac{1}{2}\rho^{1p}_{0}(\boldsymbol{r})\rho^{1q}_{1\mu}(\boldsymbol{r})\\
&\quad 2(-1)^{1-\mu}\delta_{\mu,\nu}2\sqrt{2}(-1)^{1+r}C^{1-r}_{1-p1-q}\\
&+ 2C^{0011,0}_{00,0011}\sum_{q}\sum_{\mu\lambda}\frac{(-1)^{1-\lambda}}{\sqrt{3}}(-1)^{1-q}(-1)^{1-\mu}\frac{1}{2}\rho^{0}_{1\lambda}(\boldsymbol{r})\rho^{1q}_{1\mu}(\boldsymbol{r})\\
&\quad 2(-1)^{1-q}\delta_{q,r}2\sqrt{2}(-1)^{1+\nu}C^{1-\nu}_{1-\lambda1-\mu}\\
&+ 2C^{0011,1}_{00,0011}(\sum_{pq}\sum_{\lambda}\frac{(-1)^{1-p}}{\sqrt{3}}\frac{(-1)^{1-\lambda}}{\sqrt{3}}(-1)^{1-q}\frac{1}{2}\rho^{1p}_{1\lambda}(\boldsymbol{r})\rho^{1q}_{0}(\boldsymbol{r})\\
&\quad 2(-1)^{1-\lambda}\delta_{\lambda,\nu}2\sqrt{2}(-1)^{1+r}C^{1-r}_{1-p1-q}\\
&+ \sum_{p}\sum_{\mu\lambda}\frac{(-1)^{1-p}}{\sqrt{3}}\frac{(-1)^{1-\lambda}}{\sqrt{3}}(-1)^{1-\mu}\frac{1}{2}\rho^{1p}_{1\lambda}(\boldsymbol{r})\rho^{0}_{1\mu}(\boldsymbol{r})\\
&\quad 2(-1)^{1-p}\delta_{p,r}2\sqrt{2}(-1)^{1+\nu}C^{1-\nu}_{1-\lambda1-\mu})\\
&= -4\sqrt{\frac{2}{3}}C^{0000,1}_{00,0000}\left[\left[\rho^{1}_{0}(\boldsymbol{r})\rho^{1}_{1\nu}(\boldsymbol{r})\right]_{1\nu}\right]^{1r} - 4\sqrt{\frac{2}{3}}C^{0011,0}_{00,0011}\left[\left[\rho^{0}_{1}(\boldsymbol{r})\rho^{1r}_{1}(\boldsymbol{r})\right]_{1\nu}\right]^{1r}\\
&+ \frac{4}{3}\sqrt{2}C^{0011,1}_{00,0011}(\left[\left[\rho^{1}_{0}(\boldsymbol{r})\rho^{1}_{1\nu}(\boldsymbol{r})\right]_{1\nu}\right]^{1r} + \left[\left[\rho^{0}_{1}(\boldsymbol{r})\rho^{1r}_{1}(\boldsymbol{r})\right]_{1\nu}\right]^{1r}) = 0. \qquad (5.25)
\end{aligned}
$$

From the last two lines of Eq. (5.25) we obtain the constraints among the leading-order coupling constants for the case of vector-isovector CE,

$$
\begin{aligned}
C^{0000,1}_{00,0000} &= \frac{1}{\sqrt{3}}C^{0011,1}_{00,0011}, \qquad (5.26)\\
C^{0011,0}_{00,0011} &= \frac{1}{\sqrt{3}}C^{0011,1}_{00,0011}. \qquad (5.27)
\end{aligned}
$$

In summary, we found that for the scalar-isoscalar channel ($v = 0, t = 0$), scalar-isovector ($v = 0, t = 1$), and for vector-isoscalar ($v = 1, t = 0$), all the zero-order coupling constants are unrestricted.

For the vector-isovector case ($v = 1, t = 1$) we found the constraints of Eqs. (5.26-5.27), whereas we found that the coupling constant $C^{0000,0}_{00,0000}$ is still unrestricted.

Chapter 6

Summary

The long-term goal of the study of higher-order EDFs or pseudopotentials, is of course the application in practical calculations. But before proceeding with the implementation of numerical codes, the basic derivations and the complete investigation of the properties of the functional and pseudopotential must be carried out as preliminary steps.

In this work, we contributed to this investigation, first by deriving the zero-range nuclear N^3LO pseudopotential with derivatives up to sixth order and finding the corresponding N^3LO EDF, obtained as the HF average energy of the pseudopotential. The number of terms of the pseudopotential is twice smaller then that of the most general EDF and this feature is due to the zero-range character of the pseudopotential. We found explicit linear relations between the parameters of the pseudopotential and coupling constants of the EDF. Through the dependence of the coupling constants to the parameters, we could derive linear relations between the isoscalar and isovector coupling constants. The analogous analysis was repeated for gauge-invariant pseudopotential. A separate analysis was conducted on the EDF restricted by spherical, space-inversion, and time-reversal symmetries, which are relevant for describing spherical nuclei. The reduction of the numbers of independent terms related to imposing on the EDF the pseudopotential origins in spherical nuclei is relatively small, when compared to the one for deformed, asymmetric, odd, and/or rotating nuclei.

As second main point of our analysis of the N^3LO EDFs, we have derived sets of constraints on the coupling constants of the functional that guarantee the validity of the continuity equation in the four spin-isospin channels. In the scalar-isoscalar channel, the constraints found are the same of those pertaining to the gauge-invariant functional. We extended the connection between the

validity of CE and gauge invariance, also to vector and isovector channels. In general, the validity of the continuity equations is equivalent to the local gauge invariance with respect to spin and isospin rotations, respectively, which form non-abelian groups of transformation. The contribution to CE coming from the zero-order EDF have been explicitly calculated to show the role played by the one-body pseudopotential in the derivation of the CE.

Appendix A: derivation of the condition (4.30)

In this Appendix, we are going to show the complete derivation of the condition (4.30) on the one-body pseudopotential for the validity of the CE. We introduce the isospin index t'' in order to distinguish between the isospin index in the one-body pseudopotential from index t', which denotes the isospin channel in the density matrix. Therefore, in the sum over γ is also included the isospin index t''.

The derivation starts by inserting expression (4.29) of the field in the r.h.s. of condition (4.25),

$$
\begin{aligned}
& \sum_{\sigma\sigma'\tau\tau'} \sum_{l} \sum_{\sigma''\tau''} (\hat{\Gamma}^{\sigma\sigma''}_{\tau\tau''}(\boldsymbol{r})\phi_l(\boldsymbol{r}\sigma''\tau'',t)\phi^*_l(\boldsymbol{r}'\sigma'\tau',t) \qquad (6.1)\\
- \;& \hat{\Gamma}^{\sigma'\sigma''*}_{\tau'\tau''}(\boldsymbol{r}')\phi^*_l(\boldsymbol{r}'\sigma''\tau'',t))\phi_l(\boldsymbol{r}\sigma\tau,t))\sigma^{\sigma'\sigma}_{v\lambda}\tau^{tr}_{\tau'\tau}\\
= \;& \sum_{\sigma\sigma'\tau\tau'} \sum_{\sigma''\tau''} \sum_{\gamma} (\left[\left[\left[U^{t''}_{\gamma}(\boldsymbol{r}) D_{n_\gamma L_\gamma} \right]_{v_\gamma} \sigma^{\sigma\sigma''}_{v_\gamma} \right]_0 \tau^{t''}_{\tau\tau''} \right]^0 \rho(\mathbf{r}\sigma''\tau'', \boldsymbol{r}'\sigma'\tau', t)\\
- \;& \left[\left[\left[U^{'t''}_{\gamma}(\boldsymbol{r}') D'_{n_\gamma L_\gamma} \right]_{v_\gamma} \sigma^{\sigma''\sigma'}_{v_\gamma} \right]_0 \tau^{t''}_{\tau''\tau'} \right]^0 \rho(\mathbf{r}\sigma\tau, \boldsymbol{r}'\sigma''\tau'', t))\sigma^{\sigma'\sigma}_{v\lambda}\tau^{tr}_{\tau'\tau} = 0,
\end{aligned}
$$

where the two operators $\sigma^{\sigma'\sigma}_{v\lambda}$ and $\tau^{tr}_{\tau'\tau}$ are multiplied on the right side of the condition, and the traces over the spin and isospin indices are taken in order to select the opportune spin and isospin channels of the CE under consideration. Now we can continue the derivation by applying the recouplings, that are preliminary steps needed to calculate the traces over the spin and isospin,

$$
\begin{aligned}
= & \sum_{\sigma\sigma'\tau\tau'}\sum_{\sigma''\tau''}\sum_{\gamma}\Bigg(\Bigg[\Bigg[\Big[U_{\gamma}^{t''}(\boldsymbol{r})D_{n_\gamma L_\gamma}\Big]_{v_\gamma}\sigma_{v_\gamma}^{\sigma\sigma''}\Bigg]_0\tau_{\tau\tau''}^{t''}\Bigg]^0 \\
& \frac{1}{4}\sum_{v't'}(\sqrt{3})^{v'+t'}\left[\sigma_{v'}^{\sigma''\sigma'},\left[\tau_{\tau''\tau'}^{t'},\rho_{v'}^{t'}(\boldsymbol{r},\boldsymbol{r}')\right]^0\right]_0 \\
- & \Bigg[\Bigg[\Big[U_{\gamma}^{'t''}(\boldsymbol{r}')D'_{n_\gamma L_\gamma}\Big]_{v_\gamma}\sigma_{v_\gamma}^{\sigma''\sigma'}\Bigg]_0\tau_{\tau''\tau'}^{t''}\Bigg]^0 \\
& \frac{1}{4}\sum_{v't'}(\sqrt{3})^{v'+t'}\left[\sigma_{v'}^{\sigma\sigma''},\left[\tau_{\tau\tau''}^{t'},\rho_{v'}^{t'}(\boldsymbol{r},\boldsymbol{r}')\right]^0\right]_0)\sigma_{v\lambda}^{\sigma'\sigma}\tau_{\tau'\tau}^{tr} \\
= & \sum_{\sigma\sigma'\tau\tau'}\sum_{\sigma''\tau''}\sum_{\gamma}\frac{1}{4}\sum_{v't'}(\sqrt{3})^{v'+t'}\Bigg(\Bigg[\Bigg[\Big[U_{\gamma}^{t''}(\boldsymbol{r})D_{n_\gamma L_\gamma}\Big]_{v_\gamma}\sigma_{v_\gamma}^{\sigma\sigma''}\Bigg]_0\tau_{\tau\tau''}^{t''}\Bigg]^0 \\
& \left[\sigma_{v'}^{\sigma''\sigma'},\left[\tau_{\tau''\tau'}^{t'},\rho_{v'}^{t'}(\boldsymbol{r},\boldsymbol{r}')\right]^0\right]_0-\Bigg[\Bigg[\Big[U_{\gamma}^{'t''}(\boldsymbol{r}')D'_{n_\gamma L_\gamma}\Big]_{v_\gamma}\sigma_{v_\gamma}^{\sigma''\sigma'}\Bigg]_0\tau_{\tau''\tau'}^{t''}\Bigg]^0 \\
& \left[\sigma_{v'}^{\sigma\sigma''},\left[\tau_{\tau\tau''}^{t'},\rho_{v'}^{t'}(\boldsymbol{r},\boldsymbol{r}')\right]^0\right]_0)\sigma_{v\lambda}^{\sigma'\sigma}\tau_{\tau'\tau}^{tr} \\
= & \sum_{\sigma\sigma'\tau\tau'}\sum_{\sigma''\tau''}\sum_{\gamma}\frac{1}{4}\sum_{v't'}(\sqrt{3})^{v'+t'} \\
& \Bigg(\Bigg[\Bigg[\Bigg[\Big[U_{\gamma}^{t''}(\boldsymbol{r})D_{n_\gamma L_\gamma}\Big]_{v_\gamma}\left[\sigma_{v_\gamma}^{\sigma\sigma''}\left[\tau_{\tau\tau''}^{t''}\left[\sigma_{v'}^{\sigma''\sigma'},\left[\tau_{\tau''\tau'}^{t'},\rho_{v'}^{t'}(\boldsymbol{r},\boldsymbol{r}')\right]^0\right]_0\right]^{t''}\right]_{v_\gamma}\Bigg]^0\Bigg]_0 \\
- & \Bigg[\Bigg[\Bigg[\Big[U_{\gamma}^{'t''}(\boldsymbol{r}')D'_{n_\gamma L_\gamma}\Big]_{v_\gamma}\left[\sigma_{v_\gamma}^{\sigma''\sigma'}\left[\tau_{\tau''\tau'}^{t''}\left[\sigma_{v'}^{\sigma\sigma''},\left[\tau_{\tau\tau''}^{t'},\rho_{v'}^{t'}(\boldsymbol{r},\boldsymbol{r}')\right]^0\right]_0\right]^{t''}\right]_{v_\gamma}\Bigg]^0\Bigg]_0 \\
& \sigma_{v\lambda}^{\sigma'\sigma}\tau_{\tau'\tau'}^{tr}\Bigg)=0. \qquad (6.2)
\end{aligned}
$$

A further recoupling involving the spin and isospin operators $\sigma_{v\lambda}^{\sigma'\sigma}\tau_{\tau'\tau'}^{tr}$ is required. Let us notice that the total rank of the tensor is equal to the rank v and t of the spin and isospin operators applied to select a specific channel of the CE. So, the condition in Eq. (6.2) becomes

$$
\begin{aligned}
= & \sum_{\sigma\sigma'\tau\tau'}\sum_{\sigma''\tau''}\sum_{\gamma}\frac{1}{4}\sum_{v't'}(\sqrt{3})^{v'+t'}\sum_{V=|v_\gamma-v|}^{v_\gamma+v}\sum_{T=|t''-t|}^{t''+t}\sqrt{2V+1}\sqrt{2T+1} \qquad (6.3)\\
& \left\{\begin{array}{ccc} v_\gamma & v_\gamma & 0 \\ v & v & V \end{array}\right\}\left\{\begin{array}{ccc} t'' & t'' & 0 \\ t & t & T \end{array}\right\}\Bigg(\Bigg[\Bigg[\Big[U_\gamma^{t''}(\boldsymbol{r})D_{n_\gamma L_\gamma}\Big]_{v_\gamma}\\
& \Bigg[\Bigg[\Bigg[\sigma_{v_\gamma}^{\sigma\sigma''}\left[\tau_{\tau\tau''}^{t''}\left[\sigma_{v'}^{\sigma''\sigma'},\left[\tau_{\tau''\tau'}^{t'},\rho_{v'}^{t'}(\boldsymbol{r},\boldsymbol{r}')\right]^0\right]_0\right]^{t''}\Bigg]_{v_\gamma}\sigma_v^{\sigma'\sigma}\Bigg]_V\tau_{\tau'\tau}^{t}\Bigg]^T\Bigg]_{v\lambda}\Bigg]^{tr}\\
- & \Bigg[\Bigg[\Big[U_\gamma^{'t''}(\boldsymbol{r})D_{n_\gamma L_\gamma}\Big]_{v_\gamma}\\
& \Bigg[\Bigg[\Bigg[\sigma_{v_\gamma}^{\sigma''\sigma'}\left[\tau_{\tau''\tau'}^{t''}\left[\sigma_{v'}^{\sigma\sigma''},\left[\tau_{\tau\tau''}^{t'},\rho_{v'}^{t'}(\boldsymbol{r},\boldsymbol{r}')\right]^0\right]_0\right]^{t''}\Bigg]_{v_\gamma}\sigma_v^{\sigma'\sigma}\Bigg]_V\tau_{\tau'\tau}^{t}\Bigg]^T\Bigg]_{v\lambda}\Bigg]^{tr}\Bigg)\\
= & \sum_{\sigma\sigma'\tau\tau'}\sum_{\sigma''\tau''}\sum_{\gamma}\frac{1}{4}\sum_{v't'}(\sqrt{3})^{v'+t'}\sum_{V=|v_\gamma-v|}^{v_\gamma+v}\sum_{T=|t''-t|}^{t''+t}\sqrt{2V+1}\sqrt{2T+1}\\
& \left\{\begin{array}{ccc} v_\gamma & v_\gamma & 0 \\ v & v & V \end{array}\right\}\left\{\begin{array}{ccc} t'' & t'' & 0 \\ t & t & T \end{array}\right\}\sum_{\nu=-v'}^{v'}\frac{(-1)^{v'-\nu}}{(\sqrt{3})^{v'}}\sum_{p=-t'}^{t'}\frac{(-1)^{t'-p}}{(\sqrt{3})^{t'}}\\
& \sum_{\mu=-v_\gamma}^{v_\gamma}\sum_{q=-t''}^{t''}\sum_{M_V=-V}^{V}\sum_{M_T=-T}^{T}C_{v_\gamma\mu VM_V}^{v\lambda}C_{t''qTM_T}^{tr}C_{v_\gamma-\mu v\lambda}^{VM_V}C_{t''-qtr}^{TM_T}\\
& \Big(\Big(U_\gamma^{t''-q}(\boldsymbol{r})D_{n_\gamma L_\gamma}\Big)_{v_\gamma-\mu}\sigma_{v_\gamma\mu}^{\sigma\sigma''}\tau_{\tau\tau''}^{t''q}\sigma_{v'\nu}^{\sigma''\sigma'}\tau_{\tau''\tau'}^{t'p}\rho_{v'-\nu}^{t'-p}(\boldsymbol{r},\boldsymbol{r}')\sigma_{v\lambda}^{\sigma'\sigma}\tau_{\tau'\tau}^{tr}\\
- & \Big(U_\gamma^{'t''-q}(\boldsymbol{r}')D'_{n_\gamma L_\gamma}\Big)_{v_\gamma-\mu}\sigma_{v_\gamma\mu}^{\sigma''\sigma'}\tau_{\tau''\tau'}^{t''q}\sigma_{v'\nu}^{\sigma\sigma''}\tau_{\tau\tau''}^{t'p}\rho_{v'-\nu}^{t'-p}(\boldsymbol{r},\boldsymbol{r}')\sigma_{v\lambda}^{\sigma'\sigma}\tau_{\tau'\tau}^{tr})) = 0.
\end{aligned}
$$

Now we are indeed in the position to take the traces over all the spin and isospin indices. By using the shorthand notation of Eq. (4.31) for $A(v_\gamma, v', v; t'', t', t)$ to denote the awkward factors coming from the computation of the traces, we obtain

$$
\begin{aligned}
= \quad & \sum_{\gamma} \frac{1}{4} \sum_{v't'} (\sqrt{3})^{v'+t'} \sum_{V=|v_\gamma - v|}^{v_\gamma + v} \sum_{T=|t''-t|}^{t''+t} \sqrt{2V+1}\sqrt{2T+1} \\
& \left\{ \begin{array}{ccc} v_\gamma & v_\gamma & 0 \\ v & v & V \end{array} \right\} \left\{ \begin{array}{ccc} t'' & t'' & 0 \\ t & t & T \end{array} \right\} \sum_{\nu=-v'}^{v'} \frac{(-1)^{v'-\nu}}{(\sqrt{3})^{v'}} \sum_{p=-t'}^{t'} \frac{(-1)^{t'-p}}{(\sqrt{3})^{t'}} \\
& \sum_{\mu=-v_\gamma}^{v_\gamma} \sum_{q=-t''}^{t''} \sum_{M_V=-V}^{V} \sum_{M_T=-T}^{T} C^{v\lambda}_{v_\gamma \mu V M_V} C^{tr}_{t'' q T M_T} C^{V M_V}_{v_\gamma - \mu v \lambda} C^{T M_T}_{t''-qtr} \\
& \left((-1)^{-\lambda - r} C^{v-\lambda}_{v_\gamma \mu v' \nu} C^{t-r}_{t'' q t' p} A(v_\gamma, v', v; t'', t', t) \right. \\
& \left. \left(U^{t''-q}_{\gamma}(\boldsymbol{r}) D_{n_\gamma L_\gamma} \right)_{v_\gamma - \mu} \rho^{t'-p}_{v'-\nu}(\boldsymbol{r}, \boldsymbol{r}') \right. \\
- \quad & (-1)^{v_\gamma - v' + v - \lambda} (-1)^{t''-t'+t-r} C^{v-\lambda}_{v_\gamma \mu v' \nu} C^{t-r}_{t'' q t' p} A(v_\gamma, v', v; t'', t', t) \\
& \left. \left(U^{'t''-q}_{\gamma}(\boldsymbol{r}') D'_{n_\gamma L_\gamma} \right)_{v_\gamma - \mu} \rho^{t'-p}_{v'-\nu}(\boldsymbol{r}, \boldsymbol{r}') \right) = 0. \qquad (6.4)
\end{aligned}
$$

The traces in the last step have been calculated using the following relations,

$$
Tr \left\{ \sigma^{\sigma\sigma'}_{1\mu} \right\} = 0, \qquad (6.5)
$$

$$
Tr \left\{ \sigma^{\sigma\sigma''}_{1\mu} \sigma^{\sigma''\sigma'}_{1\nu} \right\} = 2(-1)^{1+\mu} \delta_{\mu - \nu}, \qquad (6.6)
$$

and,

$$
Tr \left\{ \sigma^{\sigma\sigma''}_{1\mu} \sigma^{\sigma''\sigma'}_{1\nu} \sigma^{\sigma'\sigma}_{1\lambda} \right\} = 2\sqrt{2} i (-1)^{1+\lambda} C^{1-\lambda}_{1\mu 1\nu}. \qquad (6.7)
$$

The expression in Eq. (6.4) must be recoupled. Since the spin and isospin spaces are separated Hilbert spaces, we rewrite the condition dropping the isospin indices in such a way that we can work on a shorter formula. The recoupling on the isospin space goes on the same line. The part of the condition depending on the spin indices is then,

$$\sum_{\gamma}\frac{1}{2}\sum_{v'}(\sqrt{3})^{v'}\sum_{V=|v_\gamma-v|}^{v_\gamma+v}\sqrt{2V+1}\left\{\begin{array}{ccc} v_\gamma & v_\gamma & 0\\ v & v & V\end{array}\right\}\sum_{\nu=-v'}^{v'}\frac{(-1)^{v'-\nu}}{(\sqrt{3})^{v'}}\sum_{\mu=-v_\gamma}^{v_\gamma}$$
$$\sum_{M_V=-V}^{V}C^{v\lambda}_{v_\gamma\mu VM_V}C^{VM_V}_{v_\gamma-\mu v\lambda}C^{v-\lambda}_{v_\gamma\mu v'\nu}\big((-1)^{-\lambda}C^{v-\lambda}_{v_\gamma\mu v'\nu}A(v_\gamma,v',v)$$
$$\big(U_\gamma(\boldsymbol{r})D_{n_\gamma L_\gamma}\big)_{v_\gamma-\mu}\rho_{v'-\nu}(\boldsymbol{r},\boldsymbol{r}')$$
$$-(-1)^{v_\gamma-v'+v-\lambda}C^{v-\lambda}_{v_\gamma\mu v'\nu}A(v_\gamma,v',v)$$
$$\Big(U^{'}_{\gamma}(\boldsymbol{r}')D'_{n_\gamma L_\gamma}\Big)_{v_\gamma-\mu}\rho_{v'-\nu}(\boldsymbol{r},\boldsymbol{r}')\big), \tag{6.8}$$

where $A(v_\gamma,v',v)$ denotes obviously the part of the term in Eq. (4.31) depending only on the spin indices.

In the following part of the derivation, formula (6.9) below is useful to simplify the products of 6-j symbols with Clebsch-Gordan coefficients,

$$\begin{aligned}
&\sum_{V=|v_\gamma-v|}^{v_\gamma+v}\sum_{M_V=-V}^{V}\sqrt{2V+1}\left\{\begin{array}{ccc} v_\gamma & v_\gamma & 0\\ v & v & V\end{array}\right\}C^{v\lambda}_{v_\gamma\mu VM_V}C^{VM_V}_{v_\gamma-\mu v\lambda}\\
=&\sum_{V=|v_\gamma-v|}^{v_\gamma+v}\sum_{M_V=-V}^{V}\sqrt{2V+1}(-1)^{V+v+v_\gamma}\frac{1}{\sqrt{2v+1}}\frac{1}{\sqrt{2v_\gamma+1}}(-1)^{v_\gamma-\mu}\\
&\sqrt{2v+1}\frac{1}{\sqrt{2V+1}}C^{VM_V}_{v\lambda v_\gamma-\mu}C^{VM_V}_{v_\gamma-\mu v\lambda}\\
=&(-1)^{v_\gamma-\mu}\frac{1}{\sqrt{2v_\gamma+1}}\sum_{V=|v_\gamma-v|}^{v_\gamma+v}\sum_{M_V=-V}^{V}C^{VM_V}_{v_\gamma-\mu v\lambda}C^{VM_V}_{v_\gamma-\mu v\lambda}\\
=&(-1)^{v_\gamma-\mu}\frac{1}{\sqrt{2v_\gamma+1}}\delta_{\mu,\mu}\delta_{\lambda,\lambda}.
\end{aligned}\tag{6.9}$$

With the help of Eq. (6.9), we can simplify the expression in Eq. (6.8) and get,

$$\begin{aligned}
=&\sum_{\gamma}\frac{1}{2}(-1)^{v_\gamma}\frac{1}{\sqrt{2v_\gamma+1}}\sum_{v'}(\sqrt{3})^{v'}\sum_{\nu=-v'}^{v'}\frac{(-1)^{v'-\nu}}{(\sqrt{3})^{v'}}\sum_{\mu=-v_\gamma}^{v_\gamma}C^{v-\lambda}_{v_\gamma\mu v'\nu}(-1)^{-\mu}\\
&\big((-1)^{-\lambda}A(v_\gamma,v',v)\left(U_\gamma(\boldsymbol{r})D_{n_\gamma L_\gamma}\right)_{v_\gamma-\mu}\rho_{v'-\nu}(\boldsymbol{r},\boldsymbol{r}')\\
-&(-1)^{v_\gamma-v'+v-\lambda}A(v_\gamma,v',v)\left(U^{'}_{\gamma}(\boldsymbol{r}')D'_{n_\gamma L_\gamma}\right)_{v_\gamma-\mu}\rho_{v'-\nu}(\boldsymbol{r},\boldsymbol{r}')\big).
\end{aligned}\tag{6.10}$$

The analogous simplification in the isospin space reads,

$$\sum_{T=|t''-t|}^{t''+t}\sum_{M_T=-T}^{T}\sqrt{2T+1}\left\{\begin{array}{ccc} t'' & t'' & 0\\ t & t & T\end{array}\right\}C^{tr}_{t''qTM_T}C^{TM_T}_{t''-qtr}$$
$$=(-1)^{t''-q}\frac{1}{\sqrt{2t''+1}}\delta_{q,q}\delta_{r,r}. \tag{6.11}$$

Now, let us come back to the complete condition of Eq. (6.4) with the isospin indices included,

$$\begin{aligned}
= \quad & \sum_{\gamma}\frac{1}{4}(-1)^{v_\gamma}\frac{1}{\sqrt{2v_\gamma+1}}(-1)^{t''}\frac{1}{\sqrt{2t''+1}}\sum_{v't'}(\sqrt{3})^{v'+t'}\sum_{\nu=-v'}^{v'}\frac{(-1)^{v'-\nu}}{(\sqrt{3})^{v'}}\\
& \sum_{p=-t'}^{t'}\frac{(-1)^{t'-p}}{(\sqrt{3})^{t'}}\sum_{\mu=-v_\gamma}^{v_\gamma}\sum_{q=-t''}^{t''}(-1)^{-\mu}(-1)^{-q}C^{v-\lambda}_{v_\gamma\mu v'\nu}C^{t-r}_{t''qt'p}\\
& \big((-1)^{-\lambda-r}A(v_\gamma,v',v;t'',t',t)\\
& \left(U^{t''-q}_{\gamma}(\boldsymbol{r})D_{n_\gamma L_\gamma}\right)_{v_\gamma-\mu}\rho^{t'-p}_{v'-\nu}(\boldsymbol{r},\boldsymbol{r}')\\
- \quad & (-1)^{v_\gamma-v'+v-\lambda}(-1)^{t''-t'+t-r}A(v_\gamma,v',v;t'',t',t)\\
& \left(U^{'t''-q}_{\gamma}(\boldsymbol{r}')D'_{n_\gamma L_\gamma}\right)_{v_\gamma-\mu}\rho^{t'-p}_{v'-\nu}(\boldsymbol{r},\boldsymbol{r}')\big),
\end{aligned}\tag{6.12}$$

which becomes, by using the Clebsch-Gordan coefficient symmetry $C^{v-\lambda}_{v_\gamma\mu v'\nu}=(-1)^{v_\gamma+v'-v}C^{v\lambda}_{v_\gamma-\mu v'-\nu}$,

$$\begin{aligned}
= \quad & \sum_{\gamma}\frac{1}{4}\frac{1}{\sqrt{2v_\gamma+1}}\frac{1}{\sqrt{2t''+1}}\sum_{v't'}(-1)^{-v-t}A(v_\gamma,v',v;t'',t',t) \qquad (6.13)\\
& \Bigg(\left[\left[\left[U^{t''}_{\gamma}(\boldsymbol{r})D_{n_\gamma L_\gamma}\right]_{v_\gamma}\rho^{t'}_{v'}(\boldsymbol{r},\boldsymbol{r}')\right]_{v\lambda}\right]^{tr}\\
- \quad & (-1)^{v_\gamma-v'+v+t''-t'+t}\left[\left[\left[U^{'t''}_{\gamma}(\boldsymbol{r}')D'_{n_\gamma L_\gamma}\right]_{v_\gamma}\rho^{t'}_{v'}(\boldsymbol{r},\boldsymbol{r}')\right]_{v\lambda}\right]^{tr}\Bigg)=0.
\end{aligned}$$

A further recoupling is required in the tensor, because we want to couple the differential operators $D_{n_\gamma L_\gamma}$ with the nonlocal densities, so we have

$$
\begin{aligned}
= \quad & \sum_{\gamma} \frac{1}{4} \frac{1}{\sqrt{2v_\gamma+1}} \frac{1}{\sqrt{2t''+1}} \sum_{v't'} (-1)^{-v-t} A(v_\gamma, v', v; t'', t', t) \qquad (6.14) \\
& \sum_{J=abs(L_\gamma - v')}^{L_\gamma + v'} (-1)^{J_\gamma + L_\gamma + v + v} \sqrt{2v_\gamma+1}\sqrt{2J+1} \left\{ \begin{array}{ccc} J_\gamma & L_\gamma & v_\gamma \\ v' & v & J \end{array} \right\} \\
& \left(\left[\left[U_\gamma^{t''}(\boldsymbol{r}) \left[D_{n_\gamma L_\gamma} \rho_{v'}^{t'}(\boldsymbol{r}, \boldsymbol{r'}) \right]_J \right]_{v\lambda} \right]^{tr} \right. \\
- \quad & \left. (-1)^{v_\gamma - v' + v + t'' - t' + t} \left[\left[U_\gamma'^{t''}(\boldsymbol{r'}) \left[D'_{n_\gamma L_\gamma} \rho_{v'}^{t'}(\boldsymbol{r}, \boldsymbol{r'}) \right]_J \right]_{v\lambda} \right]^{tr} \right) = 0.
\end{aligned}
$$

Now we have to transform each term composed by the differential operator action on the density into a linear combination of secondary densities (2.19), using the relations below,

$$
D_{n_\gamma L_\gamma M_{L_\gamma}} = \sum_{rRr'R} K_{rRr'R'}^{n_\gamma L_\gamma} \sum_{M_R M'_R} C_{RM_R R' M'_R}^{L_\gamma M_{L_\gamma}} (i)^r (\frac{1}{2})^{r'} D_{r'R'M'_R} K_{rRM_R}, \qquad (6.15)
$$

or in the recoupled form,

$$
D_{n_\gamma L_\gamma} = \sum_{rRr'R} K_{rRr'R'}^{n_\gamma L_\gamma} (i)^r (\frac{1}{2})^{r'} \left[D_{r'R'} K_{rR} \right]_{n_\gamma L_\gamma}, \qquad (6.16)
$$

and,

$$
D'_{n_\gamma L_\gamma M_{L_\gamma}} = \sum_{rRr'R} K_{rRr'R'}^{n_\gamma L_\gamma} \sum_{M_R M'_R} C_{RM_R R' M'_R}^{L_\gamma M_{L_\gamma}} (-i)^r (\frac{1}{2})^{r'} D_{r'R'M'_R} K_{rRM_R}, \qquad (6.17)
$$

or in the recoupled form,

$$
D'_{n_\gamma L_\gamma} = \sum_{rRr'R} K_{rRr'R'}^{n_\gamma L_\gamma} (-i)^r (\frac{1}{2})^{r'} \left[D_{r'R'} K_{rR} \right]_{n_\gamma L_\gamma}, \qquad (6.18)
$$

where the coefficients $K_{rRr'R'}^{n_\gamma L_\gamma}$ are numerical coefficients of the expansion (they are 91 at N^3LO) and the differential operators $D_{r'R'}$ are built from the deriva-

tives operators in Eqs. (3.38)-(3.39). We make use of these relations and we find

$$\begin{aligned}
\left[D_{n_\gamma L_\gamma}\rho^{t'}_{v'}(\boldsymbol{r},\boldsymbol{r'})\right]_J &= \sum_{rRr'R} K^{n_\gamma L_\gamma}_{rRr'R'}(i)^r(\frac{1}{2})^{r'}\left[\left[D_{r'R'}K_{rR}\right]_{n_\gamma L_\gamma}\rho^{t'}_{v'}(\boldsymbol{r},\boldsymbol{r'})\right]_J \\
&= \sum_{rRr'R} K^{n_\gamma L_\gamma}_{rRr'R'}(i)^r(\frac{1}{2})^{r'}\sum_{J_\eta}(-1)^{R'+r+v'+J}\sqrt{2L_\gamma+1} \\
&\quad \sqrt{2J_\eta+1}\left\{\begin{array}{ccc} R' & R & L_\gamma \\ v' & J & J_\eta \end{array}\right\}\left[D_{r'R'}\left[K_{rR}\rho^{t'}_{v'}(\boldsymbol{r},\boldsymbol{r'})\right]_{J_\eta}\right]_J \\
&= \sum_{rRr'R} K^{n_\gamma L_\gamma}_{rRr'R'}(i)^r(\frac{1}{2})^{r'}\sum_{J_\eta}(-1)^{R'+r+v'+J}\sqrt{2L_\gamma+1} \\
&\quad \sqrt{2J_\eta+1}\left\{\begin{array}{ccc} R' & R & L_\gamma \\ v' & J & J_\eta \end{array}\right\}\rho^{t}_{r'R',rRv'J_\eta,J}(\boldsymbol{r}), \qquad (6.19)
\end{aligned}$$

where in the second step, we recoupled the differential operator K_{rR} to the non-local density in order to obtain the tensor structure of the local densities (2.18).

We insert the result of the recoupling of Eq. (6.19) in the general condition of Eq. (6.14), and we get,

$$\begin{aligned}
&= \sum_\gamma \frac{1}{4}\frac{1}{\sqrt{2v_\gamma+1}}\frac{1}{\sqrt{2t''+1}}\sum_{v't'}(-1)^{-v-t}A(v_\gamma,v',v;t'',t',t) \qquad (6.20)\\
&\quad \sum_{J=abs(L_\gamma-v')}^{L_\gamma+v'}(-1)^{J_\gamma+L_\gamma+v+v}\sqrt{2v_\gamma+1}\sqrt{2J+1}\left\{\begin{array}{ccc} J_\gamma & L_\gamma & v_\gamma \\ v' & v & J \end{array}\right\} \\
&\quad \Big(\sum_{rRr'R} K^{n_\gamma L_\gamma}_{rRr'R'}(i)^r(\frac{1}{2})^{r'}\sum_{J_\eta}(-1)^{R'+r+v'+J}\sqrt{2L_\gamma+1}\sqrt{2J_\eta+1} \\
&\quad \left\{\begin{array}{ccc} R' & R & L_\gamma \\ v' & J & J_\eta \end{array}\right\}\left[\left[U^{t''}_\gamma(\boldsymbol{r})\rho^{t}_{r'R',rRv'J_\eta,J}(\boldsymbol{r})\right]_{v\lambda}\right]^{tr} \\
&- (-1)^{v_\gamma-v'+v}(-1)^{t''-t'+t}\sum_{rRr'R} K^{n_\gamma L_\gamma}_{rRr'R'}(-i)^r(\frac{1}{2})^{r'} \\
&\quad \sum_{J_\eta}(-1)^{R'+r+v'+J}\sqrt{2L_\gamma+1}\sqrt{2J_\eta+1} \\
&\quad \left\{\begin{array}{ccc} R' & R & L_\gamma \\ v' & J & J_\eta \end{array}\right\}\left[\left[U^{'t''}_\gamma(\boldsymbol{r'})\rho^{t}_{r'R',rRv'J_\eta,J}(\boldsymbol{r'})\right]_{v\lambda}\right]^{tr}) = 0.
\end{aligned}$$

Finally, the two tensors in the previous equation have the same structure, with

the only differences being the phase $(-1)^{n_\gamma+m_a+m_d}$ in the definition of $U_\gamma^{'t''}(\boldsymbol{r}')$. Then we can write the general condition in a more compact form as,

$$\sum_\gamma \frac{1}{4}\frac{1}{\sqrt{2v_\gamma+1}}\frac{1}{\sqrt{2t''+1}}\sum_{v't'}(-1)^{-v-t}A(v_\gamma,v',v;t'',t',t) \tag{6.21}$$
$$\sum_{J=abs(L_\gamma-v')}^{L_\gamma+v'}(-1)^{J_\gamma+L_\gamma+v+v}\sqrt{2v_\gamma+1}\sqrt{2J+1}\left\{\begin{array}{ccc} J_\gamma & L_\gamma & v_\gamma \\ v' & v & J \end{array}\right\}$$
$$\sum_{rRr'R'}K_{rRr'R'}^{n_\gamma L_\gamma}(i)^r(\frac{1}{2})^{r'}\sum_{J_\eta}(-1)^{R'+r+v'+J}$$
$$\sqrt{2L_\gamma+1}\sqrt{2J_\eta+1}\left\{\begin{array}{ccc} R' & R & L_\gamma \\ v' & J & J_\eta \end{array}\right\}$$
$$\sum_{a\alpha\beta;d\delta}\left(1-(-1)^{v_\gamma-v'+v}(-1)^{t''-t'+t}(-1)^r(-1)^{n_\gamma+m_a+m_d}\right)$$
$$C_{a,\alpha}^{\beta,t''}\chi_{a,\alpha;\gamma}^{\beta;d\delta}\left[\left[\left[D_d\rho_\delta^{t''}(\boldsymbol{r}')\right]_{J_\gamma}\left[D_{r'R'}\rho_{rRv'J_\eta}^t(\boldsymbol{r}')\right]_J\right]_{v\lambda}\right]^{\tilde{tr}}=0,$$

where we have used definitions (4.27)-(4.49) of the potentials $U_\gamma^t(\boldsymbol{r})$ and their complex conjugated.

In order to conform the notation to the one adopted in paper II, we rewrite the condition changing the indices ($r'\to m_f$, $R'\to I_f$,$r\to n_\varphi$, $R\to L_\varphi$, $v'\to v_\varphi$, $J_\eta\to J_\varphi$),

$$\sum_\gamma \frac{1}{4}\frac{1}{\sqrt{2v_\gamma+1}}\frac{1}{\sqrt{2t''+1}}\sum_{v_\varphi t}(-1)^{-v-t}A(v_\gamma,v_\varphi,v;t'',t',t) \tag{6.22}$$
$$\sum_{J=abs(L_\gamma-v_\varphi)}^{L_\gamma+v_\varphi}(-1)^{J_\gamma+L_\gamma+v_\varphi+v}\sqrt{2v_\gamma+1}\sqrt{2J+1}\left\{\begin{array}{ccc} J_\gamma & L_\gamma & v_\gamma \\ v_\varphi & v & J \end{array}\right\}$$
$$\sum_{n_\varphi L_\varphi m_f I_f}K_{n_\varphi L_\varphi m_f I_f}^{n_\gamma L_\gamma}(i)^{n_\varphi}(\frac{1}{2})^{m_f}\sum_{J_\varphi}(-1)^{I_f+n_\varphi+v_\varphi+J}$$
$$\sqrt{2L_\gamma+1}\sqrt{2J_\varphi+1}\left\{\begin{array}{ccc} I_f & L_\varphi & L_\gamma \\ v_\varphi & J & J_\varphi \end{array}\right\}$$
$$\sum_{a\alpha\beta;d\delta}\left(1-(-1)^{v_\gamma-v_\varphi+v}(-1)^{t''-t'+t}(-1)^{n_\varphi}(-1)^{n_\gamma+m_a+m_d}\right)$$
$$C_{a,\alpha}^{\beta,t''}\chi_{a,\alpha;\gamma}^{\beta;d\delta}\left[\left[\left[D_d\rho_\delta^{t''}(\boldsymbol{r})\right]_{J_\gamma}\left[D_f\rho_\varphi^t(\boldsymbol{r})\right]_J\right]_{v\lambda}\right]^{\tilde{tr}}=0$$

that is exactly the condition in Eq. (4.30).

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