Contraintes sur la fonctionnelle de la densite d'energie nucleaire et nouvelles formes analytiques possibles

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Un mois après la fin de mon doctorat voici venu le temps de finaliser mon manuscript par les traditionnels remerciements, qui ont été écrit dans ma langue maternelle, contrairement au reste du manuscrit.

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Contents

Introduction

In spite of over fifty years of theoretical and experimental studies, low-energy nuclear structure remains an open and challenging area of fundamental research. While extensive progress has been made, an accurate and universal description of nuclei from first principles is still beyond reach due to the intrinsic difficulties posed by the nuclear quantum many-body problem.

Theoretical treatment of the nuclear system

The complexity of the nuclear system implies that its description depend on the degrees of freedom used to characterize it as well as on the knowledge of the interaction between them. The first choice is to treat the nucleus as made of quarks exchanging gluons ans photons. Next, the nucleus is treated as composites nucleons exchanging mesons. Eventually, nucleons can be treated as point-like fermions interacting via many-body forces that simulate the exchange of mesons. At the next level of description, dressed nuclear interactions, i.e. interaction renormalized by medium effects, are used such that dressed fermions constituted the considered degrees of freedom. The nucleus can also be described by clusters of nucleons or as a liquid drop.
Each approach has limitations, advantages and a domain of application. For instance, using quarks, gluons and photons to assess the low-energy nuclear properties is not ideal as the typical energy scale at play is too small to excite or probe such degree of freedom individually. Macroscopic approaches such as the liquid drop model [1, 2] can roughly explain bulk properties of nuclei but lack of predictive power and cannot describe elementary modes of excitations. Microscopic techniques in which point-like nucleons are the degrees of freedom constitute the tool of choice for a coherent description of all static and dynamical nuclear properties around the MeV scale. In such an approach the aim is to solve the many-body Schrödinger equation

$$H|\Psi_i\rangle = E_i|\Psi_i\rangle \ , \tag{1}$$

where E_i constitute the energy spectrum of the nucleus and $|\Psi_i\rangle$ the corresponding N-body wave-function. Still difficulties appear.

The nuclear interaction

First of all, and in opposition to systems governed by quantum electrodynamics (QED), the strong interactions between point-like nucleons cannot be derived yet from a gauge theory of interacting quarks and gluons, i.e. from quantum chromodynamics (QCD) that governs the intrinsic structure of hadrons and their interactions. As a result, the inter-nucleon interaction can only be effectively modeled in the low-energy domain, in terms of a very complicated structure [3, 4]. Nucleons are assigned to both spin and isospin SU(2) doublets, i.e. 4-component fermions interacting in various configurations stemming from general invariances of the problem, e.g. spin-orbit, tensor, quadratic spin-orbit... couplings. Beyond its complex structure, the two-nucleon (NN) force presents bound (deuteron np in the coupled $^3S_1$-$^3D_1$ channels) and virtual (di-neutron nn in the $^1S_0$ channel) states. The associated large scattering lengths, together with the short-range repulsion between nucleons closer than their classical hard sphere radii makes

the nuclear many-body problem highly non-perturbative. Finally, a treatment of three-nucleon (NNN) interactions in a theory of point-like nucleons is unavoidable, as has been quantitatively confirmed by modern calculations such as (i) differential nucleon-deuteron cross-sections [5–7], (ii) the under-estimation of the triton and light nuclei binding energies with NN forces only [8], (iii) the Tjon line problem [9], (iv) the improper-saturation of symmetric nuclear matter [10–15], or more generally the Coester line problem [16–18].
Recently, the development of chiral effective field theory (χ-EFT) has made possible the construction of reliable NN and NNN interactions, in connection with QCD [19]. The main benefits of χ-EFT are the formulation of the nuclear problem in terms of relevant low-energies degrees of freedom while retaining the symmetry of the underlying theory, and the hierarchy, called *power counting*, obtained that naturally explains why the N-body interaction is more important than (N+1)-body interaction.
Progress toward controlled nuclear calculations has long been hindered by the highly non-perturbative character of realistic nuclear interactions. Recently, χ-EFT and Renormalization Group (RG) methods [20–23] have promoted a different view point based on the fact that the Hamiltonian (potential) is not an observable that can be fixed from experiment [24]. RG methods thus proceed to a (unitary) transformation to decouple low-momentum modes from high-momentum ones that are still present in any χ-EFT-based interaction, such that nuclear interactions become softer; i.e. they make the many-body problem more perturbative from the outset.

The many-body problem

Most nuclei, i.e. nuclei with masses typically between 40 and 350, are by essence intermediates between few- and many-body systems. That is (i) ab initio techniques that describe the interacting system in terms of basic two- and three-body vacuum nuclear forces find rapidly their theoretical and computational limits, while at the same time (ii) finite-size effects play a significant part, which prevents any statistical treatment. Furthermore, a unified view of low-energy nuclear structure implies a coherent description of (i) small- and large-amplitude collective motions, (ii) closed and open systems, that is a description of the structure-reaction interface (fission, fusion, nucleon emission at the drip-line...), and (iii) stable and exotic systems, e.g. systems with large isospin asymmetry. Finally, pairing correlations are essential to describe low-energy bulk properties of nuclei, but their explicit treatment complexifies the formulation of the many-body problem.

Different approaches

Microscopic techniques keep as much as possible a connection with initial vacuum two- and three-body interactions. However, because the numerical complexity of the nuclear problem increases exponentially with the number of nucleons, necessary approximations lead to models that gradually lose the connection with vacuum forces as one goes from few- to many-body systems by (i) restricting the Hilbert space in which nucleons evolve, (ii) approximating the treatment of correlations, and/or (iii) using phenomenological corrections or full approximations based on empirical assumptions and experimental data. For three- or four-nucleon systems, essentially exact solutions of the Faddeev or Yakubowski equations can be found using realistic forces [25–27]. Likewise, in the case of very light nuclei ($A \lesssim 12$) Green function Monte-Carlo (GFMC) calculations [28–30] can describe the fully correlated few-body problem starting from realistic two- and three-body forces, using the exact evolution operator, but are restricted to local potentials and face already huge numerical challenges for ^{12}C. Other ab initio methods allow the treatment of nuclei up to $A \approx 16$ using vacuum NN and NNN forces, e.g. the no-core shell model (NSCM) [31–34] that projects the interacting problem on a given model

space defined through a harmonic oscillator basis. Coupled-cluster (CC) theory [35–39], which constructs the correlated state from a product state using a cluster expansion of the exponented n-particle n-hole operator, truncated to B-body operators (typ. $B \sim 1-4$), renders possible calculations up to $A \approx 50$ around closed shells. The same is true about self consistent Green's function method [40] that is currently being extended to singly-open-shell nuclei [41]. Note that all these methods, while giving essentially exact results, still use a truncation of some sort while preserving an explicit connection with vacuum nuclear forces. To go to heavier systems, an approximate treatment of both the interacting problem and the interaction is needed. For instance, the configuration interaction (CI) model [42, 43], or shell model (SM), constructs a model space within which valence nucleons interact through an effective interaction. Even though the latter is usually obtained as a microscopic G-matrix, certain combinations of its matrix elements (monopolar terms...) are partly refitted on experimental data within a given model space (sd, pf...). Proceeding this way, spectroscopic properties within the considered model space are described with an excellent accuracy [42, 44].

Energy Density Functional method

Eventually, the theoretical tool of choice for the microscopic description of all medium- and heavy-mass nuclei is the Energy Density Functional (EDF) method [45], often referred to as "self-consistent mean-field method". Based on relativistic or non-relativistic frameworks, it allows a unified description of nuclei over the whole nuclear chart.
Historically, such a method has been first designed in a restrictive scheme and denoted as "mean-field" and "beyond mean-field" methods. In-medium effects were re-summed through the use of an effective potential that was qualitatively related to the Brueckner matrix [46]. The construction of effective potentials eventually led to the design of a more general EDF method, where the energy density is constructed directly without any reference to an effective potential, which allows a more flexible re-summation of correlations.
Nowadays, state-of-the-art calculations are based on empirical energy functionals (Skyrme, Gogny) adjusted on experimental data, which raises the question of the predictive power of extrapolated EDF results in the terra incognita.

Pathologies

While bulk correlations are subsumed into a suitable energy density functional, long-range correlations associated with collective modes must be incorporated more explicitly, such that two successive levels of EDF calculations coexist (i) the single-reference (SR) level followed by an explicit configuration mixing within the (ii) multi-reference (MR) level. In particular, while symmetries of the underlying nuclear Hamiltonian are broken at the SR level, the finiteness of nuclei asks for their restoration at the MR level.
The beginning of the century witnessed an explosion of MR calculations, including the (sometime combined) restoration of particle number, angular momentum, parity, linear momentum and isospin. However, it was slowly realized that the "naive" implementation of the symmetry restoration concepts within the context of the general EDF method is plagued with technical and conceptual difficulties that generate spurious divergencies and steps.
At first, implicit numerical regularization schemes were used to generate "reasonable results" in practical applications. However, it was realized later on that such divergencies are in fact the visible precursor of finite un-physical contaminations related to non analyticities of the energy kernel over the complex plane that cannot be bypassed using numerical tricks [47–49].
As a result, a method was formulated to meaningfully regularize, for any symmetry restoration and configuration mixing calculation, EDF parameterizations that depend solely on integer powers of the one-body density matrices. Given that the large majority of modern parameterization

of the nuclear does not fulfill such a property, challenging questions currently faced by practitioners relate to whether (i) spuriosities that have been dealt with recently are the only ones or whether it is necessary look for other constraints in order to make MR calculations well defined within the general EDF context (ii) regularizable high-precision EDFs can be constructed, (iii) a more general regularization method that tackle non-integer powers of the density matrices can be designed, (iv) one must go back to using EDF kernels that derive from strict pseudo-potentials displaying no dependence on the trial state (e.g. no density dependence) such that problems are avoided in the first place, (v) one should rely on approximations of the full symmetry restoration that may bypass the problem from the outset (e.g. Kamhlah, Lipkin), or whether (vi) the formulation of the symmetry-restored EDF method can be guided by a first-principle many-body theory such that problems are avoided in the first place.
The present work aims at tackling questions (i) and (iv) leaving the other questions for further investigations.

Outline

The present document is organized as follows. A short introduction of the EDF formalism is provided in Chap. 1. Chap. 2 is devoted to a review of the notion of symmetry breaking and restoration on which the nuclear energy density functional method rely. Difficulties to formulate the restoration of symmetries within the general energy functional framework will be pointed out. Such problems serve as a motivation for the development of (i) new constraints to be applied on the energy density, presented in Chap. 2 and in Appendix E, and of (ii) a new Skyrme pseudo-potential. Analytical developments of such pseudo-potential are discussed in Chap. 3. The associated infinite nuclear matter properties are derived in Chap. 4. The optimization procedure of the pseudo-potential free parameters is presented in Chap. 5. Parameterizations than obtained are used to compute INM and nuclei properties in Chap. 6. Such results provide information on the quality of the fitting procedure and on the relevance of the pseudo-potential developed.

Chapter 1

Energy Density Functional method in a nutshell

Abstract: The present chapter is a short introduction to the Energy Density Functional (EDF) method [45]. It serves as a baseline for the more detailed and specific discussion provided in Chap. 2. The particular case for which the energy kernel is computed from a pseudo-potential and the resulting specific differences with the more general case are stressed.

Contents

1.1 Introduction

The most appropriate tool for the microscopic description of all medium- and heavy-mass nuclei is the Energy Density Functional (EDF) method, historically referred to as "self-consistent mean-field and beyond mean-field methods". It is based on the use of product states and thus resembles a particle, or more precisely quasi-particle, independent approximation. It however allows the re-summation of many-body correlations through the use of an effective energy functional.

1.2 Basic ingredients

1.2.1 Product states of reference

The EDF method originates from the picture of a nucleus as an ensemble of quasi-particle moving independently in their self created mean field. It is not based on the manipulation of

(an approximation to) the correlated exact N-body wave-function $|\Psi\rangle$. It however relies on the use of product states of Bogoliubov quasi-particles labelled with collective labels g

$$|\Phi(g)\rangle = \prod_{\mu} \beta_{\mu}^{(g)}|0\rangle \ , \tag{1.1}$$

where $\{\beta_{\mu}^{(g)\dagger}\}$ and $\{\beta_{\mu}^{(g)}\}$ denote quasi-particle creation and annihilation operators. Typically g represents the value of the axial quadrupole moment, Euler angles denoting the orientation of the deformed body, the value of the pairing gap, the angle in gauge space ... Quasi-particle creation and annihilation operators relate to particle ones through

$$\beta_{\mu} = \sum_{i} U_{\mu i}^{\dagger} a_i + V_{\mu i}^{\dagger} a_i^{\dagger} \ , \tag{1.2a}$$

$$\beta_{\mu}^{\dagger} = \sum_{i} V_{i\mu} a_i + U_{i\mu} a_i^{\dagger} \ , \tag{1.2b}$$

where $\{a_i\}$ denote any convenient single-particle basis and where U and V form a unitary transformation of the Bogoliubov type [50].

1.2.2 Energy functional kernel

To re-sum the bulk of correlations using such simple product states, the existence of an effective off-diagonal energy kernel is postulated

$$E[g',g] \equiv E[\langle\Phi(g')|;|\Phi(g)\rangle] = E[\rho_{ij}^{g'g}, \kappa_{ij}^{g'g}, \kappa_{ij}^{gg'\,*}] \ , \tag{1.3}$$

that is a functional, in the mathematical sense, of one-body transition density matrices defined through

$$\rho_{ij}^{g'g} \equiv \frac{\langle\Phi(g')|a_j^{\dagger}a_i|\Phi(g)\rangle}{\langle\Phi(g')|\Phi(g)\rangle} \ , \tag{1.4a}$$

$$\kappa_{ij}^{g'g} \equiv \frac{\langle\Phi(g')|a_j a_i|\Phi(g)\rangle}{\langle\Phi(g')|\Phi(g)\rangle} \ , \tag{1.4b}$$

$$\kappa_{ij}^{gg'\,*} \equiv \frac{\langle\Phi(g')|a_i^{\dagger}a_j^{\dagger}|\Phi(g)\rangle}{\langle\Phi(g')|\Phi(g)\rangle} \ . \tag{1.4c}$$

One-body transition density matrices 1.4 are calculated from a pair of product states as defined in Eq. 1.1.

1.2.3 Skyrme example

In the case of quasi-local Skyrme EDF, the energy kernel takes the form

$$E[g',g] \equiv \int d\vec{r}\ \mathcal{E}(\rho^{g'g}(\vec{r}), \tau^{g'g}(\vec{r}), \vec{j}^{g'g}(\vec{r}), \ldots) \ , \tag{1.5}$$

where $\mathcal{E}(\rho^{g'g}(\vec{r}), \tau^{g'g}(\vec{r}), \vec{j}^{g'g}(\vec{r}), \ldots)$ is a general function of a set of one-body local transition densities [45]

$$\rho^{g'g}(\vec{r}) \equiv \sum_{ij} \varphi_j^*(\vec{r})\, \varphi_i(\vec{r})\, \rho_{ij}^{g'g} \quad , \tag{1.6a}$$

$$\tau^{g'g}(\vec{r}) \equiv \sum_{ij} \left[\vec{\nabla}\varphi_j^*(\vec{r})\right] \cdot \left[\vec{\nabla}\varphi_i(\vec{r})\right] \rho_{ij}^{g'g} \quad , \tag{1.6b}$$

$$\vec{j}^{g'g}(\vec{r}) \equiv -\frac{i}{2} \sum_{ij} \left\{ \varphi_j^*(\vec{r}) \left[\vec{\nabla}\varphi_i(\vec{r})\right] - \left[\vec{\nabla}\varphi_j^*(\vec{r})\right] \varphi_i(\vec{r}) \right\} \rho_{ij}^{g'g} \quad , \tag{1.6c}$$

$$\vdots$$

For instance, in the case of a bilinear functional up to second order in gradients, neglecting spin, isospin and pairing for simplicity, one has

$$\begin{aligned} &\mathcal{E}^{ex}(\rho^{g'g}(\vec{r}), \tau^{g'g}(\vec{r}), \vec{j}^{g'g}(\vec{r})) \\ &\qquad \equiv \frac{\hbar^2}{2m}\tau^{g'g}(\vec{r}) + C^{\nabla\rho}\left(\vec{\nabla}\rho^{g'g}(\vec{r})\right)^2 + C^{\tau}\left(\rho^{g'g}(\vec{r})\tau^{g'g}(\vec{r}) - \vec{j}^{g'g}(\vec{r}) \cdot \vec{j}^{g'g}(\vec{r})\right) \quad . \end{aligned} \tag{1.7}$$

where specific constraints have been imposed onto the functional form for it to be a scalar under all transformations that leave the nuclear Hamiltonian invariant. For instance $\rho^{g'g}(\vec{r})\tau^{g'g}(\vec{r})$ and $\vec{j}^{g'g}(\vec{r}) \cdot \vec{j}^{g'g}(\vec{r})$ are correlated such that Galilean invariance is fulfilled. We refer the reader to Refs. [51–53] for the formulation of such constraints.

1.3 Symmetry breaking and restoration

The nuclear EDF method relies heavily on the concept of spontaneous symmetry breaking and (approximate) restoration. In that sense, it is intrinsically a two-step approach.

1.3.1 Single-Reference (SR-)EDF

At the single-reference (SR) level, one invokes the diagonal kernel $E[g', g]$ only, i.e. one-body density matrices are computed from a single product-state of reference $|\Phi(g)\rangle$. The state $|\Phi(g)\rangle$ may break as many symmetries of the nuclear Hamiltonian as it finds energetically favorable and thus acquires finite order-parameters that we group under the generic notation $|g|\, e^{i\mathrm{Arg}(g)}$. The unknown quantity, i.e. the reference state $|\Phi(g)\rangle$, is determined by minimizing the diagonal energy kernel

$$E^{SR} \equiv \mathrm{Min}_{|\Phi(g)\rangle}\Big\{ E[g,g] + Const[|\Phi(g)\rangle] \Big\} \quad , \tag{1.8}$$

under a set of constrains, e.g. that the average particle number in $|\Phi(g)\rangle$ is the actual number of particles in the nucleus under study. Minimization 1.8 gives rise to solving a Bogoliubov-De Gennes-like eigenvalue equation, see Sec. 3.6. This first step incorporates static collective correlations and thus provides a first approximation to observables such as binding energies, charge radii, nucleonic density distributions and effective single-particle energies.

1.3.2 Multi-Reference (MR-)EDF

The multi-reference (MR) extension further includes correlations associated with quantum collective fluctuations of the order parameter $|g|\, e^{i\mathrm{Arg}(g)}$ associated with the various symmetries of interest. In particular it treats collective vibrations and restores broken symmetries by mixing configurations corresponding to several values of $|g|$ and $\mathrm{Arg}(g)$, respectively (see Fig. 1.1). The

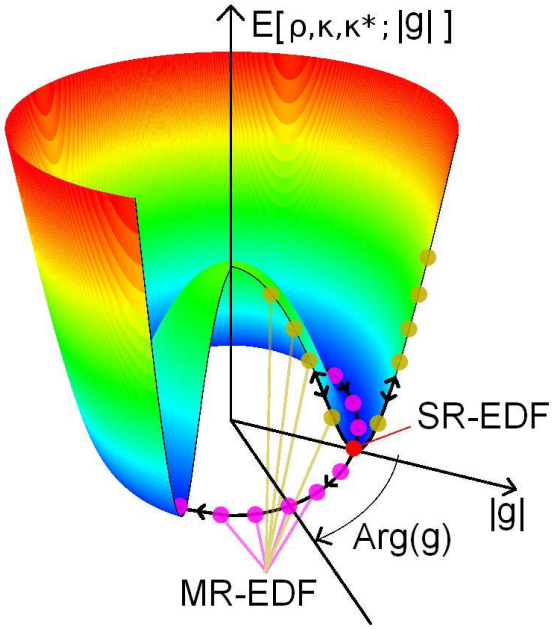

Figure 1.1: Schematic view of the energy landscape as a function of the phase and the magnitude of the order parameter q of a (possibly) spontaneously broken symmetry.

MR step thus invokes several product states $\{|\Phi(g)\rangle\}$ generated by constrained SR calculations. The MR energy mixes off-diagonal energy kernels (Eq. 1.3) associated with the chosen set of product states through

$$E_k^{MR} \equiv \mathrm{Min}_{f^k_{|g|}} \left\{ \frac{\sum_{g,g'} f^{k*}_g f^k_{g'} E[g',g] \langle\Phi(g')|\Phi(g)\rangle}{\sum_{g,g'} f^{k*}_g f^k_{g'} \langle\Phi(g')|\Phi(g)\rangle} \right\} , \tag{1.9}$$

where coefficients $f^k_{\mathrm{Arg}(g)}$ associated to symmetries restoration are determined by the structure of the symmetry groups (see Chap. 2). As a results the minimization only provides coefficients $f^k_{|g|}$ associated to collective vibrations.

1.3.3 EDF power

Correlation energy	Treatment	Scale	Vary with
Bulk	Summed into EDF kernel	$\sim 8\,A$ MeV	A
Static collective	Finite order parameter q	$\lesssim 25$ MeV	$A_{\mathrm{val}}, G_{\mathrm{deg}}$
Dynamical collective	Fluctuations of q	$\lesssim 5$ MeV	$A_{\mathrm{val}}, G_{\mathrm{deg}}$

Table 1.1: Schematic classification of correlation energies as they naturally appear in nuclear EDF methods. The quantity A_{val} denotes the number of valence nucleons while G_{deg} characterizes the degeneracy of the valence major shell.

Given the efforts needed to better formulate the EDF method (see Chaps. 2,5,6), one may question the necessity to stick to such an approach rather than to use an (ab-initio) approach that strictly computes the energy from a (state-/density-independent) Hamiltonian, e.g. through

many-body perturbation theory. Although the breaking (up to a few tens of MeV) and the restoration (up to a few MeV) of symmetries bring in both types of methods essential correlations that vary rapidly with nucleon numbers, incorporating the bulk of correlations [1] (hundreds of MeV) requires involved ab-initio calculations [55] that are still impractical for heavy open-shell nuclei. The power of the EDF approach is to parameterize bulk correlations under the form of a functional of one-body density (matrices) such that systematic calculations of heavy nuclei are tractable. The success of the overall approach, based on the resummation of bulk correlations into the EDF kernel and the further breaking and restoration of symmetries, relies on the empirical decoupling of the different categories of correlations at play, i.e. on the different scales that characterize them (see TAB. {1.1}), and on the fact that quickly varying correlations with the filling of nuclear shells are explicitly accounted for through symmetry breaking and restoration [2].

1.4 Pseudo-potential-based EDF method

A particular case of the EDF method is obtained when the energy functional kernel is derived from an effective Hamiltonian

$$\hat{H}_{\rm pseudo} = \sum_{ij} \hat{t}_{ij} a_i^\dagger a_j + \frac{1}{2!}\sum_{ijkl} \hat{v}^2_{ijkl} a_i^\dagger a_j^\dagger a_l a_k + \frac{1}{3!}\sum_{ijklmn} \hat{v}^3_{ijklmn} a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l + \cdots \ , \tag{1.10}$$

where $\hat{v}^N_{ijkl}$ denote N-body pseudo-potential, i.e. effective interactions. Such particular case might be denoted as a pseudo-potential-based EDF method. The off-diagonal energy kernel, written $E_H[g',g]$, used at each step of the method is then defined as

$$E_H[g',g] \equiv \langle \Phi(g')|H_{\rm pseudo}|\Phi(g)\rangle = E_H[\rho^{g'g}_{ij}, \kappa^{g'g}_{ij}, \kappa^{gg'\,*}_{ij}] \ , \tag{1.11}$$

which is a functional of one-body transition density matrices EQ. 1.4 as can be demonstrated by using the generalized Wick theorem [56]. The SR energy E_H^{SR} and the MR energy $E_{k,H}^{MR}$ are still obtained through EQ. 1.8 and EQ. 1.9, respectively, but using EQ. 1.11 as the energy kernel.

1.4.1 Skyrme example

Let us simplify the effective Hamiltonian 1.10 as

$$\hat{H}^{\rm ex}_{\rm pseudo} = \sum_{ij} \hat{t}_{ij} a_i^\dagger a_j + \frac{1}{2!}\sum_{ijkl} \hat{v}^{2Sk}_{ijkl}\, a_i^\dagger a_j^\dagger a_l a_k \ , \tag{1.12}$$

where $\hat{v}^{2Sk}_{ijkl}$ is a simplified form of the two-body Skyrme pseudo-potential depending on the reduced set of parameters $\{t_1, t_2\}$ (see CHAP. 3 for a presentation of such Skyrme pseudo-potential). Using EQ. 1.12 in EQ. 1.11 and applying the generalized Wick theorem provides

$$E_H^{ex}[g',g] \equiv \int d\vec{r}\ \mathcal{E}_H^{ex}(\rho^{g'g}(\vec{r}), \tau^{g'g}(\vec{r}), \vec{j}^{g'g}(\vec{r})) \ , \tag{1.13}$$

with

$$\begin{aligned}\mathcal{E}_H^{ex}&(\rho^{g'g}(\vec{r}), \tau^{g'g}(\vec{r}), \vec{j}^{g'g}(\vec{r})) \\ &\equiv \frac{\hbar^2}{2m}\tau^{g'g}(\vec{r}) + A^{\nabla\rho}\left(\vec{\nabla}\rho^{g'g}(\vec{r})\right)^2 + A^{\tau}\left(\rho^{g'g}(\vec{r})\tau^{g'g}(\vec{r}) - \vec{j}^{g'g}(\vec{r})\cdot\vec{j}^{g'g}(\vec{r})\right) \ ,\end{aligned} \tag{1.14}$$

where spin, isospin and pairing have been neglected for simplicity. One realizes that EQ. 1.14 looks identical to EQ. 1.7. However, crucial differebnces exist between the two.

1. We take as a loose definition of bulk correlations the correlation energy computed beyond a genuine Hartree-Fock approximation in terms of the vacuum (low-momentum [54]) nuclear Hamiltonian for nuclei that do not break any symmetry besides translational invariance, i.e. doubly-magic nuclei.
2. As expected by EQ. 1.9, we have in mind to add the fluctuations of the magnitude of the order parameter.

1.4.2 Specific difference with general case

In the pseudo-potential-based approach, the two functional coefficients $A^{\nabla\rho}$ and A^{τ} are both related to the free parameters $\{t_1, t_2\}$ through

$$A^{\nabla\rho} = \frac{t_1}{4} + \frac{t_2}{4} \qquad \text{and} \qquad A^{\tau} = \frac{3t_1}{16} - \frac{t_2}{16} \ . \tag{1.15}$$

Contrarily, in the general EDF approach, the free parameters are the functional coefficients $C^{\nabla\rho}$ and C^{τ}. As a result, those free parameters are not interrelated contrarily to $A^{\nabla\rho}$ and A^{τ}. It obviously comes from the fact that the functional has been postulated rather than derived as the matrix element of an operator. It is only in the latter case that the antisymmetrization is taken into account. Functional coefficients interrelations are in that sense a way for the energy functional to respect the Pauli principle that is not fulfilled a priori in the more general EDF method. Similarly, a density-dependent effective "Hamiltonian" does not ensure an entirely antisymmetrized energy functional since the density dependence does not itself derive from a matrix element of an operator.

After this short introduction, the next chapter focuses in symmetry restoration and discusses specific differences that exist in the general EDF framework as opposed to the pseudo-potential-based EDF approach.

Chapter 2

Breaking and restoring symmetries

Abstract: This chapter is devoted to a review of the notion of symmetry breaking and restoration within the frame of the nuclear energy density functional method [57]. We focus on key differences between pseudo-potential-based EDF and a more general implementation of the EDF methods. In particular, we point to difficulties to formulate the restoration of symmetries within the general EDF framework. The problems tackled recently in connection with particle-number restoration serve as a baseline to the present discussion. Reaching out to angular-momentum restoration, we identify an exact mathematical property of the energy density $\mathcal{E}^{LM}(\vec{R})$ that could be used to constrain energy density functional kernels. Consequently, we suggest possible routes towards a better formulation of symmetry restorations within energy density functional methods.

Contents

2.1 Introduction

2.1.1 Spontaneous symmetry breaking

Symmetries are essential features of classical and quantal systems. For the latter in particular, symmetries characterize the energetics of the system and provide transition matrix elements of operators with specific selection rules. In nuclear systems for example, electromagnetic and electro-weak decays display patterns associated with such selection rules.

On the other hand, certain emergent phenomena relate to the spontaneous breaking of those symmetries [58]. In the thermodynamic limit, i.e. when the number of particles N and the volume V of the system go to infinity such that N/V remains constant, a state with lower symmetry than the Hamiltonian can be rigorously used as an effective ground-state of the system. Such a state is a linear superposition of nearly-degenerate eigenstates, i.e. it is a wave-packet. In finite systems however, quantum fluctuations make such a wave-packet to relax into the symmetry-conserving ground-state and cannot be ignored; i.e. the concept of spontaneous symmetry breaking is only an intermediate description of the system that arises within certain approximations and symmetries must eventually be restored. Still, it makes physical sense to go through such an intermediate description as pseudo spontaneously-broken symmetries (i) relate to specific features of the inter-particle interactions, (ii) characterize internal correlations and (ii) leave clear fingerprints in the observed excitation spectrum of the system.

Invariance	V^{NN}	Internal correlations	Excitation patterns
Spatial translation	Short range	Spatial localization	Surface vibrations
Gauge rotation	S-wave attraction	Pairing	Energy gap
Spatial rotation	Quad.-quad. component	Angular localization	Rotational bands

Table 2.1: Links between the spontaneous breaking of translational, rotational and particle-number symmetries and features of the nuclear force, correlations in the internal motion of nucleons and patterns in the excitation spectrum.

In atomic nuclei, several symmetries, if allowed, tend to break spontaneously in approximate descriptions based on the mean-field concept. The most important ones relate to the invariance of the nuclear Hamiltonian H under spatial translations and rotations as well as to the gauge invariance associated with particle-number symmetry. As described in Tab. {2.1}, the spontaneous breaking of these three symmetries relates to the short-range and dominant quadrupole-quadrupole terms of the nucleon-nucleon interaction as well as to its strong attraction in the $L = 0$ partial-wave of relative motion. The latter in particular generates a S-wave di-neutron (di-proton) virtual state at almost zero scattering energy that is the precursor of neutron (proton) Cooper pairs and superfluidity in the nuclear medium. Even though such symmetries must be eventually enforced, their underlying breaking impacts the low-lying spectroscopy of finite nuclei through the presence of surface vibrational excitations, rotational bands and a gap in the individual excitations of even-even nuclei, respectively [50]. Parity and time-reversal are other good symmetries of H that can be spontaneously broken, while isospin symmetry is only approximate in the first place.

2.1.2 Pseudo-potential-based EDF method

As schematically shown in Fig. 2.1, quantum many-body methods separate into two categories as for the way symmetries are dealt with, i.e. (i) methods enforcing symmetries throughout

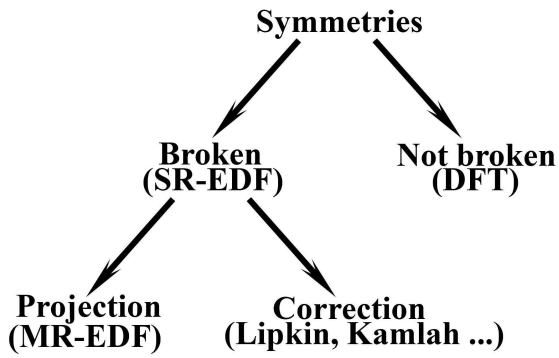

Figure 2.1: Schematic representation of the different strategies followed by many-body methods regarding the treatment of symmetries, e.g. in Density Functional Theory and nuclear Energy Density Functional approaches.

and (ii) those that explicitly single out the intermediate breaking of symmetries. Although hybrid approaches that allow the breaking of some symmetries while enforcing the others can be set up, the present chapter focuses on the EDF method that strongly relies on the concept of symmetry breaking, i.e. a method whose philosophy, apart for computational constraints, is to allow all symmetries to break spontaneously a priori. The breaking of each symmetry is monitored by the magnitude and the phase of an order parameter g, such that the (approximate) energy is independent of its phase as schematically shown in FIG. 1.1. This corresponds to the fact that a spontaneous symmetry breaking is accompanied by the presence of a zero-energy Goldstone mode. Of course, that a certain symmetry does break spontaneously usually depends on the number of elementary constituents of the system under consideration. For example, while translational symmetry (strongly) breaks in all nuclei, particle-number symmetry tend to (weakly) break in all but doubly-magic nuclei whereas rotational symmetry remains unbroken if either the neutron number or the proton number is "magic" [1]. FIG. 2.2 displays the correlation energy incorporated in ^{240}Pu and ^{120}Sn ground-states energy through the spontaneous breaking of rotational and particle-number symmetries, respectively. Such symmetry breakings may account for up to 20 MeV correlation energy out of about 2 GeV of binding energy, i.e. for about 2%, which is much larger than the targeted accuracy on nuclear masses. Incorporating such correlation energies through symmetry-conserving approaches, e.g. configuration interaction methods, would necessitate tremendous computational efforts in such heavy open-shell nuclei.

As already stated, methods authorizing the breaking of symmetries at a certain level of approximation must eventually restore them in a second stage. In pseudo-potential-based EDF methods, the single reference step relies on minimizing the average value of an effective Hamiltonian for a trial product state that does not carry good quantum numbers, i.e. which mixes irreducible representations of the symmetry group of interest. Restoring symmetries amounts to using an enriched trial state that does carry good quantum numbers. In terms of the schematic "mexican-hat" picture of FIG. 1.1, this corresponds to incorporating zero-energy fluctuations associated with the phase of the order parameter [2]. One typical approach used in the pseudo-

1. The fact that the neutron or proton number is magic is not known a priori but is based on a posteriori observations and experimental facts. In particular, the fact that traditional magic numbers, i.e. $N, Z = 2, 8, 20, 28, 50, 82, 126$, remain as one goes to very isospin-asymmetric nuclei is the subject of intense on-going experimental and theoretical investigations [59].

2. As discuss in CHAP. 1, and although it is not the focus of the present work, the restoration of symmetries must be accompanied by the inclusion of collective quantum correlations associated with the fluctuations of the *magnitude* of the order parameter, i.e. fluctuations along the radial coordinate of the "mexican-hat"

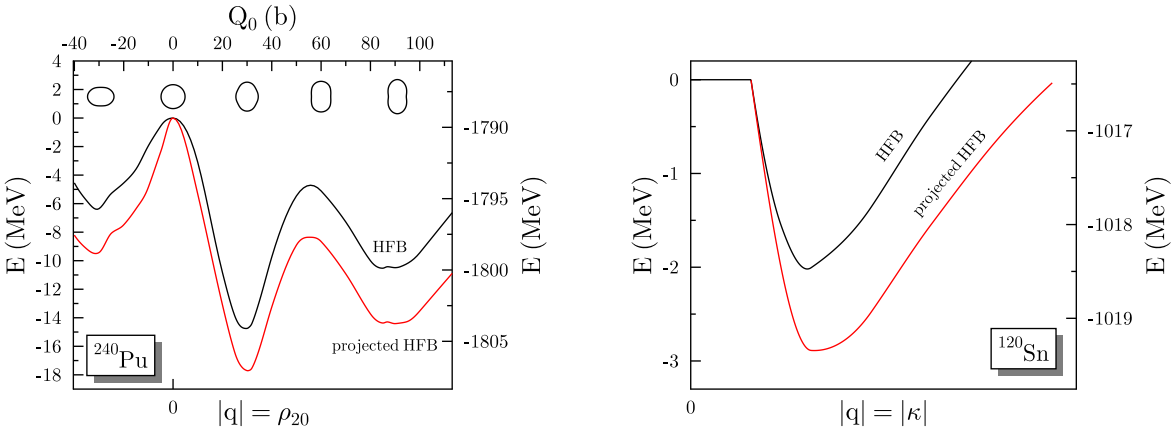

Figure 2.2: Energy gain from spontaneous symmetry breaking and symmetry restoration as a function of the magnitude of the order parameter q. Left: breaking and restoration of rotational symmetry in the ground state of ^{240}Pu as a function of the axial quadrupole moment of the single-nucleon density distribution (adapted from Ref. [65]). Right: breaking and restoration of neutron-number symmetry in the ground state of ^{120}Sn as a function of the norm of the anomalous pair density (adapted from Ref. [66]).

potential-based MR-EDF method is to project out from the symmetry-breaking product state the component that belongs to the intended irreducible representation [50]. Fig. 2.2 shows that doing so for rotational and particle-number symmetries adds a few MeV correlation energy to the ground-state binding energy of heavy nuclei. This is still significant compared to the few hundreds keV targeted accuracy on nuclear masses. As shown in Fig. 2.1, a variant consists of performing the symmetry restoration only approximately such that the calculation boils down to the minimization of a *corrected* diagonal energy kernel expressed in terms of a single symmetry-breaking product-state. Typical examples are Lipkin [60, 61] or Kamlah approximate projection methods [62, 63]. While it is likely that the strongly broken translational symmetry can be safely treated through such approximate projection methods [3], it is still unclear whether the same is true for weakly broken symmetries such as particle number symmetry or rotational symmetry in transitional nuclei.

2.1.3 General EDF method

The pseudo-potential-based EDF projection method and its variants is well formulated quantum mechanically [50]. The goal of the present chapter is to discuss the general EDF counterpart [45]. In the general framework, the MR-EDF step necessitates a prescription to extend the SR energy functional [4] associated to a single auxiliary state of reference, i.e. a diagonal energy kernel, to the non-diagonal energy kernel associated with a pair of reference states (see Sec. 2.4.2). Constraints based on physical requirements have been worked out that limit the number of possible prescriptions to do so [67]. In short, it requires the off diagonal EDF $E[g', g]$ kernel to be a functional of the bra $\langle\Phi(g')|$ and of the ket $|\Phi(g)\rangle$ as already alluded to in Eq. 1.3. Still, pathologies [68–70] of MR-EDF calculations have been recently identified and corresponding cures [47–49] have been proposed. Besides the actual successes of nuclear EDF calculations [45], the work of Refs. [47–49, 71] demonstrates that nuclear SR- and MR-EDF meth-

3. Such a statement is to be taken with a grain of salt for rather light nuclei [64].
4. The density-dependence of the effective Hamilton operator in more standard formulations.

ods must be further constrained to become satisfactory many-body approaches to finite Fermi systems. The first goal of the present chapter will be to reformulate, focusing on group-theory considerations, concerns about MR-EDF calculations that have been dealt with in Refs. [47–49, 71]. Our second objective will be to provide a new mathematical property that could be used in the case of angular-momentum restoration to constrain the form of basic EDF kernels at play.

2.1.4 Density functional theory

As the aim of the present chapter is to raise questions about the treatment of symmetries within the nuclear EDF method, let us make a few relevant statements about Density Functional Theory (DFT) [72–74] that provides a formal framework to obtain the ground-state energy and one-body density of electronic many-body systems. It has become customary in nuclear physics to assimilate the SR-EDF method, eventually including corrections *a la* Lipkin or Kamlah, with DFT, i.e. to state that the Hohenberg-Kohn theorem underlays nuclear SR-EDF calculations [75–79]. This is a misconception as distinct strategies actually support both methods. Whereas the SR-EDF method minimizes the energy with respect to a symmetry-breaking trial density(ies), DFT relies on an energy functional whose minimum must be reached for a one-body density that possesses *all* symmetries of the actual ground-state density, i.e. that displays fingerprints of the symmetry quantum numbers carried by the underlying exact ground-state [80]. As a matter of fact, generating a symmetry-breaking solution is problematic in DFT, as it lies outside the frame of the Hohenberg-Kohn theorem, and is usually referred to as the *symmetry dilemma*. To bypass the symmetry dilemma and grasp kinematical correlations associated with good symmetries, several reformulations of DFT have been proposed over the years, e.g. see Refs. [81, 82], some of which are actually close in spirit [5] to the nuclear MR-EDF method [81].

Recent efforts within the nuclear community have been devoted to formulating a Hohenberg-Kohn-like theorem in terms of the internal density, i.e. the matter distribution relative to the center of mass of the self-bound system [83, 84]. Together with an appropriate Kohn-Sham scheme [84], it allows one to reinterpret the SR-EDF method as a functional of the internal density rather than as a functional of a translational-symmetry-breaking density. This constitutes an interesting route whose ultimate consequence would be to remove entirely the notion of breaking and restoration of symmetries from the EDF approach and make the SR formulation a complete many-body method, at least in principle. To reach such a point though, the work of Refs. [83, 84] must be extended, at least, to rotational and particle-number symmetries, knowing that translational symmetry was somewhat the easy case to deal with given the explicit decoupling of internal and center of mass motions.

2.2 Symmetry group

Let us consider an arbitrary continuous compact group $\mathcal{G} \equiv \{\mathcal{R}(g)\}$ parameterized by r real parameters $g \equiv \{g_i; i = 1, \dots, r\}$ and whose transformations leave H invariant. We denote by $v_\mathcal{G}$ the volume of the group

$$v_\mathcal{G} \equiv \int_\mathcal{G} dm(g) \ , \tag{2.1}$$

where $m(g)$ is the invariant measure on $\mathcal{G}$. Having in mind to deal more specifically with particle number and rotational symmetries, we further consider $\mathcal{G}$ to be a Lie group, although this is not mandatory. We thus introduce the set of infinitesimal generators $\mathcal{C} = \{\mathcal{C}_i; i = 1, \dots, r\}$ that make up the Lie algebra and in terms of which any transformation of the group can be expressed. The Casimir of the group built from the infinitesimal generators and a non-degenerate

5. But not in the technical details

invariant bilinear form is denoted by Λ. We also denote by $R(g)$ (C) a unitary representation of $\mathcal{R}(g)$ $(\mathcal{C})$ on the Fock space of quantum mechanics and by $S^{\lambda}_{ab}(g) \equiv \langle\Theta^{\lambda a}|\, R(g)\, |\Theta^{\lambda b}\rangle$ the matrix elements of the unitary irreducible representation labeled by λ. States $|\Theta^{\lambda a}\rangle$ span the irreducible representation λ whose degree is d_λ. They are eigenstates of the Casimir Λ and of a chosen generator C_0

$$\Lambda\,|\Theta^{\lambda a}\rangle \;=\; l(\lambda)\,|\Theta^{\lambda a}\rangle \;, \tag{2.2}$$

$$C_0\,|\Theta^{\lambda a}\rangle \;=\; g(a)\,|\Theta^{\lambda a}\rangle \;, \tag{2.3}$$

where eigenvalues $l(\lambda)$ and $g(a)$ are functions of labels λ and a, respectively, with a running over d_λ values.
Noticing that $S^{\lambda}_{ab}(0) = \delta_{ab}$ for all λ, the action of two successive transformations and the unitarity of the representation can be both read off the following identity

$$\sum_c S^{\lambda\,*}_{ca}(g')\, S^{\lambda}_{cb}(g) \;=\; \sum_c S^{\lambda}_{ac}(-g')\, S^{\lambda}_{cb}(g) = S^{\lambda}_{ab}(g-g') \;, \tag{2.4}$$

where $-g$ and $g-g'$ symbolically denote the parameters of transformations $R^{-1}(g)$ and $R^{-1}(g')R(g)$, respectively. A so-called *irreducible tensor operator* T^{λ}_a and a state $|\Theta^{\lambda a}\rangle$ transform according to

$$R(g)\, T^{\lambda}_a\, R(g)^{-1} \;=\; \sum_b T^{\lambda}_b\, S^{\lambda}_{ba}(g) \;, \tag{2.5}$$

$$R(g)\,|\Theta^{\lambda a}\rangle \;=\; \sum_b |\Theta^{\lambda b}\rangle\, S^{\lambda}_{ba}(g) \;. \tag{2.6}$$

The discussion below is conducted for the energy, i.e. for a scalar operator H belonging to the trivial irreducible representation $\lambda = 0$ characterized by $S^{0}_{ba}(g) = \delta_{ab}$. However, such a discussion can be extended to any irreducible tensor operator [85].

For nuclear structure, two groups are of particular importance as discussed in the introduction, i.e. $SO(3)$ for rotations in the three-dimensional space and $U(1)$ for rotations in the gauge space associated with particle number. The group of spatial translations is also essential but corresponds to a symmetry that is strongly broken in all nuclei and that does not need to be exactly restored in practice. Consequently, Tab. {2.2} gather useful elements that characterize $U(1)$ and $SO(3)$ such that the formulae given below for a generic compact Lie group can be easily adapted to either of them.

$\mathcal{G}$	g	$dm(g)$	$v_{\mathcal{G}}$	$\{C\}$	Λ	C_0	$R(g)$	$S^{\lambda}_{ab}(g)$	d_λ
$U(1)$	φ	$d\varphi$	2π	N	N^2	-	$e^{iN\varphi}$	$e^{im\varphi}$	1
$SO(3)$	α,β,γ	$\sin\beta d\alpha d\beta d\gamma$	$16\pi^2$	$\vec{J}$	J^2	J_z	$e^{-i\alpha\hat{J}_z}\, e^{-i\beta\hat{J}_y}\, e^{-i\gamma\hat{J}_z}$	$\mathcal{D}^{J}_{MM'}(\Omega)$	$2J+1$

Table 2.2: Characteristics of $SO(3)$ and $U(1)$ relevant to the present study. The gauge angle of $U(1)$ is $\varphi \in [0, 2\pi]$ whereas Euler angles parameterizing $SO(3)$ are $\Omega \equiv (\alpha, \beta, \gamma) \in [0, 4\pi] \times [0, \pi] \times [0, 2\pi]$. The one-dimensional irreducible representations of $U(1)$ are labeled by $m \in \mathbb{Z}$ whereas the $(2J+1)$-dimensional ones of $SO(3)$ are labeled by $2J \in \mathbb{N}$ and are given by the so-called Wigner functions $D^{J}_{MM'}(\Omega)$ [86], where $(2M, 2M') \in \mathbb{Z}^2$ with $-2J \leq 2M, 2M' \leq +2J$. For $U(1)$, one has $l(N) = N^2$, whereas for $SO(3)$, with the choice $C_0 \equiv J_z$, one has $l(J) = \hbar^2 J(J+1)$ and $g(M) = M\,\hbar$.

2.3 Pseudo-potential-based EDF method

The present section describes what we denote as a pseudo-potential-based EDF method where energy kernels are *explicitly and strictly* computed as matrix elements of an effective Hamilton operator that does *not* depend on the wave-function it is used with, e.g. H does not depend on the density of the system, see CHAP. 1.

2.3.1 SR-EDF step (symmetry breaking)

The symmetry-breaking product state $|\Phi(g)\rangle$ used at the SR level can be decomposed on states with good quantum numbers according to

$$|\Phi(g)\rangle \quad = \quad \sum_{\lambda a} c_{\lambda a} |\Phi^{\lambda a}\rangle \ , \tag{2.7}$$

where $\sum_{\lambda a} |c_{\lambda a}|^2 = 1$ as we choose $|\Phi(g)\rangle$ to be normalized. Using either EQ. 2.5 or EQS. (2.6,2.7), one can easily prove that the average energy

$$E_H^{SR} \equiv \mathrm{Min}_{|\Phi(g)\rangle} \frac{\langle\Phi(g)|H|\Phi(g)\rangle}{\langle\Phi(g)|\Phi(g)\rangle} \ , \tag{2.8}$$

is a scalar under all transformations of $\mathcal{G}$, i.e. E_H^{SR} is independent of g such that we can take $g \equiv 0$ for the reference state and omit the label altogether. However, such an energy cannot be labeled by good quantum numbers (λ, a), which is the fingerprint of the symmetry-breaking character of the many-body state $|\Phi\rangle$. In the present situation, one can use the standard Wick theorem [87] to express the diagonal EDF kernel at play in EQ. 2.8 as a specific functional $E_H[\rho_{ij}, \kappa_{ij}, \kappa_{ij}^*]$ of the diagonal one-body density matrices (EQ. 1.4 with $g' = g = 0$) computed from the symmetry breaking state $|\Phi\rangle$, see SEC. 1.3.1.

2.3.2 MR-EDF step (symmetry restoration)

To formulate the symmetry restoration, one needs to consider the off diagonal energy *kernel* $E_H[g', g]$. In the pseudo-potential-based EDF method, such a kernel reads

$$E_H[g', g] \quad \equiv \quad \frac{\langle\Phi|R^{-1}(g')HR(g)|\Phi\rangle}{\langle\Phi|R^{-1}(g')R(g)|\Phi\rangle} \ , \tag{2.9}$$

where the norm overlap kernel is $N[g', g] \equiv \langle\Phi|R^{-1}(g')R(g)|\Phi\rangle$. The energy kernel at play (EQ. 2.9) can be computed in this case using the *generalized* Wick theorem [56] such that $E_H[g', g] = E_H[\rho^{g'g}, \kappa^{g'g}, \kappa^{gg'*}]$, i.e. the off-diagonal energy kernel is expressed through the same functional as the diagonal one except that diagonal one-body density matrices are replaced by *transition* one-body density matrices 1.4 involving the two transformed product states $R(g)|\Phi\rangle$ and $\langle\Phi|R(g')$. Expanding $|\Phi\rangle$ according to EQ. 2.7 and using EQ. 2.4, one obtains

$$E_H[g', g]\, N[g', g] \quad = \quad \sum_{\lambda ab} c_{\lambda a}^* \, c_{\lambda b} \, E_H^\lambda \, S_{ab}^\lambda(g - g') \ , \tag{2.10}$$

$$N[g', g] \quad = \quad \sum_{\lambda ab} c_{\lambda a}^* \, c_{\lambda b} \, S_{ab}^\lambda(g - g') \ , \tag{2.11}$$

where $\langle\Phi^{\lambda a}|H|\Phi^{\lambda' a'}\rangle \equiv E_H^\lambda \, \delta_{\lambda\lambda'} \, \delta_{aa'}$ are the symmetry-restored (MR) energies. Expressions 2.9 and 2.11 correspond to the double expansion over the volume of the group

$$F[g', g] \equiv \sum_{\lambda\lambda'} \sum_{aba'b'} F_{aba'b'}^{\lambda\lambda'} \, S_{ab}^\lambda(g') \, S_{a'b'}^\lambda(g) \ , \tag{2.12}$$

applied to any function $F[g',g] = f[g-g']$ that in fact only depends on the difference of the two arguments. In such a case, the double expansion reduces to a single expansion whose coefficients f^{λ}_{ab} are $e^{\lambda}_{H,ab} \equiv c^{*}_{\lambda a}\, c_{\lambda b}\, E^{\lambda}_{H}$ and $n^{\lambda}_{ab} \equiv c^{*}_{\lambda a}\, c_{\lambda b}$ for the functions of interest $e_H[g-g']\, n[g-g']$ and $n[g-g']$, respectively. Given that coefficients f^{λ}_{ab} transform specifically under any member of $\mathcal{G}$ [6], the ratio of two such objects, e.g. E^{λ}_{H}, transforms as a scalar as it corresponds to the scalar operator H.
Starting from $E_H[g',g]$ and $N[g',g]$, and given the orthogonality relationship

$$\int_{\mathcal{G}} dm(g)\, S^{\lambda *}_{ab}(g)\, S^{\lambda'}_{a'b'}(g) = \frac{v_{\mathcal{G}}}{d_\lambda}\, \delta_{\lambda\lambda'}\, \delta_{aa'}\, \delta_{bb'} \quad , \tag{2.13}$$

one can perform the integration

$$\left(\frac{d_\lambda}{v_{\mathcal{G}}}\right)^2 \int\!\!\int_{\mathcal{G}} dm(g')\, dm(g)\, S^{\lambda}_{ca}(g')\, S^{\lambda *}_{cb}(g)\, E_H[g',g]\, N[g',g] = e^{\lambda}_{H,ab} \quad , \tag{2.14}$$

to extract the energy E^{λ}_{H} associated with states $|\Phi^{\lambda a}\rangle$ spanning the irreducible representation λ [7]. Such a symmetry restoration stage is denoted as a *multi-reference* method in the sense that, while the energy computed through Eq. 2.8 involves a single reference state $|\Phi\rangle$, the extraction of E^{λ}_{H} involves the set of references states $|\Phi(g)\rangle \equiv R(g)|\Phi\rangle$ obtained from $|\Phi\rangle$ through all transformations of $\mathcal{G}$. It is worth noting that Eq. 2.14 is a specific application of the general expression given in Eq. 1.9 for the MR-EDF energy. In the present case the sums take the form of continuous integrals and the weights f^{k}_{g} are fixed by the structure of the symmetry group.

2.3.3 Transfer operator

Within the pseudo-potential-based EDF approach Eq. 2.14 can actually be obtained by first introducing the transfer operator [50]

$$P^{\lambda}_{ab} \equiv \frac{d_\lambda}{v_{\mathcal{G}}} \int_{\mathcal{G}} dm(g)\, S^{\lambda *}_{ab}(g)\, R(g) \quad , \tag{2.15}$$

to explicitly extract the many-body state with good symmetries

$$|\Phi^{\lambda a}\rangle = \frac{1}{c_{\lambda b}}\, P^{\lambda}_{ab}|\Phi\rangle \quad , \tag{2.16}$$

from which Eq. 2.14 can be easily recovered through

$$E^{\lambda}_{H} \equiv \frac{\langle\Phi^{\lambda a}|H|\Phi^{\lambda a}\rangle}{\langle\Phi^{\lambda a}|\Phi^{\lambda a}\rangle} \quad . \tag{2.17}$$

When dealing with a non abelian group, one must actually consider an arbitrary linear combination of states spanning a given irreducible representation such that mixing coefficients are determined through the minimization of the resulting energy. This corresponds to considering that the link between the symmetry-restored states of interest and the symmetry-breaking one is in fact given by

$$|\Phi^{\lambda a}\rangle \equiv \sum_{b} g^{\lambda b}\, P^{\lambda}_{ab}|\Phi\rangle \quad , \tag{2.18}$$

6. The corresponding law is easily obtained from the transformation of $S^{\lambda}_{ab}(g)$.
7. The fact that $E_H[g',g]$ and $N[g',g]$ only depend on the difference $g-g'$ can be exploited to extract $e^{\lambda}_{H,ab}$ through a single integral rather than through a double integral as in Eq. 2.14. The reason why we keep explicitly two integrals here will only become clear in Sec. 2.5.1.

rather than by Eq. 2.16, and to determining the $\{g^{\lambda b}\}$ through the minimization of

$$E_H^\lambda \equiv \frac{\langle \Phi^{\lambda a}|H|\Phi^{\lambda a}\rangle}{\langle \Phi^{\lambda a}|\Phi^{\lambda a}\rangle} = \frac{\sum_{bb'} g^{\lambda b*}\, g^{\lambda b'}\, e^\lambda_{H,bb'}}{\sum_{bb'} g^{\lambda b*}\, g^{\lambda b'}\, n^\lambda_{bb'}} \quad , \tag{2.19}$$

with $e^\lambda_{H,bb'}$ defined by Eq. 2.14 and $n^\lambda_{bb'}$ given by a similar equation for the kernel $N[g',g]$. Such a minimization leads to solving a Hill-Wheeler-Griffin equation [88, 89].

2.4 General EDF method

We are now interested in the general EDF formalism within which energy kernels are formulated as functionals of one-body (transition) densities as defined by Eq. 1.4.

2.4.1 SR-EDF step

The general SR-EDF method [45] relies on computing the analog to the symmetry-breaking average energy E^{SR} (Eq. 2.8) as the minimum of an a priori *general* diagonal functional $E[\rho^{gg}_{ij}, \kappa^{gg}_{ij}, \kappa^{gg\,*}_{ij}]$. As opposed to what was considered in Sec. 2.3, the diagonal kernel is *not* computed as the average value of a genuine operator H. For actual parameterizations of the nuclear EDF, we refer the reader to Ref. [45] and to Chaps. 5,6.

2.4.2 MR-EDF step

By analogy to the pseudo-potential-based method, the off-diagonal energy kernel $E[g',g]$ (Eq. 2.10) is naturally introduced over the volume of $\mathcal{G}$ through $E[g',g] \equiv E[\rho^{g'g}, \kappa^{g'g}, \kappa^{gg'\,*}]$, where $E[\rho^{gg}, \kappa^{gg}, \kappa^{gg\,*}]$ is the diagonal kernel. It is not be made clear that there is no Wick theorem to justify in the general case such a choice as the kernel is not defined as the matrix element of an operator. Such an off-diagonal kernel possesses an expansion similar to Eq. 2.10. Consequently, one can extract

$$e^\lambda_{ab} \equiv \left(\frac{d_\lambda}{v_\mathcal{G}}\right)^2 \int_\mathcal{G}\int_\mathcal{G} dm(g')\, dm(g)\, S^\lambda_{ca}(g')\, S^{\lambda\,*}_{cb}(g)\, E[g',g]\, N[g',g] \quad , \tag{2.20}$$

by analogy to Eq. 2.14. Whereas in the pseudo-potential-based method one could explicitly demonstrate the identity $e^\lambda_{H,ab} = c^*_{\lambda a}\, c_{\lambda b}\, E^\lambda_H$, this is not the case in the general EDF approach as there no possibility to perform the equivalent to the derivation that started from Eq. 2.9. Eq. 2.20 simply corresponds to the application of expansion 2.12 to the *function* $E[g',g]$ over the irreducible representations of the group, without any reference to a many-body state with good quantum numbers. As a matter of fact, and contrarily to what is often stated [45], e^λ_{ab} is *not* computed from a projected state in the general MR-EDF method, i.e. the transfer operator P^λ_{ab} *cannot* be factorized explicitly in Eq. 2.20. However, one can *implicitly* relate the MR-EDF energy E^λ to the projected state $|\Phi^{\lambda a}\rangle$ obtained from $|\Phi\rangle$ as in Eq. 2.18. With this in mind, it is natural and customary [45, 47] to *define* the symmetry-restored energy E^λ from e^λ_{ab} through the analog of Eq. 2.19, i.e.

$$E^\lambda \equiv \frac{\sum_{bb'} g^{\lambda b*}\, g^{\lambda b'}\, e^\lambda_{bb'}}{\sum_{bb'} g^{\lambda b*}\, g^{\lambda b'}\, n^\lambda_{bb'}} \quad , \tag{2.21}$$

where the $\{g^{\lambda b}\}$ are determined through the minimization of E^λ.

2.4.3 Puzzling questions

We have clarified in previous sections that general SR- and MR-EDF methods have been empirically constructed by analogy to pseudo-potential-based SR- and MR-EDF methods. The key difference with the latter is that the energy kernels at play in the general EDF method are *not* defined as matrix elements of a genuine operator between product state. For the rest, expressions utilized in both approaches, in particular regarding the extraction of the symmetry-restored energy (Eqs. (2.14,2.19) versus Eqs. (2.20,2.21)), look totally alike. Still, puzzling questions remain to be raised.

As mentioned in Sec. 1.2.3, one must require at the symmetry-breaking level that the SR energy $E[\rho^{gg}, \kappa^{gg}, \kappa^{gg\,*}]$ is a scalar under all transformations of $\mathcal{G}$. Such a requirement has led to formulating a set of constraints on the functional form of $E[\rho^{gg}, \kappa^{gg}, \kappa^{gg\,*}]$ [51–53]. The next question one may ask is the following: are those constraints imposed on the energy kernel $E[\rho^{gg}, \kappa^{gg}, \kappa^{gg\,*}]$ at the SR level sufficient to making the general MR-EDF method described in Sec. 2.4.2 well defined, in particular from a symmetry standpoint? In particular, one may wonder whether the fact that the energy kernel $E[g', g]$, which is the key ingredient to the MR-EDF calculation, is not computed as the matrix element of a (genuine) operator makes the method ill-defined in any way?

As a matter of fact, a set of physical constraints to be imposed on $E[g', g]$ have already been worked out [67]. The facts (i) that the MR energy should be real, (ii) that the kernel $E[g', g]$ only depends on the relative value $g - g'$ of its arguments, (iii) that the SR-EDF should be recovered from the Kamlah expansion and (vi) that the Random Phase Approximation based on the SR-EDF $E[\rho^{gg}, \kappa^{gg}, \kappa^{gg\,*}]$ should be recovered as a limit of the MR-EDF calculation [90], has helped limiting the energy kernel $E[g', g]$ to depend on transition densities only, e.g. $E[g', g] \equiv E[\rho^{g'g}, \kappa^{g'g}, \kappa^{gg'\,*}]$.

The aim of the present contribution is to elaborate further on the question raised above and to discuss a path that could be followed to constrain more tightly the form of the kernel $E[g', g]$ and thus MR-EDF calculations. References [47–49, 70] have already provided important elements in the case of $U(1)$, i.e. for particle-number restoration (PNR). Let us recall the main outcome of those studies prior to formulating the problem to be addressed.

2.4.4 Lessons learnt from particle-number restoration

Eq. 2.10 applied to $U(1)$ provides the Fourier decomposition

$$e[\varphi]\, n[\varphi] = \sum_{N \in \mathbb{Z}} c_N^2\, E^N\, e^{iN\varphi} \tag{2.22}$$

of the periodic function $e[\varphi]\, n[\varphi]$ over $[0, 2\pi]$. From a mathematical standpoint, the sum in Eq. 2.22 runs a priori over all irreducible representations of the group, i.e. over both positive and negative integers N. From a physics point of view though, the label N denotes the particle number of the physical system. Consequently, the sum should actually only run over positive integers, i.e. one should find $c_N^2 E^N = 0$ and $E^N = 0$ for $N \leq 0$. In the pseudo-potential-based EDF method, such a result is indeed obtained from the fact that E_H^N is computed as the average value of H in $|\Phi^N\rangle$, the latter being zero [48] for $N \leq 0$. In the EDF context, however, it was demonstrated [48, 49] that Fourier components $c_N^2 E^N$ may be different from zero for $N \leq 0$, i.e. one usually obtains a non-zero symmetry-restored energy for negative particle numbers! This problem was shown [48] to be related to unphysical mathematical properties of $e[\varphi]$. Applying the regularization method proposed in Ref. [47], the cancelation of non-physical Fourier components was recovered [48]. At the same time, components E^N for $N > 0$ were modified by up to 1 MeV, which is of the same order as the root-mean-square error on mass residuals reached by the best available particle-number-restored EDF mass fits [91]. This

demonstrates the practical need of constraining further MR-EDF calculations in order to produce fully reliable results.

2.5 Towards new constraints?

The example discussed above is particularly enlightening given that clear-cut physical arguments can be used to argue that certain coefficients in the Fourier expansion of $e[\varphi]\,n[\varphi]$ should be strictly zero, although they are not if one does not pay particular attention to it. Recovering such physical features removes at the same time non-physical contaminations from other coefficients of the expansion [48]. This proves that the MR-EDF method, as performed so far, faces the danger to be ill-defined and that new constraints on the energy kernel $E[g',g]$ must be worked out in order to make the method physically sound. The regularization method proposed in Ref. [47] that restores the validity of PNR can only be applied if the EDF kernel $E[\rho^{g'g},\kappa^{g'g},\kappa^{gg'*}]$ is a polynomial of a transition density matrices [49], which is an example of such a constraint.

For an arbitrary symmetry group, the situation might not be as transparent as for $U(1)$. Indeed, it is unlikely in general that certain coefficients of the expansion of $E[g',g]N[g',g]$ over irreducible representations of the group must be zero based on physical arguments. The challenge we face can be formulated in the following way: although expansion 2.12 that underlines the general MR-EDF method is sound from a group-theory point of view minimum, mathematical properties deduced from a pseudo-potential-based EDF method must be worked out and imposed on the analytical form of the kernel $E[g',g]$ to make e^{λ}_{ab} extracted from Eq. 2.20 physically sound. The rest of the present contribution is dedicated to briefly introducing an example of such a property in the case of $SO(3)$, i.e. for angular momentum restoration, that could be used to constrain the form of $E[\Omega',\Omega]$. Details of such an analysis are reported in Appendix E.

2.5.1 Mathematical property associated with angular-momentum conservation

We omit spin and isospin for simplicity and consider the rotationally-invariant nuclear Hamiltonian $H=T+V$ in which the central two-nucleon interaction

$$V \equiv \frac{1}{2}\int\!\!\int d\vec{r}_1 d\vec{r}_2\, v(|\vec{r}_1-\vec{r}_2|)\, a^\dagger_{\vec{r}_1}\, a^\dagger_{\vec{r}_2}\, a_{\vec{r}_2}\, a_{\vec{r}_1} \quad , \tag{2.23}$$

is local, i.e. non-antisymmetrized matrix elements are defined as

$$\langle 1:\vec{r}_1;2:\vec{r}_2|V|1:\vec{r}_3;2:\vec{r}_4\rangle \equiv v(|\vec{r}_1-\vec{r}_2|)\,\delta(\vec{r}_1-\vec{r}_3)\,\delta(\vec{r}_2-\vec{r}_4) \quad , \tag{2.24}$$

and in which three-nucleon and higher many-body forces are disregarded for simplicity. None of the conclusions drawn below would be modified by the inclusion of many-body forces or by using a non-local two-nucleon interaction. Operator $a^\dagger_{\vec{r}}$ ($a_{\vec{r}}$) creates (annihilates) a nucleon at position $\vec{r}$. Considering an eigenstate $|\Theta^{LM}\rangle$ of $\vec{L}^2$ and L_z, as well as using center of mass $\vec{R}\equiv(\vec{r}_1+\vec{r}_2)/2$ and relative coordinates $\vec{r}\equiv\vec{r}_1-\vec{r}_2$, the potential energy reads as

$$V^L \equiv \frac{\langle\Theta^{LM}|V|\Theta^{LM}\rangle}{\langle\Theta^{LM}|\Theta^{LM}\rangle} = \frac{1}{2}\int d\vec{R}\int d\vec{r}\; v(r)\,\rho^{[2]\,LMLM}_{\vec{R}\vec{r}} \tag{2.25}$$

$$\equiv \int d\vec{R}\; V^{LM}(\vec{R}) \quad , \tag{2.26}$$

which defines a local potential energy *density* $V^{LM}(\vec{R})$ in terms of the non-local two-body density matrix $\rho^{[2]\,LMLM}_{\vec{R}\vec{r}} \equiv \langle\Theta^{LM}|\,a^\dagger_{\vec{r}_2}\,a^\dagger_{\vec{r}_1}\,a_{\vec{r}_1}\,a_{\vec{r}_2}\,|\Theta^{LM}\rangle/\langle\Theta^{LM}|\Theta^{LM}\rangle$. After tedious but straightforward

calculations (Appendix E), one can demonstrate that

$$V^{LM}(\vec{R}) = \sum_{L'=0}^{2L} C^{LM}_{LML'0}\, v^{[2]}_{LL'}(R)\, Y^0_{L'}(\hat{R}) \ , \tag{2.27}$$

where the Clebsch-Gordan coefficient $C^{LM}_{LML'0}$ carries the dependence on M while Y^m_l denotes spherical harmonics. The weight $v^{[2]}_{LL'}(R)$ depends on the norm of $\vec{R}$ only and is related to a reduced matrix element of the two-body density matrix operator recoupled to a total angular momentum L'. The remarkable mathematical property identified through Eq. 2.27 states that the scalar potential energy V^L is obtained from an intermediate energy density $V^{LM}(\vec{R})$ whose dependence on the orientation of $\vec{R}$ is tightly constrained by the angular-momentum quantum number of the underlying many-body state $|\Theta^{LM}\rangle$, i.e. its expansion over spherical harmonics is limited to $L' \leq 2L$. Such a result is unchanged when adding the kinetic energy (density) to the potential energy (density) such that we restrict ourselves to the latter for simplicity. Of course, the energy eventually extracts the coefficient of the lowest harmonic, i.e. $V^L = \sqrt{4\pi}\int dR\, v^{[2]}_{L0}(R)$.

2.5.2 Pseudo-potential-based EDF method

Since property 2.27 is general, it can also be obtained within the frame of the pseudo-potential-based MR-EDF method presented in Sec. 2.3. Omitting again the kinetic energy for simplicity and using Eqs. (2.4,2.7,2.10,2.23), the pseudo-potential energy kernel reads

$$\begin{aligned} V_H[\Omega',\Omega]\, N[\Omega',\Omega] &= \frac{1}{2}\int d\vec{R}\, d\vec{r}\, V(r)\, \langle\Theta|R^\dagger(\Omega')\, \hat{\rho}^{[2]}_{\vec{R}\vec{r}}\, R(\Omega)|\Theta\rangle \\ &= \frac{1}{2}\sum_{\{L,M\}} c^*_{L_1N_1} c_{L_2N_2} D^{L_1\dagger}_{N_1M_1}(\Omega') D^{L_2}_{M_2N_2}(\Omega) \int d\vec{R}\, d\vec{r}\, V(r) \rho^{[2]\, L_1M_1L_2M_2}_{\vec{R}\vec{r}} \ , \end{aligned} \tag{2.28}$$

where $\{L,M\}$ denotes a sum over the six angular-momentum quantum numbers appearing in the formula. Applying Eq. 2.14 to the above expression (Eq. 2.28) provides, thanks to the orthogonality property 2.13, the result

$$\begin{aligned} V^L_H &= \frac{(2L+1)^2}{(8\pi^2)^2}\int d\Omega' d\Omega\, \frac{D^L_{KM}(\Omega')}{c_{LK}}\, \frac{D^{L*}_{KM}(\Omega)}{c^*_{LK}}\, V_H[\Omega',\Omega]\, N[\Omega',\Omega] \\ &= \frac{1}{2}\int d\vec{R}\, d\vec{r}\, V(r)\, \rho^{[2]\, LMLM}_{\vec{R}\vec{r}} \ , \end{aligned} \tag{2.29}$$

so that Eqs. (2.26,2.27) are recovered. To obtain such a result it is mandatory to use the double-integral formulation of Eq. 2.14 rather than the more standard single-integral formulation that takes advantage, from the outset, of the fact that $V_H[\Omega',\Omega]$ and $N[\Omega',\Omega]$ only depend on the difference $\Omega - \Omega'$. We thus insist on using the double-integral formulation in the present discussion.

2.5.3 General EDF method

Let us now come back to the general EDF method formulation given in Sec. 2.4. The point is to underline the fact that property 2.27 cannot be derived a priori given that the potential energy part of the kernel $E[\Omega',\Omega]$ is *not* explicitly related to the two-body density matrix in this case. Taking a quasi-local Skyrme EDF as an example, although this can be easily adapted to non-local EDF of the Gogny type, the energy kernel takes the form

$$\begin{aligned} E[\Omega',\Omega] &= E[\rho^{\Omega'\Omega}, \kappa^{\Omega'\Omega}, \kappa^{\Omega\Omega'*}] \\ &\equiv \int d\vec{R}\ \mathcal{E}(\rho^{\Omega'\Omega}(\vec{R}), \tau^{\Omega'\Omega}(\vec{R}), \vec{j}^{\Omega'\Omega}(\vec{R}), \ldots) \ , \end{aligned} \tag{2.30}$$

where the set of *one-body* local transition densities are given in Eq. 1.6 with $g' = \Omega'$ and $g = \Omega$, such that constraints imposed at the SR level [51–53] are fulfilled (see Sec. 2.4.3). Given such an EDF, there is no reason a priori that the energy density $\mathcal{E}^{LM}(\vec{R})$ extracted from Eqs. (2.20,2.21) displays property 2.27; i.e. the angular dependence of $\mathcal{E}^{LM}(\vec{R})$ is likely to display harmonics $Y^0_{L'}(\hat{R})$ with $L' > 2L$. One might argue that it is not an issue considering that the symmetry-restored energy E^L eventually relates to the harmonic $Y^0_0(\hat{R})$ only. However, a formalism that provides $\mathcal{E}^{LM}(\vec{R})$ with a spurious angular content will certainly also provide the coefficient $\mathcal{E}^{L0}(R)$ of the lowest harmonic with unphysical contributions. To state it differently, it is likely that constraining the MR-EDF kernels $E[\rho^{\Omega'\Omega}, \kappa^{\Omega'\Omega}, \kappa^{\Omega\Omega'*}]$ to produce an energy density $\mathcal{E}^{LM}(\vec{R})$ that fulfils the mathematical property 2.27 will impact at the same time the value of the weight $\mathcal{E}^{L0}(R)$, and thus the value of E^L. To some extent, this is similar to the situation encountered with $U(1)$ where restoring the physical property that Fourier coefficients $c_N^2 E^N$ with $N \leq 0$ should be strictly zero did impact the value of all non-zero Fourier coefficients [48].

2.6 Conclusions

We elaborate on key differences between pseudo-potential-based and more general implementations of the EDF method, and point to difficulties encountered when formulating symmetry restoration within the general EDF approach. Furthermore, we identify in a pseudo-potential-based framework a mathematical property of the energy density $\mathcal{E}^{LM}(\vec{R})$ associated with angular momentum restoration that could be used to constrain EDF kernels.
An alternative consists of sticking to a well-defined pseudo-potential-based EDF method to construct EDF parameterizations. However, there does not exist at this point in time such a parameterization of the EDF kernel that provides good enough phenomenology. The second part of the present thesis is dedicated to building such a parameterization.

Chapter 3

A new Skyrme pseudo-potential

Abstract: The present chapter is devoted to the construction of a new EDF parameterization that is safe by construction for MR-EDF calculations. The EDF kernel derives from a generalized Skyrme *pseudo-potential*. The generalization consists in adding a three-body part, to the usual density-*independent* two-body one, of the most general form up to second order in gradients.

Contents

3.1 Introduction

3.1.1 Context

Most of the existing parameterizations of the energy density functional kernel have been constructed in the general EDF formulation context, for instance using a density-dependent effective Hamiltonian. As a result and as discussed in Chap. 2, existing parameterizations of the EDF kernel are unsafe for MR-EDF calculations. This is problematic as MR-EDF calculations are necessary to access extensive spectroscopic informations while restoring symmetries that are broken at the SR level. Parameterizations of the EDF adapted to such calculations are thus needed.

As discussed in Chap. 2, the first way is to develop corrections to the EDF kernel. The regularization method developed in Ref. [47–49] gives the first step in that direction. Nevertheless, EDFs from which regularized MR-EDF calculations are done can still induce spurious contributions at this symmetry restoration level. Indeed, as the symmetry breaking energy is not computed from the average value of a genuine operator, one cannot ensure that all necessary properties of the energy density associated with the symmetry restored energies are indeed fulfilled, as explained in Chap. 2. New corrections could be elaborated to limit further spurious contributions. As of today, corrections are insufficient to consider self-interaction and ill defined symmetry restoration issues as being fully under control.
The second way to perform safe MR-EDF calculations is to compute the EDF kernel as the matrix element of strict pseudo-potential. In such a case the symmetry restored energies are well-defined such that calculations are spurious contributions free. Indeed, the Pauli principle is fully accounted for whenever the energy kernel is computed as an operator matrix element rather than postulated under the form of a functional of one-body density matrices.

Unfortunately, such a procedure also has disadvantages. First, the analytical derivation of the functional can be tedious and time consuming. The second disadvantage is that it is not *a priori* sure that strict pseudo-potentials of manageable form are flexible enough to provide high-quality EDF parameterizations. Few parameterizations have already been constructed within the pseudo-potential-based EDF formulation in the past, and they did not provide good enough phenomenology, as is the case of SIII parameterization [92]. As a matter of fact, the density dependence of existing standard Skyrme or Gogny effective interactions was introduced at the time to bypass such an apparent lack of flexibility. Thereby, the generalized pseudo-potential

has to be rich enough but also simple enough so that the fit of its free parameters remains bearable.

For this study, the pseudo-potential we aim at developping belongs to the Skyrme family. In the general context, Skyrme EDF parameterizations are postulated and constructed directly by taking all possible bilinear combinations of quasi-local densities, usually up to second order in gradients, which respect a certain set of symmetry requirements [51–53]. Recent developments have focused on increasing the power in densities [93, 94], i.e. considering bilinear, trilinear, ... terms, while keeping up to two gradients or by increasing the number of gradients while keeping bilinear terms only [95]. Similar developments are possible using pseudo-potentials. This has been done recently by Raimondi et al. [96] regarding the second option. However, developments regarding the first option still have to be done. In such a context bilinear functionals are obtained from a two-body pseudo potential, trilinear ones using three-body pseudo potential, etc. The number of gradients operators in each terms of the functional reflects the number of gradients considered in the pseudo potential.
The two-body pseudo-potential without any density dependence, or with a gradient-less three-body pseudo potential are known to be unsufficient to reproduce correctly the nuclear data. As a consequence the pseudo-potential developed presently is a three-body Skyrme operator, up to second order in gradients, added to the usual two-body one, giving rise to bilinear plus trilinear terms in the density matrices. This chapter deals with the construction of the most general three-body Skyrme pseudo-potential and the derivation of the corresponding energy functional kernel.

3.1.2 Energy density functional

The pseudo Hamiltonian used in the present work takes the form

$$\hat{H}_{\text{pseudo}} = \sum_{ij} \hat{t}_{ij} a_i^\dagger a_j + \frac{1}{2!} \sum_{ijkl} \hat{v}^{2Sk}_{ijkl} a_i^\dagger a_j^\dagger a_l a_k + \frac{1}{3!} \sum_{ijklmn} \hat{v}^{3Sk}_{ijklmn} a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l \ , \tag{3.1}$$

where $\hat{v}^{2Sk}_{ijkl}$ and $\hat{v}^{3Sk}_{ijklmn}$ denote non-antisymmetrized matrix elements of two- and three-body Skyrme effective pseudo-potentials. In Eq. 3.1. $\{a_j^\dagger, a_j\}$ denote creation and annihilation operators in an arbitrary single-particle basis. The SR energy functional kernel is obtained from the average value of the pseudo Hamiltonian

$$E \equiv \frac{\langle \Phi | \hat{H}_{\text{pseudo}} | \Phi \rangle}{\langle \Phi | \Phi \rangle} \ , \tag{3.2}$$

where the reference state $|\Phi\rangle$ is taken under the form of a Hartree-Fock-Bogoliubov product state, Chap. 1. Consequently, the SR-EDF kernel is obtained from an effective HFB problem written in terms of a pseudo Hamilton operator. The energy can be calculated using Wick theorem [87], see Appendix A.1, such that

$$E = E^{\rho}_{kin} + E^{\rho\rho}_{Sk} + E^{\kappa\kappa}_{Sk} + E^{\rho\rho\rho}_{Sk} + E^{\kappa\kappa\rho}_{Sk} \tag{3.3a}$$

$$E^{\rho}_{kin} = \sum_{ij} \langle i|\hat{t}|j\rangle \rho_{ji} \tag{3.3b}$$

$$E^{\rho\rho}_{Sk} = \frac{1}{2} \sum_{ijkl} \langle i\, j|\hat{v}^{2Sk} \mathcal{A}_{12}|k\, l\rangle \ \rho_{ki}\, \rho_{lj} \tag{3.3c}$$

$$E^{\kappa\kappa}_{Sk} = \frac{1}{4} \sum_{ijkl} \langle i\, j|\hat{v}^{2Sk} \mathcal{A}_{12}|k\, l\rangle \ \kappa^*_{ij}\, \kappa_{kl} \tag{3.3d}$$

$$E_{Sk}^{\rho\rho\rho} = \frac{1}{6}\sum_{ijklmn}\langle i\,j\,k|\hat{v}^{3Sk}\mathcal{A}_{123}|l\,m\,n\rangle\,\rho_{li}\,\rho_{mj}\,\rho_{nk} \tag{3.3e}$$

$$E_{Sk}^{\kappa\kappa\rho} = \frac{1}{4}\sum_{ijklmn}\langle i\,j\,k|\hat{v}^{3Sk}\mathcal{A}_{123}|l\,m\,n\rangle\,\kappa_{ij}^{*}\,\kappa_{lm}\,\rho_{nk}\ , \tag{3.3f}$$

where $\mathcal{A}_{12}$ and $\mathcal{A}_{123}$ are two- and three-body antisymmetrizers introduced hereafter in Sec. 3.1.5. The Coulomb energy is here omitted for simplicity. The (diagonal or SR) one-body density matrix and pairing tensor entering Eq. 3.3 are defined as

$$\rho_{ij} \equiv \frac{\langle\Phi|a_j^{\dagger}a_i|\Phi\rangle}{\langle\Phi|\Phi\rangle}\ , \tag{3.4a}$$

$$\kappa_{ij} \equiv \frac{\langle\Phi|a_j a_i|\Phi\rangle}{\langle\Phi|\Phi\rangle}\ . \tag{3.4b}$$

The normal density matrix is hermitian $\rho_{ij} = \rho_{ji}^{*}$ while the anomalous density matrix is skew symmetric $\kappa_{ij} = -\kappa_{ji}$. The SR energy kernel is computed from a local energy density $\mathcal{E}[\rho,\kappa^{*},\kappa](\vec{r})$ according to

$$E^{\mathrm{SR}} \equiv \int d\vec{r}\,\mathcal{E}[\rho,\kappa^{*},\kappa](\vec{r}) = \int d\vec{r}\left(\mathcal{E}_{kin}^{\rho}(\vec{r}) + \mathcal{E}_{Sk}^{\rho\rho}(\vec{r}) + \mathcal{E}_{Sk}^{\rho\rho\rho}(\vec{r}) + \mathcal{E}_{Sk}^{\kappa\kappa}(\vec{r}) + \mathcal{E}_{Sk}^{\kappa\kappa\rho}(\vec{r})\right)\ , \tag{3.5}$$

where it as been separated into terms that are linear in ρ_{ij}, bilinear in ρ_{ij} and in κ_{ij}, trilinear in ρ_{ij} and bilinear in κ_{ij} times ρ_{ij}. The remaining of the present document focuses on Eqs. (3.3b,3.3c,3.3e) only. Eventually, the approach proposed in the document is meant to be extended to Eqs. (3.3d,3.3f). It is simply because of a lack of time that there were excluded from the present investigation. The computation of the energy functional consists in expanding matrix elements $\hat{t}_{ij}$, $\hat{v}^{3Sk}_{ijklmn}$ and $\hat{v}^{3Sk}_{ijklmn}$ and applying gradient operators on density matrices expressed in coordinate⊗spin⊗isospin representation. For this purpose density matrices and their corresponding quasi-local counter parts are now introduced.

3.1.3 Density matrices and quasi-local densities

3.1.3.1 Coordinate representation

First, the coordinate⊗spin⊗isospin representation is defined through

$$\hat{\vec{r}}\,|\vec{r}\sigma q\rangle = \vec{r}\,|\vec{r}\sigma q\rangle\ , \tag{3.6a}$$

$$\hat{\vec{s}}^{2}\,|\vec{r}\sigma q\rangle = \frac{\hbar^2}{2}\left(\frac{1}{2}+1\right)|\vec{r}\sigma q\rangle\quad,\quad \hat{s}_z|\vec{r}\sigma q\rangle = \hbar\sigma\,|\vec{r}\sigma q\rangle\ , \tag{3.6b}$$

$$\hat{\vec{\tau}}^{2}\,|\vec{r}\sigma q\rangle = \frac{\hbar^2}{2}\left(\frac{1}{2}+1\right)|\vec{r}\sigma q\rangle\quad,\quad \hat{\tau}_z|\vec{r}\sigma q\rangle = \hbar q\,|\vec{r}\sigma q\rangle\ , \tag{3.6c}$$

and constitute a continuous orthonormal direct-product basis of $\mathcal{H}_1 = \mathcal{H}_{1,\vec{r}}\otimes\mathcal{H}_{1,\sigma}\otimes\mathcal{H}_{1,\tau}$, with $\vec{r}\in\mathbb{R}^3$ and $\sigma,q\in\{+1/2,-1/2\}$ [1]. For spin and isospin parts, a shorthand notation is used as in fact $|\sigma\rangle\equiv|1/2\sigma\rangle$ and $|q\rangle\equiv|1/2q\rangle$. Orthogonality and completeness relations are written as

$$\langle\vec{r}\sigma q|\vec{r}\,'\sigma' q'\rangle = \delta(\vec{r}-\vec{r}\,')\,\delta_{\sigma\sigma'}\,\delta_{qq'}\quad,\quad \int d\vec{r}\sum_{\sigma}\sum_{\tau}|\vec{r}\sigma\tau\rangle\langle\vec{r}\sigma\tau| = \mathbb{1}_1\ , \tag{3.7}$$

where $\mathbb{1}_1$ is the unity operator on $\mathcal{H}_1$.
Introducing, a complete orthogonal set of single-particle wave functions

$$\langle\,\vec{r}\sigma q\,|\,i\rangle \equiv \varphi_i(\vec{r}\sigma q)\ , \tag{3.8}$$

1. The quantum number q is sometimes referred to as a letter, i.e. n for neutrons and p for protons, or as a number, i.e. $+1/2$ for neutrons and $-1/2$ for protons.

creation and annihilation operators $a^\dagger(\vec{r}\sigma q)$ and $a(\vec{r}\sigma q)$ can be defined according to

$$a(\vec{r}\sigma q) \equiv \sum_i \varphi_i(\vec{r}\sigma q)\; a_i \quad ; \quad a^\dagger(\vec{r}\sigma q) \equiv \sum_i \varphi_i^*(\vec{r}\sigma q)\; a_i^\dagger \;\; . \tag{3.9}$$

One-nucleon states can eventually be written under the form of spinors

$$\langle\, \vec{r}q \,|\, i\rangle \equiv \varphi_i(\vec{r}q) \equiv \begin{pmatrix} \varphi_i(\vec{r}\,\sigma\!=\!+1/2\,q) \\ \varphi_i(\vec{r}\,\sigma\!=\!-1/2\,q) \end{pmatrix} \;\; . \tag{3.10}$$

3.1.3.2 Density matrix

The EDF will be expressed in terms of local one-body densities and their gradients. Such densities are obtained from the normal one-body density matrix expressed in coordinate⊗spin⊗isospin basis [2] through

$$\begin{aligned} \rho_q(\vec{r}\sigma, \vec{r}\,'\sigma') &\equiv \frac{\langle\Phi|a^\dagger(\vec{r}\,'\sigma' q)a(\vec{r}\sigma q)|\Phi\rangle}{\langle\Phi|\Phi\rangle} \\ &= \sum_{ij} \varphi_i(\vec{r}\sigma q)\, \varphi_j^*(\vec{r}\,'\sigma' q)\, \rho_{ij}^q \;\; , \end{aligned} \tag{3.11}$$

and from spin Pauli matrices

$$\sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \;\; . \tag{3.12}$$

Starting from Eq. 3.11, a set of the non-local densities is first introduced by applying up to two gradients and/or by folding the density matrix with a spin Pauli matrix

$$\rho_q(\vec{r}, \vec{r}\,') \equiv \sum_{ij} \varphi_j^\dagger(\vec{r}\,'q)\, \varphi_i(\vec{r}q)\, \rho_{ij}^q \;\; , \tag{3.13a}$$

$$s_{q,\nu}(\vec{r}, \vec{r}\,') \equiv \sum_{ij} \varphi_j^\dagger(\vec{r}\,'q)\, \sigma_\nu\, \varphi_i(\vec{r}q)\, \rho_{ij}^q \;\; , \tag{3.13b}$$

$$\tau_q(\vec{r}, \vec{r}\,') \equiv \sum_{\mu} \nabla_{\vec{r},\mu}\, \nabla_{\vec{r}\,',\mu}\, \rho_q(\vec{r}, \vec{r}\,') \;\; , \tag{3.13c}$$

$$T_{q,\nu}(\vec{r}, \vec{r}\,') \equiv \sum_{\mu} \nabla_{\vec{r},\mu}\, \nabla_{\vec{r}\,',\mu}\, s_{q,\nu}(\vec{r}, \vec{r}\,') \;\; , \tag{3.13d}$$

$$j_{q,\mu}(\vec{r}, \vec{r}\,') \equiv -\frac{i}{2}\left(\nabla_{\vec{r},\mu} - \nabla_{\vec{r}\,',\mu}\right)\, \rho_q(\vec{r}, \vec{r}\,') \;\; , \tag{3.13e}$$

$$J_{q,\mu\nu}(\vec{r}, \vec{r}\,') \equiv -\frac{i}{2}\left(\nabla_{\vec{r},\mu} - \nabla_{\vec{r}\,',\mu}\right)\, s_{q,\nu}(\vec{r}, \vec{r}\,') \;\; , \tag{3.13f}$$

where $\vec{\nabla}_{\vec{r}}$ is the gradient associated with coordinate $\vec{r}$. Equation 3.13 provides non-local matter, kinetic, spin kinetic, current and spin-current densities for a given isospin projection, respectively.

3.1.3.3 Quasi-local densities

Thanks to the contact character of the Skyrme pseudo-potential to be used later on the normal parts of the energy density functional, $\mathcal{E}_{Sk}^{\rho\rho}$ and $\mathcal{E}_{Sk}^{\rho\rho\rho}$, are going to be functionals of the

2. Without proton/neutron mixing, so that $\rho(\vec{r}\sigma q, \vec{r}\,'\sigma' q') = 0$ for $q \neq q'$.

following local densities

$$\rho_q(\vec{r}) \equiv \rho_q(\vec{r},\vec{r}) = \sum_{ij} \varphi_j^\dagger(\vec{r}q)\,\varphi_i(\vec{r}q)\,\rho_{ij}^q \ , \tag{3.14a}$$

$$s_{q,\mu}(\vec{r}) \equiv s_{q,\mu}(\vec{r},\vec{r}) = \sum_{ij} \varphi_j^\dagger(\vec{r}q)\,\sigma_\mu\,\varphi_i(\vec{r}q)\,\rho_{ij}^q \ , \tag{3.14b}$$

$$\tau_q(\vec{r}) \equiv \tau_q(\vec{r},\vec{r}) = \sum_{ij} \left[\vec{\nabla}\varphi_j^\dagger(\vec{r}q)\right]\cdot\left[\vec{\nabla}\varphi_i(\vec{r}q)\right]\rho_{ij}^q \ , \tag{3.14c}$$

$$T_{q,\mu}(\vec{r}) \equiv T_{q,\mu}(\vec{r},\vec{r}) = \sum_{ij} \vec{\nabla}\varphi_j^\dagger(\vec{r}q)\,\sigma_\mu\cdot\vec{\nabla}\varphi_i(\vec{r}q)\,\rho_{ij}^q \ , \tag{3.14d}$$

$$j_{q,\mu}(\vec{r}) \equiv j_{q,\mu}(\vec{r},\vec{r}) = -\frac{i}{2}\sum_{ij}\left\{\varphi_j^\dagger(\vec{r}q)\left[\nabla_\mu\varphi_i(\vec{r}q)\right] - \left[\nabla_\mu\varphi_j^\dagger(\vec{r}q)\right]\varphi_i(\vec{r}q)\right\}\rho_{ij}^q \ , \tag{3.14e}$$

$$J_{q,\mu\nu}(\vec{r}) \equiv J_{q,\mu\nu}(\vec{r},\vec{r}) = -\frac{i}{2}\sum_{ij}\left\{\varphi_j^\dagger(\vec{r}q)\,\sigma_\nu\left[\nabla_\mu\varphi_i(\vec{r}q)\right] - \left[\nabla_\mu\varphi_j^\dagger(\vec{r}q)\right]\sigma_\nu\,\varphi_i(\vec{r}q)\right\}\rho_{ij}^q \ . \tag{3.14f}$$

We further introduce the spin-orbit current as the pseudo-vector part of the spin-orbit tensor

$$J_{q,\lambda}(\vec{r}) \equiv \sum_{\mu,\nu}\epsilon_{\lambda\mu\nu}\,J_{q,\mu\nu} = -\frac{i}{2}\sum_{ij}\left\{\varphi_j^\dagger(\vec{r}q)\left[\vec{\nabla}\times\vec{\sigma}\varphi_i(\vec{r}q)\right] - \left[\vec{\nabla}\varphi_j^\dagger(\vec{r}q)\right]\times\vec{\sigma}\,\varphi_i(\vec{r}q)\right\}\rho_{ij}^q \ , \tag{3.14g}$$

where greek indexes refer to cartesian components of a vector (μ) or of a tensor (μ,ν).
All throughout this wprk, neutron and proton densities can be recoupled into isoscalar and isovector densities according to

$$\mathcal{P}^0(\vec{r}) \equiv \mathcal{P}^n(\vec{r}) + \mathcal{P}^p(\vec{r}) \ , \tag{3.15a}$$

$$\mathcal{P}^1(\vec{r}) \equiv \mathcal{P}^n(\vec{r}) - \mathcal{P}^p(\vec{r}) \ , \tag{3.15b}$$

where $(\mathcal{P}^t,\mathcal{P}^q) \in \left\{(\rho_t,\rho_q);(\vec{s}_t,\vec{s}_q);(\tau_t,\tau_q);(\vec{T}_t,\vec{T}_q);(\vec{j}_t,\vec{j}_q);(J_{t,\mu\nu},J_{q,\mu\nu})\right\}$ with $t\in\{0,1\}$ and $q\in\{n,p\}$. Similarly local densities entering the anomalous part of the quasi-local functional are obtained from the anomalous density matrix but are omitted here as pairing contributions to the EDF kernel are not discussed in the present document.

3.1.3.4 Rules for applying Quasi-local densities rules

Gradient operators coming from Skyrme pseudo-potentials will have to be applied on non-local density matrices $\rho_q(\vec{r},\vec{r}\,')$ and $s_{q,\mu}(\vec{r},\vec{r}\,')$. Rules have been derived that express the action of specific combinations of gradients on such non-local densities in terms of combinations of quasi-local densities (see Eq. 3.14) in order to facilitate the algebraic derivations [97, 98]. Those rules are proven in Appendix A.2 and work identically for $\rho_q(\vec{r},\vec{r}\,')$ or $s_{q,\nu}(\vec{r},\vec{r}\,')$.
Defining

$$\mathcal{P}^q_{\vec{r}\,\vec{r}\,'} \equiv \left\{\begin{array}{l}\rho_q(\vec{r},\vec{r}\,') \\ \vec{s}_q(\vec{r},\vec{r}\,')\end{array}\right. \ , \tag{3.16}$$

the associated rules are

$$\vec{\nabla}_r \, \mathcal{P}^q_{\vec{r}\,\vec{r}\,'} \Big|_{\vec{r}=\vec{r}\,'=\vec{r}} = \frac{1}{2}\vec{\nabla}\mathcal{P}^q_{\vec{r}} + i\vec{\mathcal{J}}^q_{\vec{r}} \ , \tag{3.17a}$$

$$\vec{\nabla}_{r'} \, \mathcal{P}^q_{\vec{r}\,\vec{r}\,'} \Big|_{\vec{r}=\vec{r}\,'=\vec{r}} = \frac{1}{2}\vec{\nabla}\mathcal{P}^q_{\vec{r}} - i\vec{\mathcal{J}}^q_{\vec{r}} \ , \tag{3.17b}$$

$$\vec{\nabla}_r \cdot \vec{\nabla}_r \, \mathcal{P}^q_{\vec{r}\,\vec{r}\,'} \Big|_{\vec{r}=\vec{r}\,'=\vec{r}} = \frac{1}{2}\Delta\mathcal{P}^q_{\vec{r}} - \mathcal{T}^q_{\vec{r}} + i\vec{\nabla}\cdot\vec{\mathcal{J}}^q_{\vec{r}} \ , \tag{3.17c}$$

$$\vec{\nabla}_{r'} \cdot \vec{\nabla}_{r'} \, \mathcal{P}^q_{\vec{r}\,\vec{r}\,'} \Big|_{\vec{r}=\vec{r}\,'=\vec{r}} = \frac{1}{2}\Delta\mathcal{P}^q_{\vec{r}} - \mathcal{T}^q_{\vec{r}} - i\vec{\nabla}\cdot\vec{\mathcal{J}}^q_{\vec{r}} \ , \tag{3.17d}$$

$$\vec{\nabla}_{r'} \cdot \vec{\nabla}_r \, \mathcal{P}^q_{\vec{r}\,\vec{r}\,'} \Big|_{\vec{r}=\vec{r}\,'=\vec{r}} = \mathcal{T}^q_{\vec{r}} \ , \tag{3.17e}$$

$$\sum_{\lambda\mu\nu} \epsilon_{\lambda\mu\nu}\nabla_{r',\lambda}\cdot\nabla_{r\mu} \, \mathcal{P}^q_{\vec{r}\,\vec{r}\,'} \Big|_{\vec{r}=\vec{r}\,'=\vec{r}} = \sum_{\lambda\mu\nu} \epsilon_{\lambda\mu\nu} i\nabla_\lambda \mathcal{J}^q_{\vec{r},\mu} \ , \tag{3.17f}$$

where

$$\left(\mathcal{P}^q_{\vec{r}} \, , \, \mathcal{T}^q_{\vec{r}} \, , \, \mathcal{J}^q_{\vec{r},\mu}\right) \equiv \begin{cases} \left(\rho_q(\vec{r}) \, , \, \tau_q(\vec{r}) \, , \, j_{q,\mu}(\vec{r})\right) \\ \left(s_{q,\nu}(\vec{r}) \, , \, T_{q,\nu}(\vec{r}) \, , \, J_{q,\mu\nu}(\vec{r})\right) \end{cases} . \tag{3.18}$$

3.1.4 Gauge transformations

Skyrme forces are locally gauge invariant, which reflects the fact that its momentum dependence has been introduced to simulate the finite-range effects of the effective interaction [99]. The gauge transformed one-body density matrix reads as

$$\rho'_q(\vec{r}\,\sigma, \vec{r}\,'\sigma') = \exp\left\{ i\left(\phi(\vec{r}) - \phi(\vec{r}\,')\right)\right\} \rho_q(\vec{r}\sigma, \vec{r}\,'\sigma') \ . \tag{3.19}$$

Galilean transformation is a special kind of local gauge transformation and represents invariance of the system under a translational motion. Galilean transformation is obtained for $\phi(\vec{r}) = \vec{p}\cdot\vec{r}/\hbar$. Quasi-local densities Eq. 3.14 calculated from the gauge transformed density matrix take the form

$$\mathcal{P}^{t/q\,\prime}_{\vec{r}} = \mathcal{P}^{t/q}_{\vec{r}} \ , \tag{3.20a}$$

$$\mathcal{T}^{t/q\,\prime}_{\vec{r}} = \mathcal{T}^{t/q}_{\vec{r}} + 2\mathcal{J}^{t/q}_{\vec{r},\mu}\nabla_\mu\phi(\vec{r}) + \mathcal{P}^{t/q}_{\vec{r}}\nabla_\mu\phi(\vec{r})\nabla_\mu\phi(\vec{r}) \ , \tag{3.20b}$$

$$\mathcal{J}^{t/q\,\prime}_{\vec{r},\mu} = \mathcal{J}^{t/q}_{\vec{r},\mu} + \mathcal{P}^{t/q}_{\vec{r}}\nabla_\mu\phi(\vec{r}) \ , \tag{3.20c}$$

where t/q denotes either isoscalar-isovector or neutron-proton indices.

3.1.5 Antisymmetrizer and exchange operators

Antisymmetrizer operators enforce the Pauli principle, i.e. the fact that two fermions cannot be in the same quantum state. In the expression of the SR energy kernel, Eq. 3.3, antisymmetrizer operators originate from the application of Wick theorem, see Appendix A.1. Antisymmetrizers can be applied to the ket, the bra or both for an identical result. Two-body $\mathcal{A}_{12}$ and three-body $\mathcal{A}_{123}$ antisymmetrisers are defined through

$$\mathcal{A}_{12}\,|i\,j\rangle \equiv |i\,j\rangle - |j\,i\rangle \ , \tag{3.21a}$$

$$\mathcal{A}_{123}\,|i\,j\,k\rangle \equiv |i\,j\,k\rangle - |j\,i\,k\rangle - |i\,k\,j\rangle - |k\,j\,i\rangle + |k\,i\,j\rangle + |j\,k\,i\rangle \ , \tag{3.21b}$$

ensuring that the result is null as soon as at least two single-particle states are the same. Antisymmetrizers can be written as functions of so-called particle-exchange operators P_{xy}, that

exchange particle x and y, so that

$$\mathcal{A}_{12} = 1 - P_{12} \ , \tag{3.22a}$$
$$\mathcal{A}_{123} = 1 - P_{12} - P_{23} - P_{13} + P_{12}P_{23} + P_{13}P_{23} \ . \tag{3.22b}$$

Although the three-particle antisymmetrizer could be written using a different choice of double exchange operators, given that

$$P_{12}P_{13}\,|ijk\rangle = P_{13}P_{23}\,|ijk\rangle \ , \tag{3.23a}$$
$$P_{13}P_{12}\,|ijk\rangle = P_{12}P_{23}\,|ijk\rangle \ , \tag{3.23b}$$
$$P_{23}P_{12}\,|ijk\rangle = P_{13}P_{23}\,|ijk\rangle \ , \tag{3.23c}$$
$$P_{23}P_{13}\,|ijk\rangle = P_{12}P_{23}\,|ijk\rangle \ , \tag{3.23d}$$

the choice made in Eq. 3.22b is kept throughout the rest of the document. In coordinate⊗spin⊗isospin representation, one can introduce coordinate P^r_{12}, spin P^σ_{12} and isospin P^τ_{12} exchange operators according to

$$P^r_{12}|\vec{r}_1\sigma_1 q_1, \vec{r}_2\sigma_2 q_2\rangle = |\vec{r}_2\sigma_1 q_1, \vec{r}_1\sigma_2 q_2\rangle \ , \tag{3.24a}$$
$$P^\sigma_{12}|\vec{r}_1\sigma_1 q_1, \vec{r}_2\sigma_2 q_2\rangle = |\vec{r}_1\sigma_2 q_1, \vec{r}_2\sigma_1 q_2\rangle \ , \tag{3.24b}$$
$$P^\tau_{12}|\vec{r}_1\sigma_1 q_1, \vec{r}_2\sigma_2 q_2\rangle = |\vec{r}_1\sigma_1 q_2, \vec{r}_2\sigma_2 q_1\rangle \ . \tag{3.24c}$$

The total particle-exchange operator $P_{xy} = P^r_{xy}P^\sigma_{xy}P^\tau_{xy}$, exchanging all three quantum numbers, is equivalent to exchanging the particles.

3.1.6 Two-body spherical state and exchange operators

The two-body Hilbert space $\mathcal{H}_2$ is the tensor product $\mathcal{H}_2 \equiv \mathcal{H}_1(1) \otimes \mathcal{H}_1(2)$ of two one-body Hilbert spaces. The direct product basis of $\mathcal{H}_2$ is obtained from those of $\mathcal{H}_1(1)$ and $\mathcal{H}_1(2)$ through

$$|1 : \vec{r}_1\sigma_1 q_1 \ , \ 2 : \vec{r}_2\sigma_2 q_2\rangle \equiv |1 : \vec{r}_1\sigma_1 q_1\rangle \otimes |2 : \vec{r}_2\sigma_2 q_2\rangle \ . \tag{3.25}$$

The convention used in the following consists in writing non-antisymmetrized direct-product two-body states without specifying the particle label. The first (second) set of quantum numbers is associated to the first (second) particle. The same convention has been used for direct-product three-body states.

3.1.6.1 Coordinate part

Two-nucleon states $|\vec{r}_1\sigma_1 q_1\, \vec{r}_2\sigma_2 q_2\rangle$ can be written as $|\vec{R}\vec{r}; \sigma_1 q_1\, \sigma_2 q_2\rangle$ by introducing relative and center of mass coordinates

$$\vec{R} \equiv \frac{\vec{r}_1 + \vec{r}_2}{2} \quad , \quad \vec{r} \equiv \vec{r}_1 - \vec{r}_2 \quad , \quad \vec{P} \equiv \vec{p}_1 + \vec{p}_2 \quad , \quad \vec{p} \equiv \frac{\vec{p}_1 - \vec{p}_2}{2} \ , \tag{3.26}$$

where $\vec{P}$ and $\vec{p}$ stands for center of mass and relative momenta. The total orbital angular-momentum of the two-body system, defined as $\hat{\vec{L}}_{tot} \equiv \hat{\vec{l}}_1 + \hat{\vec{l}}_2$ is decomposed into a center-of-mass and a relative part, $\hat{\vec{L}}_{tot} \equiv \hat{\vec{L}}_{com} + \hat{\vec{L}}$ where

$$\hat{\vec{L}}_{com} \equiv \hat{\vec{R}} \times \hat{\vec{P}}, \qquad \hat{\vec{L}} \equiv \hat{\vec{r}} \times \hat{\vec{p}} \ . \tag{3.27}$$

In spherical coordinates, $|\vec{r}\rangle \equiv |r\theta\phi\rangle$ with $r = \|\vec{r}\|$, $0 \leq \theta \leq \pi$, $0 \leq \phi \leq 2\pi$, where angles θ and ϕ provide the orientation of the relative position vector $\vec{r}$. The orbital angular momentum operator $\hat{\vec{L}}$ acts only on angular coordinates (θ, ϕ). Spherical harmonics

$$Y_L^{M_L}(\theta, \phi) \equiv \langle\theta\phi|LM_L\rangle \ , \tag{3.28}$$

are the wave functions associated with eigenstates $|LM_L\rangle$ of $\hat{\vec{L}}^2$ and $\hat{L}_z$ such that the angular part of $|\vec{r}\rangle$ can be expanded according to

$$|\theta\phi\rangle = \sum_{LM_L} Y_L^{M_L}(\theta,\phi)|LM_L\rangle \ . \tag{3.29}$$

When the two nucleons are exchanged, i.e. using P_{12}^r on the two-body state, $\vec{r}$ is changed into $-\vec{r}$, which is equivalent to changing θ and ϕ into $\pi-\theta$ and $\phi+\pi$. As $Y_L^{M_L}(\pi-\theta,\phi+\pi) = (-1)^L Y_L^{M_L}(\theta,\phi)$, the exchange of the two particles introduces a phase $(-1)^L$. Consequently, a state $|LM_L\rangle$ with L even is symmetric under the exchange of the two particles whereas a state with an odd L is antisymmetric under such an exchange. Such a property makes the basis $|r, LM_L\rangle$ of $\mathcal{H}_{2,\vec{r}}$ very suited to the construction of fully antisymmetrized states down the road.

3.1.6.2 Spin and isospin part

The two-nucleon spin operator is $\hat{\vec{S}} = \hat{\vec{\sigma}}_1 + \hat{\vec{\sigma}}_2$. Eigenstates $|SM_S\rangle$ of $\hat{\vec{S}}^2$ and $\hat{S}_z$ are expressed in terms of non-antisymmetrized direct-product spin two-body states $|\sigma_1,\sigma_2\rangle$ as

$$|0\ 0\rangle = \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} \quad , \quad \begin{cases} |1\ 1\rangle = |\uparrow\uparrow\rangle \ , \\ |1\ 0\rangle = \dfrac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} \ , \\ |1\ -1\rangle = |\downarrow\downarrow\rangle \ , \end{cases} \tag{3.30}$$

and have eigenvalues $\hbar^2 S(S+1)$ and M_S for $\hat{\vec{S}}^2$ and of $\hat{S}_z$, respectively, with possible values $S=0$ or 1 and $|M_S| \leq S$. As is customary, "spin-up" and "spin down" arrows have been used to denote $\sigma = +1/2$ and $\sigma = -1/2$, respectively. The $S=0$, or spin-singlet, state is antisymmetric under the exchange of particles 1 and 2 while $S=1$, or spin-triplet, states are symmetric. One can define the spin-exchange operator through

$$P_{12}^\sigma = \hat{\vec{S}}^2 - 1 \equiv \frac{1}{2}\Big(1 + \hat{\vec{\sigma}}_1 \cdot \hat{\vec{\sigma}}_2\Big) \ , \tag{3.31}$$

such that $P_{12}^\sigma |SM_S\rangle = (-1)^{1-S}|SM_S\rangle$. $|SM_S\rangle$ with S even, i.e. $S=0$, is antisymmetric under the exchange of the two particles whereas a state with an odd S, i.e. $S=1$, is symmetric under such an exchange. The same conclusion holds for the isospin part, replacing $\hat{\vec{S}}$ by $\hat{\vec{T}}$, $\hat{\vec{\sigma}}$ by $\hat{\vec{\tau}}$, S and M_S by T and M_T, $\uparrow$ by n and $\downarrow$ by p, respectively.

3.1.6.3 Pauli principle

A physical two-body fermion state is antisymetrized according to $\frac{1}{\sqrt{2}}\mathcal{A}_{12}|\vec{r}_1\sigma_1 q_1\,,\,\vec{r}_2\sigma_2 q_2\rangle$. The application of a particle exchange operator on this state provides

$$P_{12}\frac{1}{\sqrt{2}}\mathcal{A}_{12}|\vec{r}_1\sigma_1 q_1\,,\,\vec{r}_2\sigma_2 q_2\rangle = -\frac{1}{\sqrt{2}}\mathcal{A}_{12}|\vec{r}_1\sigma_1 q_1\,,\,\vec{r}_2\sigma_2 q_2\rangle \ , \tag{3.32}$$

as is easily proven, knowing the expression of $\mathcal{A}_{12}$, Eq. 3.22a, and using $P_{12}P_{12}=1$. The same property holds for three-body states. Such a property, rewritten $P_{12}^r P_{12}^\sigma P_{12}^\tau = -1$ when applied on an antisymmetrized state, is a transcription of the Pauli exclusion principle. Following the previous explanation, coordinate, spin and isospin exchange operators bring a phase $(-1)^L$, $(-1)^{1-S}$ and $(-1)^{1-T}$, respectively, such that

$$P_{12}^r P_{12}^\sigma P_{12}^\tau = -1 \quad \Leftrightarrow \quad (-1)^L(-1)^{1-S}(-1)^{1-T} = -1 \quad \Leftrightarrow \quad L+S+T \text{ is odd} \ . \tag{3.33}$$

3.1.6.4 Partial-waves and coordinate exchange operator

As will be seen below, Skyrme pseudo-potentials are constructed from two-body incoming and outgoing relative momentum operators, $\hat{\vec{k}}$ and $\hat{\vec{k}}'$. The angular part of $\hat{v}^{2Sk}(\hat{\vec{k}},\hat{\vec{k}}')$ can be expressed in terms of spherical harmonics, Ref. [86]

$$\hat{v}^{2Sk}(\hat{\vec{k}},\hat{\vec{k}}') = \frac{4\pi}{2l+1}\sum_{m=-l}^{l} Y_l^{m*}(\theta',\phi')Y_l^m(\theta\,,\phi\,)\;\hat{v}_l^{2Sk}(\hat{k},\hat{k}')\;\;, \tag{3.34}$$

where (θ,ϕ) and (θ',ϕ') are the incoming and outgoing relative angles, respectively. Inserting a closure relation in Eq. 3.3c and neglecting spin and isospin for now, one has

$$\begin{aligned} E_{Sk}^{\rho\rho} &= \frac{1}{2}\int d\vec{r}_1' d\vec{r}_2' d\vec{r}_1 d\vec{r}_2 \langle \vec{r}_1'\,\vec{r}_2'|\hat{v}^{2Sk}\mathcal{A}_{12}|\vec{r}_1\,\vec{r}_2\rangle \rho(\vec{r}_1,\vec{r}_1')\rho(\vec{r}_2,\vec{r}_2') \\ &= \frac{1}{2}\int d\vec{r}d\vec{r}'d\vec{R}d\vec{R}'\langle\,\vec{R}'r'\theta'\phi'\,|\,\hat{v}^{2Sk}(\hat{\vec{k}},\hat{\vec{k}}')\mathcal{A}_{12}\,|\,\vec{R}\,r\,\theta\,\phi\,\rangle\rho(\vec{R}'\vec{r}')\rho(\vec{R}\,\vec{r})\;\;. \end{aligned} \tag{3.35}$$

Inserting Eq. 3.34 into Eq. 3.35 and using Eq. 3.29 as well as the orthogonality of spherical harmonics, one sees that each term of decomposition 3.34 acts in a single partial-wave (L,M) of decomposition Eq. 3.29. Consequently, interaction terms proportional to one spherical harmonic select a unique partial-wave. Knowing that P_{12}^r applied on a state $|LM_L\rangle$ gives rise to phase $(-1)^L$ or $(-1)^{L'}$, one finds that

$$\hat{v}^{2Sk}(\hat{\vec{k}},\hat{\vec{k}}') \propto Y_l^{m*}(\theta',\phi')Y_l^m(\theta\,,\phi\,) \quad\Rightarrow\quad L=L'=l \quad\Rightarrow\quad P_{12}^r=(-1)^l\;\;, \tag{3.36}$$

such that the application of an exchange operator P_{12}^r is in fact predetermined by the partial-wave selection associated with the interaction term in front of it. For central two-body contact interactions up to second order in relative momenta, possible cases are

$$\hat{v}^{2Sk}(\hat{\vec{k}},\hat{\vec{k}}') \propto \left\{\begin{array}{l} 1 \\ \hat{\vec{k}}^{\,2}+\hat{\vec{k}}'^{2} \end{array}\right. \propto Y_0^{0*}(\theta',\phi')Y_0^0(\theta\,,\phi\,) \quad\Rightarrow\quad P_{12}^r=1 \tag{3.37a}$$

$$\hat{v}^{2Sk}(\hat{\vec{k}},\hat{\vec{k}}') \propto \hat{\vec{k}}'\cdot\hat{\vec{k}} \propto Y_1^{0*}(\theta',\phi')Y_1^0(\theta\,,\phi\,) \quad\Rightarrow\quad P_{12}^r=-1\;\;. \tag{3.37b}$$

The same reasoning holds if $\hat{v}^{2Sk}(\hat{\vec{k}},\hat{\vec{k}}')$ depends on higher powers of $\hat{\vec{k}}$ and $\hat{\vec{k}}'$. The predetermination of P_{12}^r occurs only if the interaction has been separated in terms proportional to a single spherical harmonics. Although such a feature remains in the three-body case, one has to be careful because there are three different two-body states in a given three-body state.

3.1.6.5 Relative momentum, spin matrices and scalar product

The determination of partial-waves selected by the interaction has been performed in the case of a contact interaction depending solely on relative incoming and outgoing momenta. Likewise, the same determination is possible when the interaction depends also in spin matrices. For a contact spin-orbit interaction

$$\hat{v}^{2Sk}(\hat{\vec{k}},\hat{\vec{k}}',\hat{\vec{\sigma}}_1,\hat{\vec{\sigma}}_2) = i\left(\hat{\vec{\sigma}}_1+\hat{\vec{\sigma}}_2\right)\cdot\hat{\vec{k}}'\wedge\hat{\vec{k}}\;\;, \tag{3.38}$$

the dependence on spin Pauli matrices enforces that the triplet state $S=1$ is selected such that the further application of a spin exchange operator gives $P_{12}^\sigma=+1$. The partial-wave selection is slightly more complex, however the result is that the interaction acts in $L=1$ P-wave such that $P_{12}^r=-1$.

3.2 Linear functional

Having introduced various useful tools, we now proceed to the computation of the nuclear EDF kernel, starting with the kinetic linear part E^{ρ}_{kin}. For such a purpose, Eq. 3.3b is reexpressed introducing one coordinate⊗spin⊗isospin closure relations on $\mathcal{H}_1$

$$E^{\rho}_{kin} = \int d\vec{r}' d\vec{r} \sum_{\sigma\sigma' q} \langle \vec{r}'\sigma' q|\hat{t}|\vec{r}\,\sigma\, q\rangle \rho_q(\vec{r}\,\sigma\,, \vec{r}'\sigma') \ , \tag{3.39}$$

where $\hat{t} = \dfrac{\hbar^2}{2m}\nabla_{r'}\nabla_r \delta(\vec{r} - \vec{r}')$. Such that

$$E^{\rho}_{kin} = \frac{\hbar^2}{2m}\int d\vec{r} \sum_q \tau_q \ . \tag{3.40}$$

3.3 Bilinear functional

The next part of the nuclear EDF to compute is the bilinear part $\mathcal{E}^{\rho\rho}_{Sk}$. To do so, Eq. 3.3c is reexpressed introducing two coordinate⊗spin⊗isospin closure relations on $\mathcal{H}_2$

$$\begin{aligned} E^{\rho\rho}_{Sk} = \frac{1}{2}\int d(\vec{r}\sigma q)\Big\{ &\langle \vec{r}'_1\sigma'_1 q_1\, \vec{r}'_2\sigma'_2 q_2|\hat{v}^{2Sk}\mathcal{A}_{12}|\vec{r}_1\sigma_1 q_1\, \vec{r}_2\sigma_2 q_2\rangle \\ &\rho_{q_1}(\vec{r}_1\sigma_1, \vec{r}'_1\sigma'_1)\rho_{q_2}(\vec{r}_2\sigma_2, \vec{r}'_2\sigma'_2)\Big\} \ , \end{aligned} \tag{3.41}$$

where $\displaystyle\int d(\vec{r}\sigma q)$ encompasses the continuous and discrete sum of all spatial, spin and isospin quantum numbers.

3.3.1 Construction of the pseudo potential

In the present part, we provide the procedure to construct the most general central part of the two-body Skyrme pseudo potential $\hat{v}^{2Sk}$. Such an operator is already well known and has been widely used [97, 98, 100, 101]. Consequently, the present section serves as a warming exercise in view of working out the three-body part of the pseudo potential.

3.3.1.1 Gradient part of the central pseudo potential

An essential object is the delta operator $\hat{\delta}_{r_1 r_2}$, describing an interaction between two nucleons located at the same point. Its matrix element are defined as

$$\langle \vec{r}'_1\vec{r}'_2|\hat{\delta}_{r_1 r_2}|\vec{r}_1\vec{r}_2\rangle \equiv \delta(\vec{r}_2 - \vec{r}_1)\delta(\vec{r}'_1 - \vec{r}_1)\delta(\vec{r}'_2 - \vec{r}_2) \ . \tag{3.42}$$

Gradient operators provide the interaction with a dependence on the relative momentum of the two nucleons. The gradient structure of the pseudo potential is thus constructed using incoming and outgoing relative momenta

$$\hat{\vec{k}}_{12} \equiv -\frac{i}{2}(\hat{\vec{\nabla}}_1 - \hat{\vec{\nabla}}_2) \quad , \quad \hat{\vec{k}}'_{12} \equiv +\frac{i}{2}(\hat{\nabla}'_1 - \hat{\nabla}'_2) \ . \tag{3.43}$$

Operators $\hat{\vec{k}}_{12}$ and $\hat{\vec{\nabla}}_i$, act on the ket coordinates, while operator $\hat{\vec{k}}'_{12}$ and $\hat{\vec{\nabla}}'_i$ denotes their complex conjugate acting on the bra coordinates. Operator $\hat{\vec{\nabla}}_1$ acts on the coordinates of the

first particle while $\hat{\vec{\nabla}}_2$ acts on those of the second particle. Matrix elements are defined as

$$\langle \vec{r}_1'\vec{r}_2'|\hat{\vec{k}}_{12}|\vec{r}_1\vec{r}_2\rangle \equiv \vec{k}_{\vec{r}_1\vec{r}_2}\delta_{r_1'r_1}\delta_{r_2'r_2} = -\frac{i}{2}(\vec{\nabla}_{\vec{r}_1}-\vec{\nabla}_{\vec{r}_2})\delta(\vec{r}_1'-\vec{r}_1)\delta(\vec{r}_2'-\vec{r}_2) \quad (3.44a)$$

$$\langle \vec{r}_1'\vec{r}_2'|\hat{\vec{k}}_{12}'|\vec{r}_1\vec{r}_2\rangle \equiv \vec{k}_{\vec{r}_1'\vec{r}_2'}\delta_{r_1'r_1}\delta_{r_2'r_2} = +\frac{i}{2}(\vec{\nabla}_{\vec{r}_1'}-\vec{\nabla}_{\vec{r}_2'})\delta(\vec{r}_1'-\vec{r}_1)\delta(\vec{r}_2'-\vec{r}_2)\ , \quad (3.44b)$$

where the shortcut notation $\delta_{r_i'r_j} \equiv \delta(\vec{r}_i'-\vec{r}_j)$ has been introduced for the part accounting for the local character of these operators.
The most general gradient structure of the interaction is found by forming all possible scalars from $\hat{\vec{k}}_{12}$ and $\hat{\vec{k}}_{12}'$. Invoking hermiticity, only three such scalars can be formed up to second order, i.e. 1, $\hat{\vec{k}}_{12}'^2+\hat{\vec{k}}_{12}^2$ and $\hat{\vec{k}}_{12}'\cdot\hat{\vec{k}}_{12}$. As a result the most general form of the central part of the interaction can be written as

$$\hat{v}_{\rm cent}^{2Sk} = \left[P_{\overline{12}}^{\{x^0\}} + \frac{1}{2}\left(P_{\overline{12}}^{\{x^1\}\dagger}\hat{\vec{k}}_{12}'^2 + \hat{\vec{k}}_{12}^2 P_{\overline{12}}^{\{x^1\}}\right) + \frac{1}{2}\left(P_{\overline{12}}^{\{x^2\}\dagger}\hat{\vec{k}}_{12}'\cdot\hat{\vec{k}}_{12} + \hat{\vec{k}}_{12}'\cdot\hat{\vec{k}}_{12}P_{\overline{12}}^{\{x^2\}}\right)\right]\hat{\delta}_{r_1r_2}\ , \quad (3.45)$$

where $P_{\overline{12}}^{\{x\}}$ remains to be specified to complete the construction and is discussed in the next section. The hermiticity of the interaction requires to take particular attention on where those operators $P_{\overline{12}}^{\{x\}}$ are placed.

3.3.1.2 Exchange operators

Each term in Eq. 3.45 involves a series of exchange operators multiplied by a parameter x_i, overall denoted as $P_{\overline{12}}^{\{x\}}$. The aim is to provide the various spin-isospin and partial-wave channels with different weights. The most general structure for $P_{\overline{12}}^{\{x\}}$ is

$$\begin{aligned} P_{\overline{12}}^{\{x\}} &= x_{00} + x_{01}P_{12}^{\sigma} + x_{02}P_{12}^{\tau} + x_{03}P_{12}^{\sigma}P_{12}^{\tau} \\ &\quad + x_{10}P_{12}^{r} + x_{11}P_{12}^{r}P_{12}^{\sigma} + x_{12}P_{12}^{r}P_{12}^{\tau} + x_{13}P_{12}^{r}P_{12}^{\sigma}P_{12}^{\tau}\ , \end{aligned} \quad (3.46)$$

knowing that $P_{12}^{q}P_{12}^{q} = 1$ for $q = r,s,t$, as exchanging twice the complete set of quantum numbers give back the initial two-body state. Such an operator is hermitian $P_{\overline{12}}^{\{x\}\dagger} = P_{\overline{12}}^{\{x\}}$ given that $P_{12}^{q\dagger} = P_{12}^{q}$. Equation 3.46 implies that $P_{\overline{12}}^{\{x\}}$ could contain redundant informations, i.e. it is possible that some parameters are correlated *a priori* such that only certain linear combinations of parameters $\{x_i\}$ occur eventually in the functional. Such correlations have to be identified.

3.3.1.3 Reduction of the parameter space

The first correlation between parameters appear through the application of the Pauli principle. As already explained in Sec. 3.1.6.3, the Pauli principle is equivalent to stating that $P_{12}^{r}P_{12}^{\sigma}P_{12}^{\tau}\mathcal{A}_{12}|ij\rangle = -\mathcal{A}_{12}|ij\rangle$. Thus, the three exchange operators appearing in $P_{\overline{12}}^{\{x\}}$ are correlated and only two of them are independent, e.g. one can replace P_{12}^{x} by $-P_{12}^{y}P_{12}^{z}$. As a result, $P_{\overline{12}}^{\{x\}}$ is rewritten using all possible combinations of two of the three exchange operators, e.g. P_{12}^{σ} and P_{12}^{τ}, so that the second line in Eq. 3.46 is in fact fully correlated to the first one.
Such correlations seem to only affect the $P_{\overline{12}}^{\{x\}}$ operators located to the right of gradient operators in Eq. 3.45, given that the antisymmetrizer is only applied on the ket in the matrix element 3.3. However the cyclic nature of the trace, i.e.

$$\sum_{ijkl}\langle ij|\hat{O}P_{12}|kl\rangle\rho_{ki}\rho_{lj} = \sum_{ijkl}\langle ij|P_{12}\hat{O}|kl\rangle\rho_{ki}\rho_{lj}\ , \quad (3.47)$$

where $\hat{O}$ is an arbitrary operator, allows us to transfer the antisymmetrizer on the bra and use the same reduction for those $P_{\overline{12}}^{\{x\}}$ operators located to the left of gradients. Finally, as $P_{\overline{12}}^{\{x\}}$ operator has been made independent of P_{12}^r and acts only in spin-isospin coordinates, it commutes with gradients operators such that the interaction can be rewritten as

$$\hat{v}_{\text{cent}}^{2Sk} = \left[P_{\overline{12}}^{\{x^0\}} + \frac{1}{2}\left(\hat{\vec{k}}_{12}'^2 + \hat{\vec{k}}_{12}^2\right) P_{\overline{12}}^{\{x^1\}} + \hat{\vec{k}}_{12}' \cdot \hat{\vec{k}}_{12} P_{\overline{12}}^{\{x^2\}} \right] \hat{\delta}_{r_1 r_2} \ . \tag{3.48}$$

The second correlation comes from the *a priori* knowledge of the result of applying coordinate exchange operators in connection with terms whose spatial part acts in one specific partial wave (see Sec. 3.1.6.4). The angular part of each term entering Eq. 3.48 is indeed proportional to two spherical harmonics of same angular momentum, so that $P_{12}^r = (-1)^L$ with $L = 0$ for the first two terms and $L = 1$ for the last one. Eventually, only a reduced form of $P_{\overline{12}}^{\{x\}}$ needs to be considered when applied on the right where the antisymmetrizer is as

$$P_{\overline{12}}^{\{x\}} \mathcal{A}_{12} \quad = \quad (x_{00} \mp x_{03}) + (x_{01} \mp x_{02}) P_{12}^\sigma + (x_{02} \mp x_{01}) P_{12}^\tau + (x_{03} \mp x_{00}) P_{12}^\sigma P_{12}^\tau \ , \tag{3.49}$$

where Eq. 3.22a, $P_{12} = P_{12}^r P_{12}^\sigma P_{12}^\tau$ and $P_{12}^r = (-1)^L = \pm 1$ have been used, to identify the further correlations between parameters. Eventually, the most general form actually needed for the two operators $P_{\overline{12}}^{\{x\}}$ at play in Eq. 3.48 is

$$P_{\overline{12}}^{\{x\}} = x_0 + x_1 P_{12}^\sigma \ . \tag{3.50}$$

3.3.1.4 Spin-orbit term

A spin-orbit term is to be added to the central one. It can be expressed in term of $\hat{\vec{k}}_{12}'$ and $\hat{\vec{k}}_{12}$ coupled to spin matrices $\hat{\vec{\sigma}}_1$ and $\hat{\vec{\sigma}}_2$

$$\hat{v}_{\text{S.O.}}^{2Sk} = \frac{i}{2}\left[P_{\overline{12}}'^{\{x^3\}\dagger} \left(\hat{\vec{\sigma}}_1 + \hat{\vec{\sigma}}_2\right) \cdot \hat{\vec{k}}_{12}' \wedge \hat{\vec{k}}_{12} + \left(\hat{\vec{\sigma}}_1 + \hat{\vec{\sigma}}_2\right) \cdot \hat{\vec{k}}_{12}' \wedge \hat{\vec{k}}_{12} P_{\overline{12}}'^{\{x^3\}} \right] \hat{\delta}_{r_1 r_2} \ . \tag{3.51}$$

As for the central part, $P_{\overline{12}}'^{\{x\}}$ is expressed in term of exchange operators and reduced in a second step. However, the spin structure of the spin-orbit interaction leads to an additional reduction as the interaction selects $S = 1$ spin channel, so that $P_{12}^\sigma = +1$ and $P_{\overline{12}}'^{\{x\}} = x$, see Sec. 3.1.6.4.

3.3.1.5 Final form of the two-body pseudo potential

The final form of the most general two-body pseudo potential up to two gradients is nothing but the traditional Skyrme effective interaction. After renaming the remaining parameters one has

$$\begin{aligned}
\hat{v}^{2Sk} &= t_0 \left(1 + x_0 P_{12}^\sigma\right) \hat{\delta}_{r_1 r_2} && \text{(3.52a)} \\
&+ \frac{t_1}{2} \left(1 + x_1 P_{12}^\sigma\right) \left(\hat{\vec{k}}_{12}'^2 + \hat{\vec{k}}_{12}^2\right) \hat{\delta}_{r_1 r_2} && \text{(3.52b)} \\
&+ t_2 \left(1 + x_2 P_{12}^\sigma\right) \hat{\vec{k}}_{12}' \cdot \hat{\vec{k}}_{12} \, \hat{\delta}_{r_1 r_2} && \text{(3.52c)} \\
&+ i W_0 \left(\vec{\sigma}_1 + \vec{\sigma}_2\right) \hat{\vec{k}}_{12}' \wedge \hat{\vec{k}}_{12} \ . && \text{(3.52d)}
\end{aligned}$$

Other spin-gradient coupling structures are possible, i.e. tensor structure. However, the latter has not been considered in the present study.

3.3.2 Bilinear energy density functional

Once the pseudo potential is defined, the calculation of the energy functional can proceed from Eq. 3.41. Using Eq. 3.31, the coordinate matrix elements of the operator Eq. 3.52 (using Eq. 3.44) and rules Eq. 3.17, the energy functional is expressed in terms of one-body quasi-local densities Eq. 3.14. The derivation is detailed in Appendix A.4. The bilinear energy density functional Eq. 3.5 can be decomposed into two parts invoking quasi-local densities behaving differently under time reversal transformation. The so-called time-even part reads

$$\mathcal{E}^{\rho\rho}_{Sk,\text{even}} = \sum_{t=0,1} \left\{ A^{\rho}_t \rho_t^2 + A^{\tau}_t \rho_t \tau_t + A^{\nabla\rho}_t \vec{\nabla}\rho_t \cdot \vec{\nabla}\rho_t + \sum_{\mu\nu} A^{J}_t J_{t,\mu\nu} J_{t,\mu\nu} + A^{\nabla J}_t \rho_t \vec{\nabla} \cdot \vec{J}_t \right\} , \quad (3.53)$$

whereas the time-odd part is

$$\mathcal{E}^{\rho\rho}_{Sk,\text{odd}} = \sum_{t=0,1} \left\{ A^{s}_t \vec{s}_t^{\,2} + A^{T}_t \vec{s}_t \vec{T}_t + \sum_{\mu\nu} A^{\nabla s}_t \nabla_\mu s_{t,\nu} \nabla_\mu s_{t,\nu} + A^{j}_t \vec{j}_t \cdot \vec{j}_t + A^{\nabla j}_t \vec{s}_t \cdot \vec{\nabla} \times \vec{j}_t \right\} . \quad (3.54)$$

The relation between time-even two-body functional coefficients and those of the two-body potential are given in Tab. {3.1}.

	t_0	t_0x_0	t_1	t_1x_1	t_2	t_2x_2	W_0
A^{ρ}_0 =	$+\frac{3}{8}$	$+0$	$+0$	$+0$	$+0$	$+0$	$+0$
A^{ρ}_1 =	$-\frac{1}{8}$	$-\frac{1}{4}$	$+0$	$+0$	$+0$	$+0$	$+0$
A^{s}_0 =	$-\frac{1}{8}$	$+\frac{1}{4}$	$+0$	$+0$	$+0$	$+0$	$+0$
A^{s}_1 =	$-\frac{1}{8}$	$+0$	$+0$	$+0$	$+0$	$+0$	$+0$
A^{τ}_0 =	$+0$	$+0$	$+\frac{3}{16}$	$+0$	$+\frac{5}{16}$	$+\frac{1}{4}$	$+0$
A^{τ}_1 =	$+0$	$+0$	$-\frac{1}{16}$	$-\frac{1}{8}$	$+\frac{1}{16}$	$+\frac{1}{8}$	$+0$
A^{T}_0 =	$+0$	$+0$	$-\frac{1}{16}$	$+\frac{1}{8}$	$+\frac{1}{16}$	$+\frac{1}{8}$	$+0$
A^{T}_1 =	$+0$	$+0$	$-\frac{1}{16}$	$+0$	$+\frac{1}{16}$	$+0$	$+0$
$A^{\nabla\rho}_0$ =	$+0$	$+0$	$+\frac{9}{64}$	$+0$	$-\frac{5}{64}$	$-\frac{1}{16}$	$+0$
$A^{\nabla\rho}_1$ =	$+0$	$+0$	$-\frac{3}{64}$	$-\frac{3}{32}$	$-\frac{1}{64}$	$-\frac{1}{32}$	$+0$
$A^{\nabla s}_0$ =	$+0$	$+0$	$-\frac{3}{64}$	$+\frac{3}{32}$	$-\frac{1}{64}$	$-\frac{1}{32}$	$+0$
$A^{\nabla s}_1$ =	$+0$	$+0$	$-\frac{3}{64}$	$+0$	$-\frac{1}{64}$	$+0$	$+0$
A^{j}_0 =	$+0$	$+0$	$-\frac{3}{16}$	$+0$	$-\frac{5}{16}$	$-\frac{1}{4}$	$+0$
A^{j}_1 =	$+0$	$+0$	$+\frac{1}{16}$	$+\frac{1}{8}$	$-\frac{1}{16}$	$-\frac{1}{8}$	$+0$
A^{J}_0 =	$+0$	$+0$	$+\frac{1}{16}$	$-\frac{1}{8}$	$-\frac{1}{16}$	$-\frac{1}{8}$	$+0$
A^{J}_1 =	$+0$	$+0$	$+\frac{1}{16}$	$+0$	$-\frac{1}{16}$	$+0$	$+0$
$A^{\nabla J}_0$ =	$+0$	$+0$	$+0$	$+0$	$+0$	$+0$	$-\frac{3}{4}$
$A^{\nabla J}_1$ =	$+0$	$+0$	$+0$	$+0$	$+0$	$+0$	$-\frac{1}{4}$
$A^{\nabla j}_0$ =	$+0$	$+0$	$+0$	$+0$	$+0$	$+0$	$-\frac{3}{4}$
$A^{\nabla j}_1$ =	$+0$	$+0$	$+0$	$+0$	$+0$	$+0$	$-\frac{1}{4}$

Table 3.1: Two-body functional (3.53,3.54) coefficients are expressed in terms of pseudo potential parameters Eq. 3.52.

3.3.2.1 Galilean invariance

The fact that $A_t^{\mathcal{J}} = -A_t^{\mathcal{T}}$, where $t \in \{0,1\}$ and $(\mathcal{T},\mathcal{J}) \in \Big\{(\tau,j);(T,J)\Big\}$, and that $A_t^{\nabla j} = A_t^{\nabla J}$ reflects the Galilean invariance of the functional. Indeed, the functional is gauge invariant if

$$\mathcal{E}_{Sk}^{\rho\rho'} - \mathcal{E}_{Sk}^{\rho\rho} = 0 \ , \tag{3.55}$$

where $\mathcal{E}_{Sk}^{\rho\rho'}$ is the Galilean transformed energy density. Using quasi-local densities transformation Eq. 3.20, the latter condition is equivalent to fulfilling

$$\begin{aligned}&\sum_{t=0,1}\sum_{(\mathcal{P},\mathcal{T},\mathcal{J})}\Big(A_t^{\mathcal{T}} + A_t^{\mathcal{J}}\Big)\Big(2\mathcal{P}_{\vec{r}}^t\mathcal{J}_{\vec{r},\mu}^t\nabla_\mu\phi(\vec{r}) + \mathcal{P}_{\vec{r}}^t\mathcal{P}_{\vec{r}}^t\nabla_\mu\phi(\vec{r})\nabla_\mu\phi(\vec{r})\Big)\\ &+\sum_{t=0,1}\Big(A_t^{\nabla j} - A_t^{\nabla J}\Big)\Big(\vec{\nabla}\rho_t(\vec{r})\cdot\vec{\nabla}\phi(\vec{r})\times\vec{s}_t(\vec{r})\Big) = 0 \ ,\end{aligned} \tag{3.56}$$

for $(\mathcal{P},\mathcal{T},\mathcal{J}) \in \Big\{(\rho,\tau,\vec{j});(\vec{s},\vec{T},J_{\mu\nu})\Big\}$ and ϕ being an arbitrary gauge function. The condition is indeed fulfilled thanks to $A_t^{\mathcal{T}} = -A_t^{\mathcal{J}}$ and $A_t^{\nabla j} = A_t^{\nabla J}$.

3.4 Trilinear functional

3.4.1 Introduction

Usually, density dependencies are added to the two-body Skyrme pseudo-potential (Eq. 3.52), in order to account for medium effects. Such density dependencies do not embody quantum operators such that the EDF kernel thus obtained does not derive strictly from a pseudo-potential. Medium effects thus inserted lead to a breaking of the Pauli principle as the density dependence does not derive from an antisymmetrized matrix element but is rather added by hand. The three-body pseudo-potentiel aims at replacing such density dependencies by generating a safe trilinear part of the EDF.
The first property a three-body operator $\hat{v}_{123}$ should respect is the symmetry under the exchange of any two particles, i.e. $v_{123}^{3Sk} = v_{213}^{3Sk} = v_{321}^{3Sk} = v_{132}^{3Sk}$. Therefore, any three-body interaction can be decomposed into three terms, each of them being symmetric only with respect to the exchange of two of the three particles [102]

$$\hat{v}^{3Sk} \equiv \hat{v}_{\overline{123}}^{3Sk} + \hat{v}_{\overline{312}}^{3Sk} + \hat{v}_{\overline{231}}^{3Sk} \ , \tag{3.57}$$

where $\overline{123}$ means that the interaction is symmetric under the exchange of particles 1 and 2 only. These three parts are formally identical but act on different particles. Two of these terms can be rewritten in terms of the third one and a selection of two-body exchange operators, e.g.

$$\hat{v}^{3Sk} \equiv \hat{v}_{\overline{123}}^{3Sk} + P_{23}P_{12}v_{\overline{123}}^{3sk}P_{12}P_{23} + P_{23}P_{13}v_{\overline{123}}^{3sk}P_{13}P_{23} \ , \tag{3.58}$$

As in the two-body case Eq. 3.32, the Pauli principle implies that

$$\begin{aligned}P_{xy}P_{yz}\mathcal{A}_{123}|\vec{r}_1\sigma_1q_1\,,\,\vec{r}_2\sigma_2q_2\,,\,\vec{r}_3\sigma_3q_3\rangle &= -P_{xy}\mathcal{A}_{123}|\vec{r}_1\sigma_1q_1\,,\,\vec{r}_2\sigma_2q_2\,,\,\vec{r}_3\sigma_3q_3\rangle\\ &= \mathcal{A}_{123}|\vec{r}_1\sigma_1q_1\,,\,\vec{r}_2\sigma_2q_2\,,\,\vec{r}_3\sigma_3q_3\rangle \ ,\end{aligned} \tag{3.59}$$

with $x,y,z \in \{1,2,3\}$. The cyclic nature of the trace also stands in the three-body case

$$\sum_{ijklmn}\langle ijk|\hat{O}P_{xy}|lmn\rangle\rho_{li}\rho_{mj}\rho_{nk} = \sum_{ijklmn}\langle ijk|P_{xy}\hat{O}|lmn\rangle\rho_{li}\rho_{mj}\rho_{nk} \quad \forall x,y \in \{1,2,3\} \ , \tag{3.60}$$

such that the three-body antisymmetrizer can be applied on the left or on the right in Eq. 3.3e. Taking into account the two latter properties, the EDF kernel derived from the three body pseudo potential can be expressed using only one term from Eq. 3.57, i.e. Eq. 3.3e can be rewritten as

$$E_{Sk}^{\rho\rho\rho} = \frac{1}{2}\sum_{ijklmn} \langle ijk|\hat{v}_{\overline{123}}^{3Sk}\mathcal{A}_{123}|lmn\rangle\, \rho_{li}\, \rho_{mj}\, \rho_{kn} \ . \tag{3.61}$$

As a result the construction of the three-body interaction only requires to specify $\hat{v}_{\overline{123}}^{3Sk}$, although the latter does not embody the complete interaction. Eventually, energy Eq. 3.3e is reexpressed introducing two coordinate⊗spin⊗isospin closure relations on $\mathcal{H}_3$

$$\begin{aligned} E_{Sk}^{\rho\rho\rho} = \frac{1}{2}\int d(\vec{r}\sigma q)\Big\{ &\langle \vec{r}_1'\sigma_1' q_1\, \vec{r}_2'\sigma_2' q_2\, \vec{r}_3'\sigma_3' q_3|\hat{v}_{\overline{123}}^{3Sk}\mathcal{A}_{123}|\vec{r}_1\sigma_1 q_1\, \vec{r}_2\sigma_2 q_2\, \vec{r}_3\sigma_3 q_3\rangle \\ &\rho_{q_1}(\vec{r}_1\sigma_1,\vec{r}_1'\sigma_1')\rho_{q_2}(\vec{r}_2\sigma_2,\vec{r}_2'\sigma_2')\rho_{q_3}(\vec{r}_3\sigma_3,\vec{r}_3'\sigma_3')\Big\} \ , \end{aligned} \tag{3.62}$$

where $\int d(\vec{r}\sigma q)$ denotes the continuous and discrete sums over all spatial, spin and isospin quantum numbers.

3.4.2 Construction of the pseudo potential

The procedure to construct the pseudo potential follows the same steps as in the two body case. Let us first introduce the product of delta operators $\hat{\delta}_{r_1r_3}\hat{\delta}_{r_2r_3}$ whose matrix elements are

$$\langle \vec{r}_1'\vec{r}_2'\vec{r}_3'|\hat{\delta}_{r_1r_3}\hat{\delta}_{r_2r_3}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle = \delta(\vec{r}_1-\vec{r}_3)\delta(\vec{r}_2-\vec{r}_3)\delta(\vec{r}_1'-\vec{r}_1)\delta(\vec{r}_2'-\vec{r}_2)\delta(\vec{r}_3'-\vec{r}_3) \ . \tag{3.63}$$

Using a condensed notation, $v_{\overline{123}}^{3Sk}$ is written as

$$\hat{v}_{\overline{123}}^{3Sk} \equiv \sum_{i=1}^{N_{cent}} G_{\overline{123}}^{i}(P_{123}^{\{x^i\}},\hat{\vec{k}}',\hat{\vec{k}})\,\hat{\delta}_{r_1r_3}\hat{\delta}_{r_2r_3} \ , \tag{3.64}$$

where exchange operators $P_{123}^{\{x\}}$ contain a set of tree the parameters and play the same role as in the two-body case, i.e. they provide various spin-isospin channels with different weights. Functions $G_{\overline{123}}^{i}$ depend on relative momentum operators $\hat{\vec{k}}_{xy}'$ and $\hat{\vec{k}}_{xy}$, where $\{x,y\}$ denotes two of the three particles, and on exchange operators $P_{123}^{\{x^i\}}$. N_{cent} denotes the number of possible terms eventually entering $\hat{v}_{\overline{123}}^{3Sk}$.

The two functions $P_{123}^{\{x^i\}}$ and $G_{\overline{123}}^{i}$ are going to be determined for a central interaction. One could have constructed the three-body Skyrme interaction by naive analogy with the two-body case, i.e.

$$N_{cent} \equiv 3 \tag{3.65a}$$

$$P_{123}^{\{x^i\}} \equiv (x_0^i + x_1^i P_{12}^{\sigma}) \tag{3.65b}$$

$$G_{\overline{123}}^{i}(P_{123}^{\{x^i\}},\hat{\vec{k}}',\hat{\vec{k}}) \equiv \left[P_{123}^{\{x^1\}}\ ,\ P_{123}^{\{x^2\}}\left(\hat{\vec{k}}_{12}'^2+\hat{\vec{k}}_{12}^2\right)\ ,\ P_{123}^{\{x^3\}}\left(\hat{\vec{k}}_{12}'\cdot\hat{\vec{k}}_{12}\right)\right] \ , \tag{3.65c}$$

as has been partially or entirely done in the few existing papers on the topic [103–105]. We are however trying here to identify the most general (central) three-body pseudo-potential of the Skyrme type.

3.4.2.1 Gradient functions $G^i_{\overline{123}}$

The first limit regarding $G^i_{\overline{123}}$ is to be of second order in gradients. Therefore, the interaction will be bilinear in operators $\hat{\vec{k}}_{ij}$ and their complex conjugates. To obtain a central interaction, the possible structures made out of gradient operators are limited to terms of the form $\hat{\vec{k}}_{ij}\cdot\hat{\vec{k}}_{kl}+\hat{\vec{k}}'_{ij}\cdot\hat{\vec{k}}'_{kl}$ and $\hat{\vec{k}}_{ij}\cdot\hat{\vec{k}}'_{kl}$, where $i,j,k,l\in\{1,2,3\}$. One has to determine on which particles the gradients can act. The presence of a third particle suggests that new choices may appear, in addition to those displayed in Eq. 3.65c where $i=k=1$ and $j=l=2$. Taking into account the fact that $\hat{v}^{3Sk}_{\overline{123}}$ has to be symmetric with respect to the exchange of particle 1 and 2, the number of new choices is reduced. Indeed, possible combinations actually belong to interaction term $\hat{v}^{3Sk}_{\overline{231}}$ and $\hat{v}^{3Sk}_{\overline{132}}$, e.g. $i=k=1$ and $j=l=3$ belong to $\hat{v}^{Sk}_{\overline{132}}$. Nevertheless, new choices such as $\hat{\vec{k}}_{13}\cdot\hat{\vec{k}}_{23}+\hat{\vec{k}}'_{13}\cdot\hat{\vec{k}}'_{23}$, and $\hat{\vec{k}}_{13}\cdot\hat{\vec{k}}'_{23}+\hat{\vec{k}}_{23}\cdot\hat{\vec{k}}'_{13}$ have to be considered. Eventually, taking $P^{\{x^i\}}_{123}$ equal to identity for now, five hermitian gradient structures are available

$$G^1_{\overline{123}}(\hat{\vec{k}},\hat{\vec{k}}') \equiv 1 \tag{3.66a}$$

$$G^2_{\overline{123}}(\hat{\vec{k}},\hat{\vec{k}}') \equiv \frac{1}{2}\left[\hat{\vec{k}}'_{12}\cdot\hat{\vec{k}}'_{12} + \hat{\vec{k}}_{12}\cdot\hat{\vec{k}}_{12}\right] \tag{3.66b}$$

$$G^3_{\overline{123}}(\hat{\vec{k}},\hat{\vec{k}}') \equiv \frac{1}{2}\left[\hat{\vec{k}}'_{23}\cdot\hat{\vec{k}}'_{13} + \hat{\vec{k}}_{23}\cdot\hat{\vec{k}}_{13}\right] \tag{3.66c}$$

$$G^4_{\overline{123}}(\hat{\vec{k}},\hat{\vec{k}}') \equiv \hat{\vec{k}}_{12}\cdot\hat{\vec{k}}'_{12} \tag{3.66d}$$

$$G^5_{\overline{123}}(\hat{\vec{k}},\hat{\vec{k}}') \equiv \frac{1}{2}\left[\hat{\vec{k}}_{23}\cdot\hat{\vec{k}}'_{13} + \hat{\vec{k}}'_{23}\cdot\hat{\vec{k}}_{13}\right] \quad . \tag{3.66e}$$

Eventually, exchange operators $P^{\{x^i\}}_{123}$ have to be incorporated taking into account the overall hermiticity and the symmetry under the exchange of particles 1 and 2.

3.4.2.2 Exchange operators $P^{\{x\}}_{123}$

The presence of a third particle allows many more combinations of exchange operators than in the two-body case. All possible combinations of coordinate, spin and isospin two-particle exchange operators determine the function $P^{\{x\}}_{123}$. Using the notations

$$\mathcal{Q}^r_1\equiv 1\ ,\quad \mathcal{Q}^r_2\equiv P^r_{12}\ ,\quad \mathcal{Q}^r_3\equiv P^r_{13}\ ,\quad \mathcal{Q}^r_4\equiv P^r_{23}\ ,\quad \mathcal{Q}^r_5\equiv P^r_{12}P^r_{23}\ ,\quad \mathcal{Q}^r_6\equiv P^r_{13}P^r_{23}\ , \tag{3.67a}$$

$$\mathcal{Q}^\sigma_1\equiv 1\ ,\quad \mathcal{Q}^\sigma_2\equiv P^\sigma_{12}\ ,\quad \mathcal{Q}^\sigma_3\equiv P^\sigma_{13}\ ,\quad \mathcal{Q}^\sigma_4\equiv P^\sigma_{23}\ ,\quad \mathcal{Q}^\sigma_5\equiv P^\sigma_{12}P^\sigma_{23}\ ,\quad \mathcal{Q}^\sigma_6\equiv P^\sigma_{13}P^\sigma_{23}\ , \tag{3.67b}$$

$$\mathcal{Q}^\tau_1\equiv 1\ ,\quad \mathcal{Q}^\tau_2\equiv P^\tau_{12}\ ,\quad \mathcal{Q}^\tau_3\equiv P^\tau_{13}\ ,\quad \mathcal{Q}^\tau_4\equiv P^\tau_{23}\ ,\quad \mathcal{Q}^\tau_5\equiv P^\tau_{12}P^\tau_{23}\ ,\quad \mathcal{Q}^\tau_6\equiv P^\tau_{13}P^\tau_{23}\ , \tag{3.67c}$$

one gets

$$P^{\{x\}}_{123} = \sum_{i=1}^{6}\sum_{j=1}^{6}\sum_{k=1}^{6} x_{ijk}\mathcal{Q}^r_i\mathcal{Q}^\sigma_j\mathcal{Q}^\tau_k\ , \tag{3.68}$$

where x_{ijk} denotes the different parameters which are multiplied by the different combinations of spatial, spin and isospin exchange operators. Double exchange in Eq. 3.67 are limited to two terms thanks to Eq. 3.23. Due to double exchange operators one can note that $P^{\{x\}\dagger}_{123}\neq P^{\{x\}}_{123}$, which is a crucial feature to keep track of in order to obtain a real energy functional. The use of the Pauli principle, i.e. $P^r_{xy}P^\sigma_{xy}P^\tau_{xy}\mathcal{A}_{123}|lmn\rangle = -\mathcal{A}_{123}|lmn\rangle$, with $\{xy\}\in\{12,23,13\}$ allows one to rewrite

$$P^{\{x\}}_{123} = \sum_{j=1}^{6}\sum_{k=1}^{6} x_{1jk}\mathcal{Q}^\sigma_j\mathcal{Q}^\tau_k\ , \tag{3.69}$$

as the three exchange operators P^r_{xy}, P^σ_{xy} and P^τ_{xy} are reducible to only two. The simplest choice has been made, i.e. write $P^{\{x\}}_{123}$ as a function of spin and isospin exchange operators only. Consequently, $P^{\{x\}}_{123}$ commutes with gradient operators $\hat{\vec{k}}_{ij}$ and $\hat{\vec{k}}'_{ij}$ which simplifies significantly the algebra. Parameters x_{1jk} are now renamed x_{jk}.

3.4.2.3 Gradient functions $G^i_{\overline{123}}$ depending on $P^{\{x\}}_{123}$

Gradient structures Eqs. (3.66a,3.66b,3.66c,3.66d) are composed of bilinear gradient operators which are individually symmetric under the exchange of particles 1 and 2. As a result exchange operators $P^{\{x^i\}}_{123}$ and their hermitian conjugates that are combined with the latter gradient structures, have to be symmetric under the exchange of particles 1 and 2 such that interaction $\hat{v}^{3Sk}_{\overline{123}}$ is. To do so, certain parameters x_{jk} of $P^{\{x^i\}}_{123}$ have to be correlated such that one obtains

$$\begin{aligned}
P^{\{x\}}_{\overline{123}} &= x_{00} + x_{01}P^\sigma_{12} + x_{02}\left(P^\sigma_{13}+P^\sigma_{23}\right) + x_{03}\left(P^\sigma_{12}P^\sigma_{23}+P^\sigma_{13}P^\sigma_{23}\right)\\
&+ x_{10}P^\tau_{12} + x_{11}P^\sigma_{12}P^\tau_{12} + x_{12}\left(P^\sigma_{13}P^\tau_{12}+P^\sigma_{23}P^\tau_{12}\right) + x_{13}\left(P^\sigma_{12}P^\sigma_{23}P^\tau_{12}+P^\sigma_{13}P^\sigma_{23}P^\tau_{12}\right)\\
&+ x_{20}\left(P^\tau_{13}+P^\tau_{23}\right) + x_{21}\left(P^\sigma_{12}P^\tau_{13}+P^\sigma_{12}P^\tau_{23}\right) + x_{22}\left(P^\sigma_{13}P^\tau_{13}+P^\sigma_{23}P^\tau_{23}\right)\\
&+ x_{23}\left(P^\sigma_{23}P^\tau_{13}+P^\sigma_{13}P^\tau_{23}\right) + x_{24}\left(P^\sigma_{12}P^\sigma_{23}P^\tau_{13}+P^\sigma_{13}P^\sigma_{23}P^\tau_{23}\right) + x_{25}\left(P^\sigma_{13}P^\sigma_{23}P^\tau_{13}+P^\sigma_{12}P^\sigma_{23}P^\tau_{23}\right)\\
&+ x_{30}\left(P^\tau_{12}P^\tau_{23}+P^\tau_{13}P^\tau_{23}\right) + x_{31}\left(P^\sigma_{12}P^\tau_{12}P^\tau_{23}+P^\sigma_{12}P^\tau_{13}P^\tau_{23}\right) + x_{32}\left(P^\tau_{12}P^r_{23}P^\sigma_{13}+P^\sigma_{23}P^\tau_{13}P^\tau_{23}\right)\\
&+ x_{33}\left(P^\sigma_{23}P^\tau_{12}P^\tau_{23}+P^\sigma_{13}P^\tau_{13}P^\tau_{23}\right) + x_{34}\left(P^\sigma_{12}P^\sigma_{23}P^\tau_{12}P^\tau_{23}+P^\sigma_{13}P^\sigma_{23}P^\tau_{13}P^\tau_{23}\right)\\
&+ x_{35}\left(P^\sigma_{13}P^\sigma_{23}P^\tau_{12}P^\tau_{23}+P^\sigma_{12}P^\sigma_{23}P^\tau_{13}P^\tau_{23}\right)\ .
\end{aligned} \tag{3.70}$$

In Eq. 3.66e, however, the bilinear gradient operators are not individually symmetric under the exchange of particles 1 and 2. Consequently, using $P^{\{x\}}_{\overline{123}}$ does provide an interaction that is symmetric under exchange of particle 1 and 2, but in fact correlates *a priori* parameters that should not be correlated. For instance, one has

$$\begin{aligned}
x_{02}\left(P^\sigma_{13}+P^\sigma_{23}\right)\left[\hat{\vec{k}}_{23}\cdot\hat{\vec{k}}'_{13}\ +\ \hat{\vec{k}}'_{23}\cdot\hat{\vec{k}}_{13}\right] &= +\,x_{02}\left[P^\sigma_{13}\,\hat{\vec{k}}_{23}\cdot\hat{\vec{k}}'_{13}\ +\ P^\sigma_{23}\,\hat{\vec{k}}'_{23}\cdot\hat{\vec{k}}_{13}\right]\\
&\quad + x_{02}\left[P^\sigma_{23}\,\hat{\vec{k}}_{23}\cdot\hat{\vec{k}}'_{13}\ +\ P^\sigma_{13}\,\hat{\vec{k}}'_{23}\cdot\hat{\vec{k}}_{13}\right]\ ,
\end{aligned} \tag{3.71}$$

giving two terms that are separately symmetric under the exchange of particle 1 and 2, such that they should be considered as being potentially independent from each other. As a result, one has to treat differently the part of $P^{\{x\}}_{\overline{123}}$ depending on exchange operators that are individually symmetric under exchange of particles 1 and 2, named $P^{\{x^i\}}_{\overline{12}}$ and equal to

$$P^{\{x\}}_{\overline{12}} = x_{00} + x_{01}P^\sigma_{12} + x_{10}P^\tau_{12} + x_{11}P^\sigma_{12}P^\tau_{12}\ , \tag{3.72}$$

and the remaining part named $P^{\{x^i\}}_{\underline{12}3}$ and $P^{\{x^i\}}_{\underline{13}2}$

$$\begin{aligned}
P^{\{x\}}_{\underline{12}3} &= +x_{02}P^\sigma_{13} + x_{03}P^\sigma_{12}P^\sigma_{23} + x_{12}P^\sigma_{13}P^\tau_{12} + x_{13}P^\sigma_{12}P^\sigma_{23}P^\tau_{12} + x_{20}P^\tau_{13} + x_{21}P^\sigma_{12}P^\tau_{13} + x_{22}P^\sigma_{13}P^\tau_{13}\\
&+ x_{23}P^\sigma_{23}P^\tau_{13} + x_{24}P^\sigma_{12}P^\sigma_{23}P^\tau_{13} + x_{25}P^\sigma_{13}P^\sigma_{23}P^\tau_{13} + x_{30}P^\tau_{12}P^\tau_{23} + x_{31}P^\sigma_{12}P^\tau_{12}P^\tau_{23} + x_{32}P^\sigma_{13}P^\tau_{12}P^\tau_{23}\\
&+ x_{33}P^\sigma_{23}P^\tau_{12}P^\tau_{23} + x_{34}P^\sigma_{12}P^\sigma_{23}P^\tau_{12}P^\tau_{23} + x_{35}P^\sigma_{13}P^\sigma_{23}P^\tau_{12}P^\tau_{23}
\end{aligned} \tag{3.73}$$

$$\begin{aligned}
P^{\{x\}}_{\underline{13}2} &= +x_{02}P^\sigma_{23} + x_{03}P^\sigma_{13}P^\sigma_{23} + x_{12}P^\sigma_{23}P^\tau_{12} + x_{13}P^\sigma_{13}P^\sigma_{23}P^\tau_{12} + x_{20}P^\tau_{23} + x_{21}P^\sigma_{12}P^\tau_{23} + x_{22}P^\sigma_{23}P^\tau_{23}\\
&+ x_{23}P^\sigma_{13}P^\tau_{23} + x_{24}P^\sigma_{13}P^\sigma_{23}P^\tau_{23} + x_{25}P^\sigma_{12}P^\sigma_{23}P^\tau_{23} + x_{30}P^\tau_{13}P^\tau_{23} + x_{31}P^\sigma_{12}P^\tau_{13}P^\tau_{23} + x_{32}P^\sigma_{23}P^\tau_{13}P^\tau_{23}\\
&+ x_{33}P^\sigma_{13}P^\tau_{13}P^\tau_{23} + x_{34}P^\sigma_{13}P^\sigma_{23}P^\tau_{13}P^\tau_{23} + x_{35}P^\sigma_{12}P^\sigma_{23}P^\tau_{13}P^\tau_{23}\ .
\end{aligned} \tag{3.74}$$

Finally, our investigation leads to the following set of possible structures in the three-body pseudo potential.

$$G^1_{\overline{123}} \equiv \frac{1}{2}\left[P^{\{x^1\}\dagger}_{\overline{123}} + P^{\{x^1\}}_{\overline{123}}\right] \tag{3.75a}$$

$$G^2_{\overline{123}} \equiv \frac{1}{2}\left[P^{\{x^2\}\dagger}_{\overline{123}}\,\hat{\vec{k}}'_{12}\cdot\hat{\vec{k}}'_{12} + P^{\{x^2\}}_{\overline{123}}\,\hat{\vec{k}}_{12}\cdot\hat{\vec{k}}_{12}\right] \tag{3.75b}$$

$$G^3_{\overline{123}} \equiv \frac{1}{2}\left[P^{\{x^3\}\dagger}_{\overline{123}}\,\hat{\vec{k}}'_{23}\cdot\hat{\vec{k}}'_{13} + P^{\{x^3\}}_{\overline{123}}\,\hat{\vec{k}}_{23}\cdot\hat{\vec{k}}_{13}\right] \tag{3.75c}$$

$$G^4_{\overline{123}} \equiv \frac{1}{2}\left[P^{\{x^4\}\dagger}_{\overline{123}}\,\hat{\vec{k}}_{12}\cdot\hat{\vec{k}}'_{12} + P^{\{x^4\}}_{\overline{123}}\,\hat{\vec{k}}'_{12}\cdot\hat{\vec{k}}_{12}\right] \tag{3.75d}$$

$$G^5_{\overline{123}} \equiv \frac{1}{4}\left[P^{\{x^5\}\dagger}_{\overline{12}}\left(\hat{\vec{k}}_{23}\cdot\hat{\vec{k}}'_{13} + \hat{\vec{k}}'_{23}\cdot\hat{\vec{k}}_{13}\right) + P^{\{x^5\}}_{\overline{12}}\left(\hat{\vec{k}}'_{23}\cdot\hat{\vec{k}}_{13} + \hat{\vec{k}}_{23}\cdot\hat{\vec{k}}'_{13}\right)\right] \tag{3.75e}$$

$$G^6_{\overline{123}} \equiv \frac{1}{4}\left[P^{\{x^6\}\dagger}_{\underline{13}\overline{2}}\,\hat{\vec{k}}'_{13}\cdot\hat{\vec{k}}_{23} + P^{\{x^6\}\dagger}_{\underline{12}\overline{3}}\,\hat{\vec{k}}'_{23}\cdot\hat{\vec{k}}_{13} + P^{\{x^6\}}_{\underline{13}\overline{2}}\,\hat{\vec{k}}'_{23}\cdot\hat{\vec{k}}_{13} + P^{\{x^6\}}_{\underline{12}\overline{3}}\,\hat{\vec{k}}'_{13}\cdot\hat{\vec{k}}_{23}\right] \tag{3.75f}$$

$$G^7_{\overline{123}} \equiv \frac{1}{4}\left[P^{\{x^7\}\dagger}_{\underline{12}\overline{3}}\,\hat{\vec{k}}'_{13}\cdot\hat{\vec{k}}_{23} + P^{\{x^7\}\dagger}_{\underline{13}\overline{2}}\,\hat{\vec{k}}'_{23}\cdot\hat{\vec{k}}_{13} + P^{\{x^7\}}_{\underline{12}\overline{3}}\,\hat{\vec{k}}'_{23}\cdot\hat{\vec{k}}_{13} + P^{\{x^7\}}_{\underline{13}\overline{2}}\,\hat{\vec{k}}'_{13}\cdot\hat{\vec{k}}_{23}\right], \tag{3.75g}$$

3.4.2.4 Reduction of the parameter space

Again, one is interested in finding correlations that exist *a priori* between the parameters of the postulated pseudo-potential, in order to reduce the set to the necessary ones only. In particular, correlations coming from properties of the angular part of interaction Eq. 3.75, are more difficult to highlight in the three-body case. As before, two-body relative momenta give information regarding which two-body partial-waves are selected by a given interaction term, so that the coordinate exchange operator between the two particles can be replaced by ± 1. However, in the three-body pseudo potential Eq. 3.75, three relative momenta associated with the three possible pairs of particles are to be considered. In this situation, the action of a given coordinate exchange operator can only be anticipated for interaction terms constructed solely out of the relative momentum operators associated with that pair of particles, e.g. P^r_{12} is equal to $(-1)^L$ only for Eqs. (3.66a,3.66b,3.66d), while P^r_{13} and P^r_{23} cannot be trivially guessed for Eqs. (3.66b,3.66c,3.66d,3.66e). The gradient-less term Eq. 3.66a still allows one to replace all coordinate exchange operators by $+1$. For a mathematical proof of the present discussion, see Appendix A.3.

As a result, the number of remaining parameters is still large. However, other correlations might have not been identified yet. Even if it would be convenient to identify all correlations between the parameters *a priori* so that the calculation of the functional is simplified, any correlation for which that has not been possible can anyway become apparent when the energy functional is computed. As the functional is computed via a computer software, Sec. 3.4.4.1, there is no practical disadvantage in missing correlations in Eq. 3.70 in the first place as they will be identified automatically in the end.

3.4.3 Parameters correlation study

3.4.3.1 Problematic

Let us now introduce the method used in the present study to identify non-obvious correlations between parameters. First, let us remark that correlations already pointed out could have been identified using the following method, such that all the previous discussion on how to reduce the parameter space was only given for clarity.

One considers the EDF derived from the pseudo-potential and define the pseudo-potential pa-

rameters vector $\vec{U}$ as well as the functional coefficients vector $\vec{B}$ through

$$\vec{U} \equiv \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix} \quad , \quad \vec{B} \equiv \begin{pmatrix} B_1 \\ B_2 \\ \vdots \\ B_m \end{pmatrix} \quad , \tag{3.76a}$$

where m denotes the number of functional terms and n the number of pseudo-potential parameters. Functional coefficients are related to pseudo-potential parameters through a real matrix

$$C = \begin{pmatrix} c_{11} & \dots & c_{1n} \\ c_{21} & \dots & c_{2n} \\ \vdots & \ddots & \vdots \\ c_{m1} & \dots & c_{mn} \end{pmatrix} \quad , \tag{3.77}$$

following

$$\vec{B} = C\vec{U} \quad , \tag{3.78}$$

such that, functional coefficients $\vec{B}$ are linear combinations of pseudo-potential parameters $\vec{U}$. For instance, Tab. {3.1} provides the C matrix for our final two-body interaction 3.52. Correlations between parameters $\vec{U}$ are found by identifying linear combinations of $\vec{U}$ that appear in all the functional coefficients. For instance, if $n > m$ there is necessarily at least $n - m$ linear combinations of parameters that are not independent. In such a case the n parameters can be reduced at least to m independent parameters. If $n \leq m$, it is still possible that the number of independent parameters is eventually smaller than n, and their identification can be obtained performing the singular value decomposition of C.

3.4.3.2 Singular value decomposition

The singular value decomposition generalizes the eigenvalue decomposition for non-squared matrices. Let us called M a general matrix of size $m * n$. Its singular values s are defined by

$$Mv = su \quad \textbf{and} \quad M^\dagger u = sv \quad , \tag{3.79}$$

where v and u are called right-singular and left-singular vectors of size n and m, respectively. $M^\dagger$ is the conjugate transpose of M and is a $n * m$ matrix. Consequently, there exists for M the following decomposition

$$M = USV^\dagger \quad , \tag{3.80}$$

where U and V are unitary $m * m$ and $n * n$ matrices, respectively, and where S is a diagonal matrix of size $m * n$, e.g.

$$S = \begin{pmatrix} s_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & s_n \\ \vdots & \ddots & \vdots \\ 0 & \dots & 0 \end{pmatrix} \quad \text{for } m > n \quad , \quad S = \begin{pmatrix} s_1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & s_m & \dots & 0 \end{pmatrix} \quad \text{for } m < n \ . \tag{3.81}$$

The singular value decomposition of M can be related to the diagonalization of an auxiliary matrix. Indeed, using Eq. 3.80 one has

$$MM^\dagger = USV^\dagger VS^\dagger U^\dagger = U(SS^\dagger)U^\dagger \quad , \tag{3.82a}$$

$$M^\dagger M = VS^\dagger U^\dagger USV^\dagger = V(S^\dagger S)V^\dagger \quad , \tag{3.82b}$$

where $SS^\dagger$ and $S^\dagger S$ are two diagonal square matrices, providing the eigenvalue decomposition of $MM^\dagger$ and $M^\dagger M$ square matrices, respectively. As a result, U and V are also eigenvectors of $MM^\dagger$ and $M^\dagger M$, respectively, while non-zero singular values of M are the square roots of the (positive) non-zero eigenvalues of $MM^\dagger$ and $M^\dagger M$.

3.4.3.3 Correlations

Correlations, i.e. redundant linear combinations of parameters, can be identified by extracting right-singular vectors corresponding to zero singular values of matrix C (Eq. 3.77). Denoting $v^{0\dagger} = (v_1^0, \cdots, v_n^0)$ one of the zero singular-value right-singular vector, one has

$$Cv^0 = 0 \ , \tag{3.83}$$

equivalent to the system of m equation

$$v_1^0\, c_{i1} + v_2^0\, c_{i2} + \cdots + v_n^0\, c_{in} = 0 \quad , \quad \forall i \in \{1, \cdots, m\} \ , \tag{3.84}$$

such that

$$c_{in} = -\sum_{j=1}^{n-1} \frac{v_j^0}{v_n^0}\, c_{ij} \quad , \quad \forall i \in \{1, \cdots, m\} \ , \tag{3.85}$$

where c_{in} was chosen as a matrix element with non-zero component in vector v^0. Thus, one column of the coefficient matrix is determined by the others. Consequently,

$$\begin{aligned} B_i &= \sum_{j=1}^{n} c_{ij} u_j \\ &= \sum_{j=1}^{n-1} c_{ij} (u_j - \frac{v_j^0}{v_n^0} u_n) \\ &\equiv \sum_{j=1}^{n-1} c_{ij} u'_j \quad , \quad \forall i \in \{1, \cdots, m\} \ , \end{aligned} \tag{3.86}$$

such that instead of adjusting n parameters one has to adjust only $n-1$ of them.

3.4.3.4 Final form of the pseudo potential

Investigating the structure of the EDF kernel obtained from Eqs. (3.64,3.75), many correlations between parameters have been identified using such a method. First gradient terms Eq. 3.75c and Eqs. (3.75e,3.75f,3.75g) are fully correlated to standard central terms 3.75b and 3.75d, respectively. Second, exchange operators happen to be highly correlated, leaving only room for the spin exchange operator P_{12}^σ for terms Eqs. (3.75a,3.75b), and spin exchange operator P_{12}^σ and $P_{13}^\sigma + P_{23}^\sigma$ for term Eq. 3.75d. A last reduction appears for gradient-less terms, where the spin exchange operator term, x_{01} in Eq. 3.70 provides a null contribution to the EDF kernel. The final form of the most general central three-body Skyrme-like pseudo potential is

$$\hat{v}_{\overline{123}}^{3Sk} = P_{\overline{123}}^{\{u_0\}} \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \tag{3.87a}$$

$$+ \frac{1}{2} \left[P_{\overline{123}}^{\{u_1\}\dagger}\, \hat{\vec{k}}'_{12} \cdot \hat{\vec{k}}'_{12} \ + \ P_{\overline{123}}^{\{u_1\}}\, \hat{\vec{k}}_{12} \cdot \hat{\vec{k}}_{12} \right] \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \tag{3.87b}$$

$$+ \frac{1}{2} \left[P_{\overline{123}}^{\{u_2\}\dagger}\, \hat{\vec{k}}_{12} \cdot \hat{\vec{k}}'_{12} \ + \ P_{\overline{123}}^{\{u_2\}}\, \hat{\vec{k}}'_{12} \cdot \hat{\vec{k}}_{12} \right] \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \ , \tag{3.87c}$$

with

$$P_{\overline{123}}^{\{u_0\}} = u_0 \tag{3.88a}$$

$$P_{\overline{123}}^{\{u_1\}} = u_1\Big[1 + y_1 P_{12}^{\sigma}\Big] \tag{3.88b}$$

$$P_{\overline{123}}^{\{u_2\}} = u_2\Big[1 + y_{21} P_{12}^{\sigma} + y_{22}(P_{13}^{\sigma} + P_{23}^{\sigma})\Big] \ , \tag{3.88c}$$

where $u_0, u_1, y_1, u_2, y_{21}, y_{22}$ denote the six remaining free parameters. The complete interaction, Eq. 3.57, is obtained adding the analog $\hat{v}_{\overline{132}}^{3Sk}$ and $\hat{v}_{\overline{231}}^{3Sk}$ terms. As it can be seen Eq. 3.87 and Eq. 3.88 the final three-body pseudo-potential could not have been constructed in full "naive" analogy with the two-body case. For this reason, three-body Skyrme pseudo potential already used in the litterature [103, 105] do not constitute the most general three-body Skyrme-like interaction but only a simplified version of the one developped in the present study.

3.4.4 Trilinear contribution to the EDF kernel

As for the two body case, the energy density functional Eq. 3.5 is obtained by computing Eq. 3.62 starting from Eq. 3.87 and using Eqs. (3.17,3.31,3.44). An example of such a derivation is provided in Appendix A.4.

3.4.4.1 Formal computation

Unfortunately, the calculation of the trilinear functional is much more cumbersome than for the bilinear. The number of terms in the antisymmetrizer $\mathcal{A}_{123}$ coupled to the number of new exchange operators in the pseudo potential is responsible for that. Nevertheless, the intrinsic difficulty of the calculation is the same. The fact that some coordinate exchange operators cannot be simplified, represents the only one subtlety, as one has to take care of which non-local density gradients applied. Finally, the main challenge of the calculation is to avoid inattention mistakes, much more frequent when one has to manipulate thousands of terms. For this reason, a formal calculation code has been developped. The program is based on shape recognition and has been written in Linux shell programming. The main steps performed by the code follow closely those of the derivation presented in Appendix A.4.

Input

The two inputs for the code are the gradient structure and the exchange operators $P_{123}^{\{x\}}$, that have to be written in a file, respecting scrupulously a given format. For instance, if one would like to determine the EDF kernel deriving from potential Eqs. (3.87,3.88), the input has to read

```
####################################
TERM NUMBER
0
GRAD
+3/12 ;
PX
a_0
####################################
TERM NUMBER
1
GRAD
-3/48 k 1 2 u k 1 2 u ;
PX
a_0
```

a_1 Ps12
##
TERM NUMBER
2
GRAD
+3/48 kp 1 2 u k 1 2 u ;
PX
a_0
a_1 Ps12
a_2 Ps13
a_2 Ps23

In this input file one can identify three blocks separated by a line of character ♯. Each block has three different parts

1. TERM NUMBER : labels the free parameters associated with a given potential term. Note that a potential term can be given in more than one block. It has not been needed for terms of potential Eqs. (3.87,3.88).
2. GRAD : gives the gradient structure multiplied by the absolute factor. kp and k denotes $-2i\hat{\vec{k}}'_{xy}$ and $2i\hat{\vec{k}}_{xy}$ operators respectively, x, y given by the two numeric numbers following, here 1 and 2, and the last letter is the Cartesian index of the vector operators. The absolute factor in front of the gradient structure includes various coefficients coming up in the functional calculation
   - $\frac{1}{6}$: coming from the definition of the energy Eq. 3.3e
   - 3 : due to the fact that $\hat{v}^{\overline{123}^{3Sk}}$ has been used instead of $\hat{v}^{3Sk}$, see Eq. 3.57
   - $(-2i)^{-n_p}(2i)^{-n}$: the absolute factors of definition Eq. 3.43, where n_p and n are the numbers of $\hat{\vec{k}}'$ and $\hat{\vec{k}}$ operators, respectively
   - $\frac{1}{2}$: because the calculation of the functional is done for the input interaction times $P^{\{x\}}_{\overline{123}}$ and its hermitian interaction as expressed in Eq. 3.75
3. Px : displays operator $P^{\{x\}}_{\overline{123}}$. Each line represents one term of $P^{\{x\}}_{\overline{123}}$, so that one has to add all the lines to have the complete exchange operator. Each term is multiplied by a generic parameter, symbolized by a letter taken in $\{a, b, c, d, e, f\}$ and an integer taken in $\{0, 1, 2, 3, 4, 5\}$. Possible exchange operators are $P^r_{xy}, P^\sigma_{xy}, P^\tau_{xy}$ than are represented in the input file by Prxy, Psxy, Ptxy, respectively.

Non-local energy functional

Once the input is read, the code first derives the non-local density matrix energy functional, i.e. the functional depending on non-local densities Eq. 3.16 and on gradients, obtained through the application of all exchange operators coming from $P^{\{x\}}_{\overline{123}}$ and $\mathcal{A}_{123}$. Each combination of exchange operators P^r_{xy}, P^σ_{xy} and P^τ_{xy} gives a definite trilinear non-local energy functional, such that rules are easily expressed, Eq. A.65 and Tab. {A.2}, and used in the code. The results takes the form of a file where coefficients of each term of the non-local energy functional, that depend on parameters given in input, are stored. The file is a list of

...
BR^{p_{12}s_{23}s_{31}}_{113} = +1a2_0/1+1a2_1/2
...

where

- BR are coefficients coming from the part of the interaction where $P^{\{x\}}_{\overline{123}}$ is applied on the right, whereas BL stands for those applied on the left. Thus, the functional is divided in

two part one on which gradients applied are those given in input and with coefficient BR and one on which gradients applied are the hermitian of those given in input and with coefficient BL. In the case of interaction Eq. 3.75, $P^{\{x\}}_{\overline{123}}$ can be applied on the right or on the left equivalently because it do not depend on coordinate exchange operator, however the code is able to treat $P^{\{x\}}_{\overline{123}}$ that depend on those.
- p and s stands for normal and spin densities obtained through spin exchange operators.
- {xy} denotes the indexes of the density matrix coordinates $\vec{r}'_x$ and $\vec{r}_y$. Remember that even if $P^{\{x\}}_{\overline{123}}$ does not depend on coordinate exchange operators $\mathcal{A}_{123}$ does such that $x \neq y$ in general.
- {xyz} denotes the isospin value of the three density matrices q_x, q_y and q_z.
- The coefficient is expressed in term of parameters a2_y where a_y is the parameter given in input and 2 the potential term label.

Thus, in this case the coefficient is the one in front of the non-local density matrix energy functional term

$$\rho_{q_1}(\vec{r}'_1,\vec{r}_2)\vec{s}_{q_1}(\vec{r}'_2,\vec{r}_3)\vec{s}_{q_3}(\vec{r}'_3,\vec{r}_1) \ , \tag{3.89}$$

coming from the application of $P^{\{x\}}_{\overline{123}}$ on the right, and with the gradient structure $\hat{\vec{k}}'_{12}\cdot\hat{\vec{k}}_{12}$.

Application of the gradients

Once the non-local density matrix energy functional is obtained, gradients are applied to generate the quasi-local functional, following rules laid out in Sec. 3.1.3.4. The result takes the form of a list of three quasi-local densities times the non-local density matrix energy functional coefficients of the term on which gradients have been applied, for instance

```
...
+ 3/24 BR^{p_{12}s_{23}s_{31}}_{113} ({densT p 1 u u }) ({densP s 1 }) ({densP s 3 })
...
```

where
- densP, densT and densJ mean $\mathcal{P}$, $\mathcal{T}$ and $\mathcal{J}$ in Eq. 3.18.
- p or s decide if $(\mathcal{P},\mathcal{T},\mathcal{J})$ is equal to $(\rho,\tau,\vec{j})$ or $(\vec{s},\vec{T},J_{\mu\nu})$.
- The integer that follow stands for the isospin.

Finally, that stands for the quasi-local functional term

$$\tau_{q_1}(\vec{r})\vec{s}_{q_1}(\vec{r})\cdot\vec{s}_{q_3}(\vec{r}) \ , \tag{3.90}$$

coming from the application of a part of the gradients on the density matrices Eq. 3.89.

Recombination

One must recombine many contributions to the quasi-local density functional. Indeed, the application of gradients on a given term of the non-local density matrix energy functional can generate the same quasi-local terms than those obtained starting from another term. The recombination gives rise to two types of files,

1. one that contains the factorized quasi-local functional

   ```
   ...
   B^{Tp_1 s_1 s_2} ({densT p 1 u u }) ({densP s 1 }) ({densP s 2 })
   ...
   ```

2. one that contains the quasi-local functional coefficients in terms of non-local density matrix energy functional coefficients

```
...
B^{Tp_1 s_1 s_2} = ... + 3/24 BR^{p_{12}s_{23}s_{31}}_{113} + ...
...
```

Rules Sec. 3.1.3.4 make appear imaginary and real term so that these two files are created for the real and for the imaginary part of the functional, separately.

Coefficients calculation
The last step is the calculation of quasi-local functional coefficients in terms of potential parameters rather than in terms of non-local density matrix energy functional coefficients. For this purpose, The previous output file, where the latter are expressed in terms of the former, is used. One has to note that coefficients corresponding to the imaginary part of the quasi-local functional must canceled.

Others functionalities
Others functionalities have been inserted in the code.

- The EDF is given in terms of neutron and proton quasi-local densities. For practical reason, one would like to have the same functional in isoscalar-isovector representation using Eq. 3.15. It can be done with the code such that the functional can be given in both representations at will.
- The code also finds correlations between two pseudo-potential parameters. To find more general correlations using the method explained in see Sec. 3.4.3, one must use a Mathematica sheet given in output.
- Derivatives of the functional with respect to quasi-local densities are computed. This is used to obtain one-body fields and Landau parameters, see Sec. 3.6 and Chap. 4.
- Bulk properties of infinite nuclear matter are computed, see Chap. 4.
- Inputs, the EDF in both representations, correlations between parameters, functional coefficients, infinite nuclear matter properties, one-body fields and Landau parameters are written in a Latex file and compiled to generate a pdf file, see Appendix B and Appendix C.

Bilinear functional
To treat the entire functional in a consistent way, the code has been extended to also compute the bilinear functional deriving from the traditional two-body Skyrme pseudo-potential. This part works identically to the three-body one and possesses the same features.

3.4.4.2 Result

The trilinear Skyrme quasi-local energy density deriving from the three-body pseudo potential Eq. 3.87 is decomposed in its time-even part

$$\mathcal{E}^{\rho\rho\rho}_{Sk,\text{even}} = \sum_{t=0,1} \Big\{ B^{\rho}_t[\rho_0]\rho_t^2 + B^{\tau}_t[\rho_0]\rho_t\tau_t + B^{\nabla\rho}_t[\rho_0]\vec{\nabla}\rho_t\cdot\vec{\nabla}\rho_t + \sum_{\mu\nu} B^{J}_t[\rho_0]J_{t,\mu\nu}J_{t,\mu\nu} \Big\}$$
$$+ B^{\tau}_{10}[\rho_1]\rho_1\tau_0 + B^{\nabla\rho}_{10}[\rho_1]\vec{\nabla}\rho_1\cdot\vec{\nabla}\rho_0 + \sum_{\mu\nu} B^{J}_{10}[\rho_1]J_{1,\mu\nu}J_{0,\mu\nu}\,, \qquad (3.91)$$

and its time-odd part

$$\begin{aligned}\mathcal{E}^{\rho\rho\rho}_{Sk,\text{odd}} = \sum_{t=0,1}\Big\{ & B^s_t[\rho_0]\vec{s}_t^{\,2} + B^T_t[\rho_0]\vec{s}_t\cdot\vec{T}_t + \sum_{\mu\nu} B^{\nabla s}_t[\rho_0]\nabla_\mu s_{t,\nu}\nabla_\mu s_{t,\nu} + B^j_t[\rho_0]\vec{j}_t\cdot\vec{j}_t \\ & + B^T_{t\bar{t}}[\rho_1]\vec{s}_t\cdot\vec{T}_{\bar{t}} + B^{\tau s}_t[\vec{s}_0]\vec{s}_t\tau_t + \sum_{\mu\nu}\Big[B^{\nabla\rho s}_t[s_{0,\nu}]\nabla_\mu\rho_t\nabla_\mu s_{t,\nu} \\ & + B^{\nabla\rho s}_{t\bar{t}}[s_{1,\nu}]\nabla_\mu\rho_t\nabla_\mu s_{\bar{t},\nu} + B^{Js}_t[s_{0,\nu}]j_{t,\mu}J_{t,\mu\nu} + B^{Js}_{t\bar{t}}[s_{1,\nu}]j_{t,\mu}J_{\bar{t},\mu\nu}\Big] \\ & + \sum_{\mu\nu\lambda k}\epsilon_{\nu\lambda k}\Big[B^{\nabla sJ}_t[s_{0,k}]\nabla_\mu s_{t,\nu}J_{t,\mu\lambda} + B^{\nabla sJ}_{t\bar{t}}[s_{1,k}]\nabla_\mu s_{t,\nu}J_{\bar{t},\mu\lambda}\Big]\Big\} \\ & + B^s_{10}[\rho_1]\vec{s}_1\cdot\vec{s}_0 + B^{\nabla s}_{10}[\rho_1]\nabla_\mu s_{1,\nu}\nabla_\mu s_{0,\nu} + B^j_{10}[\rho_1]\vec{j}_1\cdot\vec{j}_0 + B^{\tau s}_{10}[\vec{s}_1]\vec{s}_1\tau_0\,. \end{aligned} \tag{3.92}$$

The trilinear functional has been written under the form of a bilinear functional with density-dependent coefficients. That might seems disturbing as one starts from an actual three-body pseudo-potential and not from a two-body one depending effectively on the density. It is in fact possible to write the trilinear functional $\mathcal{E}^{\rho\rho\rho}$ under the form of the two-body one $\mathcal{E}^{\rho\rho[\rho_0]}$, with scalar isoscalar density-dependent coefficients, plus an extra trilinear functional $\mathcal{E}^{\rho\rho\rho}_{\text{extra}}$ that cannot be obtained from a density-dependent two-body potential

$$\mathcal{E}^{\rho\rho\rho} = \mathcal{E}^{\rho\rho[\rho_0]} + \mathcal{E}^{\rho\rho\rho}_{\text{extra}}\ . \tag{3.93}$$

This means that, the Pauli principle is fulfilled not only thanks to the interdependence of functional coefficients entering $\mathcal{E}^{\rho\rho[\rho_0]}$, but also thanks to the presence of $\mathcal{E}^{\rho\rho\rho}_{\text{extra}}$. The relation between coefficients of the time-even part of the trilinear functional and those of the three-body pseudo-potential are given in Tab. {3.2}. For the time-odd part, see Tab. {3.3}. The trilinear functional

	u_0	u_1	u_1y_1	u_2	u_2y_{21}	u_2y_{22}
B^ρ_0 =	$+\frac{3}{16}$	$+0$	$+0$	$+0$	$+0$	$+0$
B^ρ_1 =	$-\frac{3}{16}$	$+0$	$+0$	$+0$	$+0$	$+0$
B^τ_0 =	$+0$	$+\frac{3}{32}$	$+0$	$+\frac{15}{64}$	$+\frac{3}{16}$	$+\frac{3}{32}$
B^τ_{10} =	$+0$	$-\frac{1}{32}$	$+\frac{1}{32}$	$-\frac{5}{64}$	$-\frac{1}{16}$	$-\frac{7}{32}$
B^τ_1 =	$+0$	$-\frac{1}{16}$	$-\frac{1}{32}$	$+\frac{1}{32}$	$+\frac{1}{16}$	$-\frac{1}{16}$
$B^{\nabla\rho}_0$ =	$+0$	$+\frac{15}{128}$	$+0$	$-\frac{15}{256}$	$-\frac{3}{64}$	$-\frac{3}{128}$
$B^{\nabla\rho}_{10}$ =	$+0$	$-\frac{5}{64}$	$+\frac{1}{32}$	$+\frac{5}{128}$	$+\frac{1}{32}$	$+\frac{7}{64}$
$B^{\nabla\rho}_1$ =	$+0$	$-\frac{5}{128}$	$-\frac{1}{32}$	$-\frac{7}{256}$	$-\frac{1}{32}$	$-\frac{5}{128}$
B^J_0 =	$+0$	$+\frac{1}{32}$	$-\frac{1}{16}$	$-\frac{7}{64}$	$-\frac{1}{8}$	$+\frac{1}{32}$
B^J_{10} =	$+0$	$-\frac{1}{16}$	$+\frac{1}{16}$	$+\frac{1}{32}$	$+0$	$+\frac{3}{16}$
B^J_1 =	$+0$	$+\frac{1}{32}$	$+0$	$-\frac{7}{64}$	$-\frac{1}{16}$	$-\frac{1}{32}$

Table 3.2: Trilinear functional 3.91 coefficients expressed in terms of pseudo-potential parameters, (Eq. 3.88). Functional coefficients are expressed without the density dependence.

used in Ref. [103], which was obtained starting from potential terms Eqs. (3.87a,3.87b) without any exchange operator, can be exactly recovered from our more general study. By contrast, the one obtained in Ref. [105], where the interaction Eq. 3.87 without parameter y_{22} was used,

		u_0	u_1	u_1y_1	u_2	u_2y_{21}	u_2y_{22}
B_0^s	=	$-\frac{3}{16}$	$+0$	$+0$	$+0$	$+0$	$+0$
B_{10}^s	=	$+\frac{3}{8}$	$+0$	$+0$	$+0$	$+0$	$+0$
B_1^s	=	$-\frac{3}{16}$	$+0$	$+0$	$+0$	$+0$	$+0$
B_0^T	=	$+0$	$-\frac{1}{16}$	$+\frac{1}{32}$	$+\frac{1}{32}$	$+\frac{1}{16}$	$+\frac{1}{8}$
B_{10}^T	=	$+0$	$+\frac{1}{16}$	$-\frac{1}{32}$	$-\frac{1}{32}$	$-\frac{1}{16}$	$-\frac{1}{8}$
B_{01}^T	=	$+0$	$+\frac{1}{16}$	$+0$	$-\frac{1}{32}$	$+0$	$+0$
B_1^T	=	$+0$	$-\frac{1}{16}$	$+0$	$+\frac{1}{32}$	$+0$	$+0$
$B_0^{\tau s}$	=	$+0$	$-\frac{1}{32}$	$-\frac{1}{32}$	$-\frac{5}{64}$	$-\frac{1}{16}$	$+\frac{5}{32}$
$B_{10}^{\tau s}$	=	$+0$	$-\frac{1}{32}$	$+0$	$-\frac{5}{64}$	$-\frac{1}{16}$	$-\frac{1}{32}$
$B_1^{\tau s}$	=	$+0$	$+\frac{1}{16}$	$+\frac{1}{32}$	$-\frac{1}{32}$	$-\frac{1}{16}$	$+\frac{1}{16}$
$B_0^{\nabla s}$	=	$+0$	$-\frac{5}{128}$	$+\frac{1}{32}$	$-\frac{7}{256}$	$-\frac{1}{32}$	$+\frac{1}{128}$
$B_{10}^{\nabla s}$	=	$+0$	$+\frac{5}{64}$	$-\frac{1}{32}$	$+\frac{1}{128}$	$+0$	$+\frac{3}{64}$
$B_1^{\nabla s}$	=	$+0$	$-\frac{5}{128}$	$+0$	$-\frac{7}{256}$	$-\frac{1}{64}$	$-\frac{1}{128}$
$B_0^{\nabla \rho s}$	=	$+0$	$-\frac{5}{64}$	$-\frac{1}{32}$	$+\frac{5}{128}$	$+\frac{1}{32}$	$-\frac{5}{64}$
$B_{01}^{\nabla \rho s}$	=	$+0$	$-\frac{5}{64}$	$+0$	$+\frac{5}{128}$	$+\frac{1}{32}$	$+\frac{1}{64}$
$B_{10}^{\nabla \rho s}$	=	$+0$	$+\frac{5}{64}$	$+0$	$+\frac{1}{128}$	$+\frac{1}{32}$	$+\frac{1}{64}$
$B_1^{\nabla \rho s}$	=	$+0$	$+\frac{5}{64}$	$+\frac{1}{32}$	$+\frac{1}{128}$	$+0$	$-\frac{3}{64}$
B_0^{Js}	=	$+0$	$+\frac{1}{16}$	$+\frac{1}{16}$	$+\frac{5}{32}$	$+\frac{1}{8}$	$-\frac{5}{16}$
B_{01}^{Js}	=	$+0$	$+\frac{1}{16}$	$+0$	$+\frac{5}{32}$	$+\frac{1}{8}$	$+\frac{1}{16}$
B_{10}^{Js}	=	$+0$	$-\frac{1}{16}$	$+0$	$+\frac{1}{32}$	$+\frac{1}{8}$	$+\frac{1}{16}$
B_1^{Js}	=	$+0$	$-\frac{1}{16}$	$-\frac{1}{16}$	$+\frac{1}{32}$	$+0$	$-\frac{3}{16}$
$B_0^{\nabla sJ}$	=	$+0$	$+0$	$+0$	$-\frac{3}{64}$	$-\frac{3}{32}$	$+\frac{3}{32}$
$B_{01}^{\nabla sJ}$	=	$+0$	$+0$	$+\frac{1}{16}$	$-\frac{3}{64}$	$-\frac{1}{32}$	$+\frac{1}{32}$
$B_{10}^{\nabla sJ}$	=	$+0$	$+0$	$-\frac{1}{32}$	$-\frac{3}{64}$	$-\frac{1}{32}$	$+\frac{1}{32}$
$B_1^{\nabla sJ}$	=	$+0$	$+0$	$-\frac{1}{32}$	$-\frac{3}{64}$	$-\frac{1}{32}$	$+\frac{1}{32}$
B_0^j	=	$+0$	$-\frac{3}{32}$	$+0$	$-\frac{15}{64}$	$-\frac{3}{16}$	$-\frac{3}{32}$
B_{10}^j	=	$+0$	$+\frac{1}{16}$	$-\frac{1}{16}$	$+\frac{5}{32}$	$+\frac{1}{8}$	$+\frac{7}{16}$
B_1^j	=	$+0$	$+\frac{1}{32}$	$+\frac{1}{16}$	$-\frac{7}{64}$	$-\frac{1}{8}$	$-\frac{5}{32}$

Table 3.3: Trilinear Functional 3.92 coefficients expressed in terms of pseudo potential parameters, (Eq. 3.88). Functional coefficients are expressed without the density dependence.

differs from our EDF and the one derived by Waroquier. In any case, only the time-even part of the EDF kernel was provided in those two papers.

3.4.4.3 Gauge invariance

The gauge invariant condition is

$$\mathcal{E}_{Sk}^{\rho\rho\rho\prime} - \mathcal{E}_{Sk}^{\rho\rho\rho} \equiv \left[\mathcal{E}_{Sk}^{\rho\rho\rho}\right]_{\mathcal{P}\prime-\mathcal{P}} = 0 \ , \tag{3.94}$$

where $\mathcal{E}_{Sk}^{\rho\rho\rho\prime}$ is the gauge-transformed energy density obtained using Eq. 3.19, while $\mathcal{P}\prime - \mathcal{P}$ means that one makes the difference between the energy density computed in terms of gauge transformed densities and the one computed from non-transformed densities. Condition Eq. 3.94 is fulfilled for a general trilinear functional if specific correlations between its coefficients are indeed present. Whenever the EDF kernel is directly postulated and does not derive from a pseudo potential, gauge invariant combinations are used to build the functional. For this reason, we do not just check that functional Eqs. (3.91,3.92) respects gauge invariance but also provide generic gauge invariant combinations of trilinear functional terms.

Gauge-invariant combinations of trilinear terms are more complex to work out than usual bilinear ones. Gauge transformation only affects densities $\mathcal{T}^t = (\tau_t, \vec{T}_t)$ and $\mathcal{J}^t = (\vec{j}_t, J_{t,\mu\nu})$ following Eq. 3.20. The fact that $\mathcal{T}^{t\prime} - \mathcal{T}^t$ and $\mathcal{J}^{t\prime} - \mathcal{J}^t$ depend on associated densities $\mathcal{J}^t$ and $\mathcal{P}^t$ in addition to the gauge function ϕ, implies that correlations only involve coefficients multiplying densities $\mathcal{T}^t$ and $\mathcal{J}^t$ of same spin and isospin character.

For a bilinear central functional the two densities are either both isoscalar or both isovector and both scalar or both vector, such that each gauge invariant combination involves only two terms of the functional. As a result condition Eq. 3.55 is equivalent to

$$\left[A_t^{\mathcal{T}}\ \mathcal{T}^t\mathcal{P}^t + A_t^{\mathcal{J}}\ \mathcal{J}^t\mathcal{J}^t\right]_{\mathcal{P}\prime-\mathcal{P}} = 0 \ , \quad \forall t \in \{0,1\}, \forall (\mathcal{P},\mathcal{T},\mathcal{J}) \in \left\{(\rho,\tau,\vec{j}),(\vec{s},\vec{T},J_{\mu\nu})\right\} \ , \tag{3.95}$$

and is thus fulfilled whenever $A_t^{\mathcal{T}} = -A_t^{\mathcal{J}}$.

For trilinear functionals, such combinations can involve many more terms as two isovector or vector densities are always multiplied by an isoscalar or scalar density. Eventually condition Eq. 3.94 gives rise to five independent gauge invariant conditions that read

$$\left[B_0^{\tau}[\rho_0]\tau_0\rho_0 + B_0^{j}[\rho_0]\, j_{0,\mu}j_{0,\mu}\right]_{\mathcal{P}\prime-\mathcal{P}} = 0 \tag{3.96a}$$

$$\left[B_0^{T}[\rho_0]T_{0,\nu}s_{0,\nu} + B_0^{\tau s}[s_{0,\nu}]\tau_0 s_{0,\nu} + B_0^{J}[\rho_0]J_{0,\mu\nu}J_{0,\mu\nu} + B_0^{Js}[s_{0,\nu}]j_{0,\mu}J_{0,\mu\nu}\right]_{\mathcal{P}\prime-\mathcal{P}} = 0 \tag{3.96b}$$

$$\left[B_1^{\tau}[\rho_0]\tau_1\rho_1 + B_{10}^{\tau}[\rho_1]\tau_0\rho_1 + B_1^{j}[\rho_0]j_{1,\mu}j_{1,\mu} + B_{10}^{j}[\rho_1]j_{1,\mu}j_{0,\mu}\right]_{\mathcal{P}\prime-\mathcal{P}} = 0 \tag{3.96c}$$

$$\left[B_1^{T}[\rho_0]T_{1,\nu}s_{1,\nu} + B_{10}^{\tau s}[s_{1,\nu}]\tau_0 s_{1,\nu}s_{1,\nu} + B_1^{J}[\rho_0]J_{1,\mu\nu}J_{1,\mu\nu} + B_{01}^{Js}[s_{1,\nu}]j_{0,\mu}J_{1,\mu\nu}\right]_{\mathcal{P}\prime-\mathcal{P}} = 0 \tag{3.96d}$$

$$\left[B_{10}^{T}[\rho_1]T_{0,\nu}s_{1,\nu} + B_{01}^{T}[\rho_1]T_{1,\nu}s_{0,\nu} + B_1^{\tau s}[s_{0,\nu}]\tau_1 s_{1,\nu}\right. \tag{3.96e}$$

$$\left. + B_{10}^{J}[\rho_1]J_{1,\mu\nu}J_{0,\mu\nu} + B_1^{Js}[s_{0,\nu}]j_{1,\mu}J_{1,\mu\nu} + B_{10}^{Js}[s_{1,\nu}]j_{1,\mu}J_{0,\mu\nu}\right]_{\mathcal{P}\prime-\mathcal{P}} = 0$$

$$\left[\epsilon_{\nu\lambda k}B_0^{\nabla sJ}[s_{0,k}]\nabla_\mu s_{0,\nu}J_{0,\mu\lambda}\right]_{\mathcal{P}\prime-\mathcal{P}} = 0 \tag{3.96f}$$

$$\left[+ \epsilon_{\nu\lambda k}B_1^{\nabla sJ}[s_{0,k}]\nabla_\mu s_{1,\nu}J_{1,\mu\lambda} + \epsilon_{\nu\lambda k}B_{10}^{\nabla sJ}[s_{1,k}]\nabla_\mu s_{1,\nu}J_{0,\mu\lambda}\right. \tag{3.96g}$$

$$+\epsilon_{\nu\lambda k} B_{01}^{\nabla sJ}[s_{1,k}]\nabla_\mu s_{0,\nu} J_{1,\mu\lambda}\Big]_{\mathcal{P}'-\mathcal{P}} = 0 \ ,$$

where repeated indexes are summed over. Those conditions have been classified in terms of isospin and spin contents. Condition 3.96a involved all the functional terms with isoscalar densities and without spin densities. As well, condition 3.96b involved all the functional terms with isoscalar densities and with two spin densities. Condition 3.96c involved all the functional terms with two isovector densities and without spin densities. Conditions (3.96d,3.96e) involved all the functional terms with two isovector densities and two spin densities. The first one Eq. 3.96d where the two isovector densities are the two spin densities, and the second one Eq. 3.96e where only one spin density is an isovector density. Condition 3.96f involved all the functional terms with three isoscalar spin densities. Finally, condition 3.96g involved all the functional terms with three spin densities with two of them are isovector densities. Taking into account only two-body density dependent part of the functional $\mathcal{E}^{\rho\rho[\rho_0]}$, i.e. considering only functional coefficients depending on ρ_0, one has the usual two body conditions Eq. 3.95. The complexity thus comes from the part that cannot be derived from two-body density dependent interaction, $\mathcal{E}^{\rho\rho\rho}_{\rm extra}$. Correlations between functional coefficients resulting from conditions Eq. 3.96 are derived in Appendix A.5 and read

$$\text{Eq. 3.96a} \quad \Rightarrow \quad B_0^\tau + B_0^j = 0 \tag{3.97a}$$

$$\text{Eq. 3.96b} \quad \Rightarrow \quad \left\{ \begin{array}{l} 2B_0^{\tau s} + B_0^{Js} = 0 \\ 2B_0^T + 2B_0^J + B_0^{Js} = 0 \\ B_0^T + B_0^{\tau s} + B_0^J + B_0^{Js} = 0 \end{array} \right. \tag{3.97b}$$

$$\text{Eq. 3.96c} \quad \Rightarrow \quad \left\{ \begin{array}{l} 2B_{10}^\tau + B_{10}^j = 0 \\ 2B_1^\tau + 2B_1^j + B_{10}^j = 0 \\ B_1^\tau + B_{10}^\tau + B_1^j + B_{10}^j = 0 \end{array} \right. \tag{3.97c}$$

$$\text{Eq. 3.96d} \quad \Rightarrow \quad \left\{ \begin{array}{l} 2B_{10}^{\tau s} + B_{01}^{Js} = 0 \\ 2B_1^T + 2B_1^J + B_{01}^{Js} = 0 \\ B_1^T + B_{10}^{\tau s} + B_1^J + B_{01}^{Js} = 0 \end{array} \right. \tag{3.97d}$$

$$\text{Eq. 3.96e} \quad \Rightarrow \quad \left\{ \begin{array}{l} 2B_1^{\tau s} + B_1^{Js} + B_{10}^{Js} = 0 \\ 2B_{10}^T + B_{10}^J + B_{10}^{Js} = 0 \\ 2B_{01}^T + B_{10}^J + B_1^{Js} = 0 \\ B_{10}^T + B_{01}^T + B_1^{\tau s} + B_{10}^J + B_1^{Js} + B_{10}^{Js} = 0 \end{array} \right. \tag{3.97e}$$

$$\text{Eq. 3.96g} \quad \Rightarrow \quad B_1^{\nabla sJ} - B_{10}^{\nabla sJ} = 0 \ , \tag{3.97f}$$

where the coefficients B_0^τ, etc are those of functionals (3.91,3.92) from which the density dependence have been removed.

3.5 Energy functional in MR-EDF methods

The energy functional proposed in the present study, is obtained adding the linear kinetic 3.40, bilinear (3.53,3.54) and trilinear (3.91,3.92) part. When derived from two- and three-body pseudo potentials the functional coefficients are expressed in terms of pseudo-potential parameters through Tabs. {3.1-3.2-3.3}.
In such a case the functional is safe for MR-EDF computation, as long as the pairing part is not treated. Indeed, the pairing functional using the presently proposed two- and three-body

pseudo potential, Eqs. (3.52,3.87,3.88) has not been derived yet [3]. Such a derivation is however in progress.
Nevertheless, one may want to use a functional for which the constraints on coefficients, i.e. their interdependence, are released except for those imposed by Gauge invariance, in which case the regularization method proposed in Ref. [47–49] has to be used to perform MR-EDF calculations.

3.6 One-body fields

Once the bilinear and trilinear parts of the functional have been calculated, one must derive the associated one-body fields necessary for the resolution of the Bogoliubov-De Gennes equations. The equation of motion are determined self-consistently by minimizing

$$\mathcal{E}[\rho,\kappa^*,\kappa] - \frac{1}{2}\lambda\Big(\mathrm{Tr}\{\rho\} + \mathrm{Tr}\{\rho^*\}\Big) - \mathrm{Tr}\Big\{\Lambda(\mathcal{R}^2-\mathcal{R})\Big\} \ , \tag{3.98}$$

under the constrains that

$$\mathrm{Tr}\{\rho\} = \mathrm{Tr}\{\rho^*\} = \langle\Phi|\hat{N}|\Phi\rangle = N \ , \tag{3.99a}$$
$$\mathcal{R}^2 = \mathcal{R} \ , \tag{3.99b}$$

where Eq. 3.99a and Eq. 3.99b are used such that (i) the particle number is equal to N, the total number of nucleons (ii) $|\Phi\rangle$ remains a Bogoliubov product state during the minimzation. Minimization 3.98 leads to

$$\mathrm{Tr}\{\mathcal{H}'\delta\mathcal{R}\} = 0 \tag{3.100}$$

where the Bogoliubov-De Gennes matrix has been introduced through

$$\mathcal{H}' \equiv \begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix} \ , \tag{3.101}$$

and the generalized density matrix through

$$\mathcal{R} \equiv \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix} \ , \tag{3.102}$$

whereas particle-hole and particle-particle (pairing) fields are respectively defined as

$$h_{ji} \equiv \frac{\delta E[\rho,\kappa]}{\delta\rho^q_{ij}} \ , \qquad \Delta_{ij} \equiv \frac{\delta E[\rho,\kappa]}{\delta\kappa^{q\,*}_{ij}} \ , \tag{3.103a}$$
$$h^*_{ji} \equiv \frac{\delta E[\rho,\kappa]}{\delta\rho^{q\,*}_{ij}} \ , \qquad \Delta^*_{ij} \equiv \frac{\delta E[\rho,\kappa]}{\delta\kappa^q_{ij}} \ , \tag{3.103b}$$

3. It is important to note that such pairing functional will depend on the same set of free parameters than functional (3.91,3.92).

for $j \leq i$. Having the particle-hole Skyrme functional at hand Eqs. (3.53,3.54,3.91,3.92), we can obtain h_{ji}, for $j \leq i$ through

$$\begin{aligned} h^q_{ji} = \int d\vec{r} \Bigg\{ & \frac{\delta\mathcal{E}}{\delta\rho_q(\vec{r})}\frac{\delta\rho_q(\vec{r})}{\delta\rho^q_{ij}} + \frac{\delta\mathcal{E}}{\delta\tau_q(\vec{r})}\frac{\delta\tau_q(\vec{r})}{\delta\rho^q_{ij}} \\ & + \sum_{\mu\nu}\frac{\delta\mathcal{E}}{\delta J_{q,\mu\nu}(\vec{r})}\frac{\delta J_{q,\mu\nu}(\vec{r})}{\delta\rho^q_{ij}} \\ & + \sum_{\mu}\frac{\delta\mathcal{E}}{\delta s_{q,\mu}(\vec{r})}\frac{\delta s_{q,\mu}(\vec{r})}{\delta\rho^q_{ij}} \\ & + \sum_{\mu}\frac{\delta\mathcal{E}}{\delta T_{q,\mu}(\vec{r})}\frac{\delta T_{q,\mu}(\vec{r})}{\delta\rho^q_{ij}} \\ & + \sum_{\mu}\frac{\delta\mathcal{E}}{\delta j_{q,\mu}(\vec{r})}\frac{\delta j_{q,\mu}(\vec{r})}{\delta\rho^q_{ij}} \\ & + \sum_{\mu}\frac{\delta\mathcal{E}}{\delta F_{q,\mu}(\vec{r})}\frac{\delta F_{q,\mu}(\vec{r})}{\delta\rho^q_{ij}} \Bigg\} \ . \end{aligned} \tag{3.104}$$

The functional derivatives of the densities, expressed in coordinate space, with respect to matrix elements of the normal density matrix in configuration space read, for $j \leq i$, as

$$\frac{\delta\rho_q(\vec{r})}{\delta\rho^q_{ij}} = \varphi^\dagger_j(\vec{r}q)\,\varphi_i(\vec{r}q) \ , \tag{3.105a}$$

$$\frac{\delta\tau_q(\vec{r})}{\delta\rho^q_{ij}} = \left[\vec{\nabla}\varphi^\dagger_j(\vec{r}q)\right]\cdot\left[\vec{\nabla}\varphi_i(\vec{r}q)\right] \ , \tag{3.105b}$$

$$\frac{\delta J_{q,\mu\nu}(\vec{r})}{\delta\rho^q_{ij}} = -\frac{i}{2}\Big\{\varphi^\dagger_j(\vec{r}q)\,\sigma_\nu\,\nabla_\mu\varphi_i(\vec{r}q) - \nabla_\mu\varphi^\dagger_j(\vec{r}q)\,\sigma_\nu\,\varphi_i(\vec{r}q)\Big\} \ , \tag{3.105c}$$

$$\frac{\delta s_{q,\mu}(\vec{r})}{\delta\rho^q_{ij}} = \varphi^\dagger_j(\vec{r}q)\,\sigma_\mu\,\varphi_i(\vec{r}q) \ , \tag{3.105d}$$

$$\frac{\delta T_{q,\mu}(\vec{r})}{\delta\rho^q_{ij}} = \vec{\nabla}\varphi^\dagger_j(\vec{r}q)\,\sigma_\mu\cdot\vec{\nabla}\varphi_i(\vec{r}q) \ , \tag{3.105e}$$

$$\frac{\delta j_{q,\mu}(\vec{r})}{\delta\rho^q_{ij}} = -\frac{i}{2}\Big\{\varphi^\dagger_j(\vec{r}q)\left[\nabla_\mu\varphi_i(\vec{r}q)\right] - \left[\nabla_\mu\varphi^\dagger_j(\vec{r}q)\right]\varphi_i(\vec{r}q)\Big\} \ , \tag{3.105f}$$

$$\frac{\delta F_{q,\mu}(\vec{r})}{\delta\rho^q_{ij}} = \frac{1}{2}\Big\{\left[\vec{\nabla}\cdot\vec{\sigma}\,\varphi_j(\vec{r}q)\right]^\dagger\nabla_\mu\varphi_i(\vec{r}q) + \nabla_\mu\varphi^\dagger_j(\vec{r}q)\,\vec{\nabla}\cdot\vec{\sigma}\varphi_i(\vec{r}q)\Big\} \ . \tag{3.105g}$$

The functional derivatives with respect to ρ^{q*}_{ij}, for $j \leq i$, are obtained from the previous expression by performing the permutation $i \leftrightarrow j$ since, because of the hermiticity of ρ, one finds that

$$\begin{aligned} \frac{\delta\rho_q(\vec{r})}{\delta\rho^{q\,*}_{ij}} &= \frac{\delta}{\delta\rho^{q\,*}_{ij}}\sum_{\mu\nu}\varphi^\dagger_\nu(\vec{r}q)\varphi_\mu(\vec{r}q)\rho^q_{\nu\mu} \\ &= \frac{\delta}{\delta\rho^{q\,*}_{ij}}\sum_{\mu\nu}\varphi^\dagger_\nu(\vec{r}q)\varphi_\mu(\vec{r}q)\rho^{q\,*}_{\mu\nu} \\ &= \varphi^\dagger_i(\vec{r}q)\varphi_j(\vec{r}q) \ , \end{aligned} \tag{3.106}$$

and similarly for the others densities. The functional derivatives of the EDF with respect to local densities expressed in coordinate space lead to introducing local multiplicative potentials

of the form

$$U_q(\vec{r}) \equiv \frac{\delta\mathcal{E}}{\delta\rho_q(\vec{r})} \ , \tag{3.107a}$$

$$B_q(\vec{r}) \equiv \frac{\delta\mathcal{E}}{\delta\tau_q(\vec{r})} \ , \tag{3.107b}$$

$$W_{q,\mu\nu}(\vec{r}) \equiv \frac{\delta\mathcal{E}}{\delta J_{q,\mu\nu}(\vec{r})} \ , \tag{3.107c}$$

$$S_{q,\mu}(\vec{r}) \equiv \frac{\delta\mathcal{E}}{\delta s_{q,\mu}(\vec{r})} \ , \tag{3.107d}$$

$$C_{q,\mu}(\vec{r}) \equiv \frac{\delta\mathcal{E}}{\delta T_{q,\mu}(\vec{r})} \ , \tag{3.107e}$$

$$A_{q,\mu}(\vec{r}) \equiv \frac{\delta\mathcal{E}}{\delta j_{q,\mu}(\vec{r})} \ , \tag{3.107f}$$

$$D_{q,\mu}(\vec{r}) \equiv \frac{\delta\mathcal{E}}{\delta F_{q,\mu}(\vec{r})} \ , \tag{3.107g}$$

The explicit expression of such multiplicative potential resulting from the bilinear and trilinear functionals are provided by the code output, see Appendix B.3 and Appendix C.3. Finally, matrix elements of the fields can be written as

$$h^q_{ji} \equiv \int d\vec{r}\, \varphi^\dagger_j(\vec{r}q)\, h_q(\vec{r})\, \varphi_i(\vec{r}q) \ , \tag{3.108}$$

in order to introduce the complete particle-hole field expressed in coordinate space

$$\begin{aligned} h_q(\vec{r}) = &- \vec{\nabla}\cdot B_q(\vec{r})\vec{\nabla} + U_q(\vec{r}) + \vec{S}_q(\vec{r})\cdot\vec{\sigma} - \vec{\nabla}\cdot\Big[\vec{C}_q(\vec{r})\cdot\vec{\sigma}\Big]\vec{\nabla} - \frac{i}{2}\Big[\vec{A}_q(\vec{r})\cdot\vec{\nabla} + \vec{\nabla}\cdot\vec{A}_q(\vec{r})\Big] \\ &- \frac{i}{2}\Big[\overleftrightarrow{W}_q(\vec{r})\otimes\overleftrightarrow{\nabla}\sigma + \overleftrightarrow{\nabla}\sigma\otimes\overleftrightarrow{W}_q(\vec{r})\Big] - \frac{1}{2}\Big[\vec{\nabla}\cdot\vec{D}_q(\vec{r})\,\vec{\sigma}\cdot\vec{\nabla} + \vec{\sigma}\cdot\vec{\nabla}\,\vec{D}_q(\vec{r})\cdot\vec{\nabla}\Big] \ , \end{aligned} \tag{3.109}$$

where all gradients act to their right on the fields and the wave-function whereas Pauli matrices act to their right on the wave function only (the fields are not spinors). A shorthand notation for tensor products has been used $\overleftrightarrow{A}\otimes\overleftrightarrow{B} \equiv \sum_{\mu\nu} A_{\mu\nu}B_{\mu\nu}$, knowing that, for two vector $\vec{u}$ and $\vec{v}$, $\overleftrightarrow{uv}$ denotes the tensor with cartesian components $u_\mu v_\nu$. The structure of field Eq. 3.109 is identical of the one obtained for traditional Skyrme EDFs, the only difference being the expressions of the multiplicative potentials 3.107.

Chapter 4

Infinite Nuclear Matter

Abstract: In the present chapter, the infinite nuclear matter (INM) properties associated with the new Skyrme EDF derived in Chap. 3 are presented. Most of the results are obtained using the formal computation code and are thus given in the LaTeX output file created by the code and reproduced for the bilinear (trilinear) part of the EDF in Appendix B (Appendix C).

Contents

4.1 Introduction

4.1.1 Definitions

Infinite nuclear matter is a homogeneous medium without boundary where protons do not interact via the Coulomb interaction. In the present case, and as is often done, pairing correlations are omitted as well. Properties of infinite nuclear matter are often used to characterize nuclear interactions. The four basic degrees of freedom characterizing homogeneous INM are the scalar-isoscalar density ρ_0, the scalar-isovector density ρ_1, the vector-isoscalar density s_0, and the vector-isovector density s_1. They can be expressed through usual neutron and proton,

as well as spin-up and spin-down densities in the following way

$$\rho_0 = \rho_{n\uparrow} + \rho_{n\downarrow} + \rho_{p\uparrow} + \rho_{p\downarrow} = \rho_n + \rho_p \ , \tag{4.1a}$$
$$\rho_1 = \rho_{n\uparrow} + \rho_{n\downarrow} - \rho_{p\uparrow} - \rho_{p\downarrow} = \rho_n - \rho_p \ , \tag{4.1b}$$
$$s_0 = \rho_{n\uparrow} - \rho_{n\downarrow} + \rho_{p\uparrow} - \rho_{p\downarrow} = s_n + s_p \ , \tag{4.1c}$$
$$s_1 = \rho_{n\uparrow} - \rho_{n\downarrow} - \rho_{p\uparrow} + \rho_{p\downarrow} = s_n - s_p \ , \tag{4.1d}$$

such that the inverse relationships read

$$\rho_{n\uparrow} = \frac{1}{4}\Big(\rho_0 + \rho_1 + s_0 + s_1\Big) = \frac{1}{4}\Big(1 + I_\tau + I_\sigma + I_{\sigma\tau}\Big)\rho_0 \ , \tag{4.2a}$$
$$\rho_{n\downarrow} = \frac{1}{4}\Big(\rho_0 + \rho_1 - s_0 - s_1\Big) = \frac{1}{4}\Big(1 + I_\tau - I_\sigma - I_{\sigma\tau}\Big)\rho_0 \ , \tag{4.2b}$$
$$\rho_{p\uparrow} = \frac{1}{4}\Big(\rho_0 - \rho_1 + s_0 - s_1\Big) = \frac{1}{4}\Big(1 - I_\tau + I_\sigma - I_{\sigma\tau}\Big)\rho_0 \ , \tag{4.2c}$$
$$\rho_{p\downarrow} = \frac{1}{4}\Big(\rho_0 - \rho_1 - s_0 + s_1\Big) = \frac{1}{4}\Big(1 - I_\tau - I_\sigma + I_{\sigma\tau}\Big)\rho_0 \ , \tag{4.2d}$$

where

$$I_\tau \equiv \rho_1/\rho_0 \ , \tag{4.3a}$$
$$I_\sigma \equiv s_0/\rho_0 \ , \tag{4.3b}$$
$$I_{\sigma\tau} \equiv s_1/\rho_0 \ , \tag{4.3c}$$

are the relative isospin, spin, and spin-isospin excess, respectively ($-1 \leq I_i \leq 1$). Degrees of freedom 4.1 take specific values for the various types of infinite nuclear matter treated. In symmetric nuclear matter one has $I_i = 0$, whereas, in asymmetric nuclear matter $I_\tau \neq 0$, in polarized nuclear matter $I_\sigma \neq 0$ and in asymmetric polarized nuclear matter $I_{\sigma\tau} \neq 0$.

4.1.2 Matter density and Fermi momenta

Infinite nuclear matter being translationally invariant, nucleonic wave-functions take the form

$$\varphi_{\vec{k}}(\vec{r}\sigma q) \ = \ (2\pi)^{-\frac{3}{2}} \ \exp(i\vec{k}\cdot\vec{r}) \ \chi_\sigma \chi_q \ , \tag{4.4}$$

where $q\sigma = \{n\uparrow, n\downarrow, p\uparrow, p\downarrow\}$ and where χ_σ and χ_q denote the spin 1/2 and isospin 1/2 parts of the wave function. Starting from Eq. 4.4, quasi-local densities 3.14 can be calculated. In the EDF approach of the nuclear matter the density matrix for one type of spin and isospin particle $\rho_{ij}^{q\sigma}$, is an heavyside function, i.e. is equal to 1 when $|\vec{k}| \leq k_{F,q\sigma}$ and 0 otherwise where $k_{F,q\sigma}$ is the spin and isospin dependent Fermi momentum. Thus, the sum over all the state i and j in Eq. 3.14 becomes an integral on $\vec{p}$ over the sphere of radius $k_{F,q\sigma}$. The local density $\rho_{q\sigma}$ thus reads

$$\begin{aligned}
\rho_{q\sigma} &= \int_{|\vec{k}|\leq k_{F,q\sigma}} d^3\vec{k} \ \varphi^*_{\vec{k}}(\vec{r}\sigma q) \, \varphi_{\vec{k}}(\vec{r}\sigma q) \\
&= \left(\frac{1}{2\pi}\right)^3 \int_{|\vec{k}|\leq k_{F,q\sigma}} d^3\vec{k} \\
&= \frac{1}{6\pi^2} k^3_{F,q\sigma} \ ,
\end{aligned} \tag{4.5}$$

such that using Eq. 4.2 $k_{F,q\sigma}$ related to spin, isospin and spin-isospin excess through

$$k_{F,n\uparrow} = (6\pi^2)^{\frac{1}{3}}\rho_{n\uparrow}^{\frac{1}{3}} = \left(\frac{3\pi^2}{2}\right)^{\frac{1}{3}}\left(1 + I_\tau + I_\sigma + I_{\sigma\tau}\right)^{\frac{1}{3}}\rho_0^{\frac{1}{3}} \ , \tag{4.6a}$$

$$k_{F,n\downarrow} = (6\pi^2)^{\frac{1}{3}}\rho_{n\downarrow}^{\frac{1}{3}} = \left(\frac{3\pi^2}{2}\right)^{\frac{1}{3}}\left(1 + I_\tau - I_\sigma - I_{\sigma\tau}\right)^{\frac{1}{3}}\rho_0^{\frac{1}{3}} \ , \tag{4.6b}$$

$$k_{F,p\uparrow} = (6\pi^2)^{\frac{1}{3}}\rho_{p\uparrow}^{\frac{1}{3}} = \left(\frac{3\pi^2}{2}\right)^{\frac{1}{3}}\left(1 - I_\tau + I_\sigma - I_{\sigma\tau}\right)^{\frac{1}{3}}\rho_0^{\frac{1}{3}} \ , \tag{4.6c}$$

$$k_{F,p\downarrow} = (6\pi^2)^{\frac{1}{3}}\rho_{p\downarrow}^{\frac{1}{3}} = \left(\frac{3\pi^2}{2}\right)^{\frac{1}{3}}\left(1 - I_\tau - I_\sigma + I_{\sigma\tau}\right)^{\frac{1}{3}}\rho_0^{\frac{1}{3}} \ . \tag{4.6d}$$

Usually a total Fermi momentum k_F is defined from the scalar-isoscalar density according to

$$\begin{aligned}\rho_0 &= \sum_{\sigma q}\int_{|\vec{k}|\leq k_F} d^3\vec{p}\ \varphi^*_{\vec{k}}(\vec{r}\sigma q)\,\varphi_{\vec{k}}(\vec{r}\sigma q) \\ &\equiv \frac{2}{3\pi^2}k_F^3 \ ,\end{aligned} \tag{4.7}$$

such that one has not simply

$$k_F \neq \sum_{\sigma q} k_{F,q\sigma} \ . \tag{4.8}$$

4.1.3 Kinetic density and Fermi momenta

Similarly

$$\begin{aligned}\tau_{q\sigma} &= \int_{|\vec{k}|\leq k_{F,q\sigma}} d^3\vec{k}\ \left[\vec{\nabla}\varphi^*_{\vec{k}}(\vec{r}\sigma q)\right]\cdot\left[\vec{\nabla}\varphi_{\vec{k}}(\vec{r}\sigma q)\right] \\ &= \left(\frac{1}{2\pi}\right)^3\int_0^{k_F}\int_0^{\pi}\int_0^{2\pi} dk\sin(\theta)d\theta d\phi\ k^4 \\ &= \frac{3}{20}\,\frac{2}{3\pi^2}\,k_{F,q\sigma}^5 \ ,\end{aligned} \tag{4.9}$$

whereas others quasi-local densities fulfill

$$\Delta\rho_{q\sigma} = \vec{\nabla}\rho_{q\sigma} = \Delta\vec{s}_{q\sigma} = \nabla_\mu s_{q\sigma,\nu} = \vec{j}_{q\sigma} = J_{q\sigma,\mu\nu} = 0 \ . \tag{4.10}$$

The kinetic density can also be calculated from the total Fermi momentum thanks to

$$\tau_0 = \frac{3}{5}\,\frac{2}{3\pi^2}\,k_F^5 \tag{4.11a}$$

$$= \frac{3}{5}\,k_F^2\rho_0 \tag{4.11b}$$

$$= \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{2/3}\rho_0^{5/3} \ . \tag{4.11c}$$

Using Eqs. (4.9,4.6), one relates spin-isospin kinetic densities to spin, isospin and spin-isospin excess [106, 107]

$$\tau_0 = \tau_{n\uparrow} + \tau_{n\downarrow} + \tau_{p\uparrow} + \tau_{p\downarrow} = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \rho_0^{\frac{5}{3}} F_{5/3}^{(0)}(I_\tau, I_\sigma, I_{\sigma\tau}) \ , \tag{4.12a}$$

$$\tau_1 = \tau_{n\uparrow} + \tau_{n\downarrow} - \tau_{p\uparrow} - \tau_{p\downarrow} = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \rho_0^{\frac{5}{3}} F_{5/3}^{(\tau)}(I_\tau, I_\sigma, I_{\sigma\tau}) \ , \tag{4.12b}$$

$$T_0 = \tau_{n\uparrow} - \tau_{n\downarrow} + \tau_{p\uparrow} - \tau_{p\downarrow} = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \rho_0^{\frac{5}{3}} F_{5/3}^{(\sigma)}(I_\tau, I_\sigma, I_{\sigma\tau}) \ , \tag{4.12c}$$

$$T_1 = \tau_{n\uparrow} - \tau_{n\downarrow} - \tau_{p\uparrow} + \tau_{p\downarrow} = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \rho_0^{\frac{5}{3}} F_{5/3}^{(\sigma\tau)}(I_\tau, I_\sigma, I_{\sigma\tau}) \ , \tag{4.12d}$$

where $F^{(0)}, F^{(\tau)}, F^{(\sigma)}$ and $F^{(\sigma\tau)}$ are defined through

$$F_m^{(0)}(I_\tau, I_\sigma, I_{\sigma\tau}) \equiv \frac{1}{4}\Big[(1 + I_\tau + I_\sigma + I_{\sigma\tau})^m + (1 + I_\tau - I_\sigma - I_{\sigma\tau})^m + (1 - I_\tau + I_\sigma - I_{\sigma\tau})^m + (1 - I_\tau - I_\sigma + I_{\sigma\tau})^m\Big] \ , \tag{4.13a}$$

$$F_m^{(\tau)}(I_\tau, I_\sigma, I_{\sigma\tau}) \equiv \frac{1}{4}\Big[(1 + I_\tau + I_\sigma + I_{\sigma\tau})^m + (1 + I_\tau - I_\sigma - I_{\sigma\tau})^m - (1 - I_\tau + I_\sigma - I_{\sigma\tau})^m - (1 - I_\tau - I_\sigma + I_{\sigma\tau})^m\Big] \ , \tag{4.13b}$$

$$F_m^{(\sigma)}(I_\tau, I_\sigma, I_{\sigma\tau}) \equiv \frac{1}{4}\Big[(1 + I_\tau + I_\sigma + I_{\sigma\tau})^m - (1 + I_\tau - I_\sigma - I_{\sigma\tau})^m + (1 - I_\tau + I_\sigma - I_{\sigma\tau})^m - (1 - I_\tau - I_\sigma + I_{\sigma\tau})^m\Big] \ , \tag{4.13c}$$

$$F_m^{(\sigma\tau)}(I_\tau, I_\sigma, I_{\sigma\tau}) \equiv \frac{1}{4}\Big[(1 + I_\tau + I_\sigma + I_{\sigma\tau})^m - (1 + I_\tau - I_\sigma - I_{\sigma\tau})^m - (1 - I_\tau + I_\sigma - I_{\sigma\tau})^m + (1 - I_\tau - I_\sigma + I_{\sigma\tau})^m\Big] \ . \tag{4.13d}$$

To calculate INM properties, derivatives of F-functions are also needed

$$\frac{\partial F_m^{(\tau)}}{\partial I_\tau} = \frac{\partial F_m^{(\sigma)}}{\partial I_\sigma} = \frac{\partial F_m^{(\sigma\tau)}}{\partial I_{\sigma\tau}} = m F_{m-1}^{(0)} \ , \tag{4.14a}$$

$$\frac{\partial F_m^{(0)}}{\partial I_\tau} = \frac{\partial F_m^{(\sigma)}}{\partial I_{\sigma\tau}} = \frac{\partial F_m^{(\sigma\tau)}}{\partial I_\sigma} = m F_{m-1}^{(\tau)} \ , \tag{4.14b}$$

$$\frac{\partial F_m^{(0)}}{\partial I_\sigma} = \frac{\partial F_m^{(\tau)}}{\partial I_{\sigma\tau}} = \frac{\partial F_m^{(\sigma\tau)}}{\partial I_\tau} = m F_{m-1}^{(\sigma)} \ , \tag{4.14c}$$

$$\frac{\partial F_m^{(0)}}{\partial I_{\sigma\tau}} = \frac{\partial F_m^{(\tau)}}{\partial I_\sigma} = \frac{\partial F_m^{(\sigma)}}{\partial I_\tau} = m F_{m-1}^{(\sigma\tau)} \ , \tag{4.14d}$$

while their second derivatives are

$$\frac{\partial^2 F_m^{(j)}}{\partial I_i^2} = m(m-1) F_{m-2}^{(j)} \ , \tag{4.15}$$

for any $i, j = 0, \tau, \sigma, \sigma\tau$. Specific values are obtained for different values of m

$$F_0^{(0)} = 1 \ , \ F_0^{(i)} = 0 \ , \tag{4.16a}$$

$$F_1^{(0)} = 1 \ , \ F_1^{(i)} = I_i \ , \tag{4.16b}$$

and for different types of INM

$$F_m^{(0)}(0,0,0) = 1 \ , \tag{4.17a}$$
$$F_m^{(i)}(0,0,0) = 0 \ , \tag{4.17b}$$
$$F_m^{(\tau)}(0,1,0) = F_m^{(\tau)}(0,0,1) = 0 \ , \tag{4.17c}$$
$$F_m^{(\sigma)}(1,0,0) = F_m^{(\sigma)}(0,0,1) = 0 \ , \tag{4.17d}$$
$$F_m^{(\sigma\tau)}(1,0,0) = F_m^{(\sigma\tau)}(0,1,0) = 0 \ , \tag{4.17e}$$
$$F_m^{(0)}(1,0,0) = F_m^{(0)}(0,1,0) = F_m^{(0)}(0,0,1) = 2^{m-1} \ , \tag{4.17f}$$
$$F_m^{(\tau)}(1,0,0) = F_m^{(\sigma)}(0,1,0) = F_m^{(\sigma\tau)}(0,0,1) = 2^{m-1} \ , \tag{4.17g}$$
$$F_m^{(0)}(1,1,1) = F_m^{(i)}(1,1,1) = 4^{m-1} \ , \tag{4.17h}$$

where $i = \tau, \sigma, \sigma\tau$.

4.2 Nuclear matter properties

Basic nuclear matter properties are computed in the present section, leaving out the derivation of the Landau parameters for the next section. The fact that most of the local densities are zero in infinite nuclear matter implies that nuclear matter properties can be expressed in terms of a limited number of functional coefficients. For the bilinear EDF the only linear combinations of Skyrme parameters entering into account are A_0^ρ, A_1^ρ, A_0^τ and A_1^τ, which are given in Tab. {3.1}. For the trilinear functional only B_0^ρ, B_1^ρ, B_0^τ, B_1^τ and B_{10}^τ given in Tabs. {3.2-3.3} are involved. Traditionally specific linear combinations of Skyrme parameters denoted as Θ_s and Θ_v have been used for the bilinear functional instead of A_0^τ and A_1^τ [108]. They provide a more natural separation into scalar and vector nuclear matter properties, as will be seen below. The same reasoning can be done for the trilinear functional that leads to defining linear combinations Θ_{3s}, Θ_{3v} and Θ'_{3v}. All such linear combinations are given by

$$\Theta_s \equiv 16A_0^\tau = 3t_1 + t_2\left(5 + 4x_2\right) \ , \tag{4.18a}$$
$$\Theta_v \equiv 8\left(A_0^\tau - A_1^\tau\right) = t_1\left(2 + x_1\right) + t_2\left(2 + x_2\right) \ , \tag{4.18b}$$
$$\Theta_{3s} \equiv 16B_0^\tau = \frac{3}{4}\left[2u_1 + u_2\left(5 + 4y_{21} + 2y_{22}\right)\right] \ , \tag{4.18c}$$
$$\Theta_{3v} \equiv 8\left(B_0^\tau - B_1^\tau - B_{10}^\tau\right) = \frac{3}{4}\left[2u_1 + u_2\left(3 + 2y_{21} + 4y_{22}\right)\right] \ , \tag{4.18d}$$
$$\Theta'_{3v} \equiv 16B_{10}^\tau = -\frac{1}{4}\left[2u_1\left(1 - y_1\right) + u_2\left(5 + 4y_{21} + 14y_{22}\right)\right] \ . \tag{4.18e}$$

Note that all the results presented here, except for effective masses, can be found in Appendix B.4 and Appendix C.4 where they are expressed as a function of functional coefficients. All results are derived automatically by the formal computation code. The contribution of the kinetic energy to INM properties can however only be found in the present section. We also define for the rest of the section $c_s \equiv \left(\frac{3\pi^2}{2}\right)^{2/3}$ and $c_n \equiv \left(3\pi^2\right)^{2/3}$.

4.2.1 Symmetric infinite nuclear matter (SNM)

Symmetric nuclear matter is characterized by an equal number of protons and neutrons as well as of spin up and spin down particles. Consequently, $\rho_1 = I_\tau = 0$ and $I_\sigma = I_{\sigma\tau} = 0$. Only two quasi-local densities ρ_q and τ_q subsist. Since $N = Z$, one has $\rho_n = \rho_p = \frac{1}{2}\rho_0$ and $\tau_n = \tau_p = \frac{1}{2}\tau_0$. The main quantity of interest for nuclear matter is its equation of state (EOS)

providing the energy per particle of the nuclear fluid as a function of its density. For symmetric nuclear matter a stable state exists such that a minimum energy is obtained for a finite density $\rho_{\rm sat}$. The binding energy per nucleon in SNM is obtained from EQS. (3.40,3.53,3.54,3.91,3.92) and reads

$$\frac{E}{A} \equiv \frac{\mathcal{E}}{\rho_0} = \frac{3}{5}\frac{\hbar^2}{2m} c_s \rho_0^{2/3} + \frac{3}{8} t_0 \rho_0 + \frac{3}{16} u_0 \rho_0^2 + \frac{3}{80} c_s \Theta_s \rho_0^{5/3} + \frac{3}{80} c_s \Theta_{3s} \rho_0^{8/3} \quad . \tag{4.19}$$

The pressure of the fluid relates to the first derivative of the equation of state with respect to the density and allows one to find $\rho_{\rm sat}$ at which the fluid is stable. In SNM the pressure is

$$P \equiv \rho_0^2 \frac{\partial E/A}{\partial \rho_0}\Big|_A = \rho_0 \left[\frac{2}{5}\frac{\hbar^2}{2m} c_s \rho_0^{2/3} + \frac{3}{8} t_0 \rho_0 + \frac{3}{8} u_0 \rho_0^2 + \frac{1}{16} c_s \Theta_s \rho_0^{5/3} + \frac{1}{10} c_s \Theta_{3s} \rho_0^{8/3}\right] \quad . \tag{4.20}$$

The equilibrium density $\rho_{\rm sat}$ is obtained as the solution of $P(\rho_{\rm sat}) = 0$.
The incompressibility of the nuclear fluid relates to the second derivative of the equation of state with respect to the density and expresses the energy cost to compress the nuclear fluid. It is defined as

$$K \equiv \frac{18P}{\rho_0} + 9\rho_0^2 \frac{\partial^2 E/A}{\partial \rho_0^2} \quad , \tag{4.21}$$

such that at equilibrium density one has

$$K_\infty \equiv 9\rho_0^2 \frac{\partial^2 E/A}{\partial \rho_0^2}\Big|_{\rho_0=\rho_{\rm sat}} = -\frac{6}{5}\frac{\hbar^2}{2m} c_s \rho_0^{2/3} + \frac{27}{8} u_0 \rho_0^2 + \frac{3}{8} c_s \Theta_s \rho_0^{5/3} + \frac{3}{2} c_s \Theta_{3s} \rho_0^{8/3} \quad , \tag{4.22}$$

which needs to be positive for the system to be stable against density fluctuations.
The energy of a nucleon in the nuclear medium is written as a kinetic term plus a momentum dependent self-energy term coming from the interaction of this particle with all the others. This individual energy can be rewritten as a kinetic energy with an effective mass. The neutron m_n^* and proton m_p^* effective masses are thus for general isospin excess

$$\begin{aligned}
\frac{\hbar^2}{2m_q^*(I_\tau)} &\equiv \frac{\partial \mathcal{E}}{\partial \tau_q} \\
&= \frac{\hbar^2}{2m} + \frac{1}{16} A_0^\tau \rho_0 + q I_\tau A_1^\tau \rho_0 + B_0^\tau \rho_0^2 + q I_\tau B_1^\tau \rho_0^2 + I_\tau^2 B_{10}^\tau \rho_0^2 \\
&= \frac{\hbar^2}{2m} + \frac{1}{16}\Theta_s \rho_0 + q I_\tau \left(\frac{1}{16}\Theta_s - \frac{1}{8}\Theta_v\right)\rho_0 \\
&\quad + \frac{1}{16}\Theta_{3s}\rho_0^2 + q I_\tau \left(\frac{1}{16}\Theta_{3s} - \frac{1}{8}\Theta_{3v} - \frac{1}{16}\Theta'_{3v}\right)\rho_0^2 + I_\tau^2 \frac{1}{16}\Theta'_{3v}\rho_0^2 \quad ,
\end{aligned} \tag{4.23}$$

where $q = +1, -1$ respectively for neutrons and protons. In the particular case of SNM, i.e. $I_\tau = 0$, proton and neutron effective masses are equal to the so called isoscalar effective mass m_0^*, which is also defined through

$$\frac{m}{m_0^*} \equiv \frac{2m}{\hbar^2}\frac{\partial \mathcal{E}}{\partial \tau_0} = 1 + \frac{1}{16}\frac{2m}{\hbar^2}\left(\Theta_s \rho_0 + \Theta_{3s}\rho_0^2\right) = 1 + \kappa_0 \quad , \tag{4.24}$$

where κ_0 is the isoscalar enhancement factor.

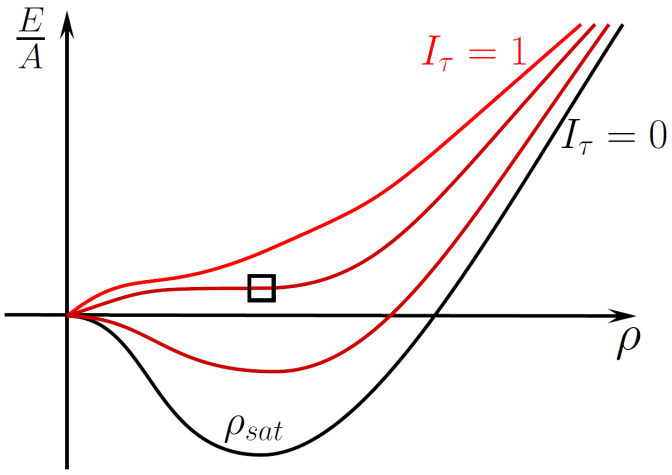

Figure 4.1: Equation of state for different value of I_τ. The square design the density where the saturation point disappear

4.2.2 Asymmetric infinite nuclear matter (ANM)

Asymmetric nuclear matter is characterized by a number of protons that differs from its number of neutrons; i.e. $I_\tau \neq 0$. The equation of state of such a nuclear fluid is

$$\begin{aligned}\frac{E}{A} = &\frac{3}{5}\frac{\hbar^2}{2m} c_s F_{5/3}^{(0)}(I_\tau,0,0)\,\rho_0^{2/3} + \frac{3}{8}t_0\,\rho_0 + \frac{3}{16}u_0\,\rho_0^2 - \frac{1}{8}t_0\,(2x_0+1)\,I_\tau^2\rho_0 - \frac{3}{16}u_0\,I_\tau^2\rho_0^2 \\ &+ \frac{3}{80}c_s\Theta_s F_{5/3}^{(0)}(I_\tau,0,0)\,\rho_0^{5/3} + \frac{3}{80}c_s\,(\Theta_s - 2\Theta_v)\,I_\tau F_{5/3}^{(\tau)}(I_\tau,0,0)\,\rho_0^{5/3} \\ &+ \frac{3}{80}c_s\Theta_{3s} F_{5/3}^{(0)}(I_\tau,0,0)\,\rho_0^{8/3} + \frac{3}{80}c_s\,(\Theta_{3s} - 2\Theta_{3v})\,I_\tau F_{5/3}^{(\tau)}(I_\tau,0,0)\,\rho_0^{8/3} \\ &+ \frac{3}{80}c_s\Theta'_{3v}\,I_\tau\left(1-I_\tau^2\right)F_{2/3}^{(\tau)}(I_\tau,0,0)\,\rho_0^{8/3}\quad . \end{aligned} \tag{4.25}$$

For $I_\tau = 0$ a saturation point can be found as the solution of $\dfrac{\partial P}{\partial \rho} = 0$. However, such a saturation point no longer exists beyond a certain value of the isospin asymmetry $0 < I_{\tau,crit} \leq 1$, see Fig. 4.1. This critical point is obtained when the first and the second derivative of the pressure cancel, see Appendix B.4.2 and Appendix C.4.2.
The symmetry energy is the analog of the incompressibility K_∞ but with respect to the isospin excess. The latter gives the stiffness of the EOS around the saturation point with respect to a change of the density while the former provides the stiffness of the EOS with respect to a non-zero isospin excess I_τ. It has to be positive for the saturation point of SNM to be stable. The symmetry energy a_τ is obtained as the second derivative of the energy per particle with respect to I_τ, $S \equiv \dfrac{1}{2}\dfrac{\partial^2 E/A}{\partial I_\tau^2}$ computed at $I_\tau = 0$

$$\begin{aligned} a_\tau \equiv & S\Big|_{I_\tau=0} \\ = & \frac{1}{3}\frac{\hbar^2}{2m}c_s\rho_0^{2/3} - \frac{1}{8}t_0\,(1+2x_0)\,\rho_0 - \frac{3}{16}u_0\,\rho_0^2 + \frac{1}{24}c_s\,(2\Theta_s - 3\Theta_v)\,\rho_0^{5/3} \\ & + \frac{1}{24}c_s\,(2\Theta_{3s} - 3\Theta_{3v})\,\rho_0^{8/3} - \frac{1}{40}c_s\,\Theta'_{3v}\rho_0^{8/3}\quad . \end{aligned} \tag{4.26}$$

Two more properties of asymmetric nuclear matter can be related to the difference between neutron and proton radius [109], i.e. the skin thickness, in asymmetric heavy nuclei. Those are the density-symmetry coefficient L

$$\begin{aligned} L \equiv & 3\rho \frac{\partial S}{\partial \rho}\Big|_{I_\tau=0} \\ = & \frac{2}{3}\frac{\hbar^2}{2m} c_s \rho_0^{2/3} - \frac{3}{8} t_0 (1+2x_0)\rho_0 - \frac{9}{8} u_0 \rho_0^2 + \frac{5}{24} c_s (2\Theta_s - 3\Theta_v)\rho_0^{5/3} \\ & + \frac{1}{3} c_s (2\Theta_{3s} - 3\Theta_{3v})\rho_0^{8/3} + \frac{1}{5} c_s \Theta'_{3v} \rho_0^{8/3} \quad , \end{aligned} \tag{4.27}$$

and the symmetry compressibility

$$\begin{aligned} K_{sym} \equiv & 9\rho^2 \frac{\partial^2 S}{\partial \rho^2}\Big|_{I_\tau=0,\rho=\rho_0} \\ = & -\frac{2}{3}\frac{\hbar^2}{2m} c_s \rho_0^{2/3} - \frac{27}{8} u_0 \rho_0^2 + \frac{5}{12} c_s (2\Theta_s - 3\Theta_v)\rho_0^{5/3} \\ & + \frac{5}{3} c_s (2\Theta_{3s} - 3\Theta_{3v})\rho_0^{8/3} + c_s \Theta'_{3v} \rho_0^{8/3} \quad . \end{aligned} \tag{4.28}$$

4.2.3 Pure neutron matter (PNM)

For $I_\tau = 1$, infinite nuclear matter is composed uniquely of neutrons. The EOS reads

$$\frac{E}{A} = \frac{3}{5}\frac{\hbar^2}{2m} c_n \rho_0^{2/3} + \frac{1}{4} t_0 (1-x_0)\rho_0 + \frac{3}{40} c_n (\Theta_s - \Theta_v)\rho_0^{5/3} + \frac{3}{40} c_n (\Theta_{3s} - \Theta_{3v})\rho_0^{8/3} \quad . \tag{4.29}$$

One can also compute proton and neutron effective masses in neutron matter, using Eq. 4.23

$$\left(\frac{m}{m^*}\right)_n = \frac{2m}{\hbar^2}\frac{\partial \mathcal{E}}{\partial \tau_n} = 1 + \frac{1}{8}\frac{2m}{\hbar^2}\left[\Big(\Theta_s - \Theta_v\Big)\rho_0 + \Big(\Theta_{3s} - \Theta_{3v}\Big)\rho_0^2\right] \quad , \tag{4.30a}$$

$$\left(\frac{m}{m^*}\right)_p = \frac{2m}{\hbar^2}\frac{\partial \mathcal{E}}{\partial \tau_p} = 1 + \frac{1}{8}\frac{2m}{\hbar^2}\left[\Theta_v \rho_0 + \left(\Theta_{3v} + \Theta'_{3v}\right)\rho_0^2\right] \quad . \tag{4.30b}$$

4.2.4 Spin-isospin polarized nuclear matter (PANM)

The general case where I_σ, I_τ and $I_{\sigma\tau}$ are not equal to zero, corresponds to the spin-isospin polarized nuclear matter. The corresponding EOS is a function of more combinations of Skyrme parameters. Consequently, it has not been derived in terms of Θ combinations and the result in terms of functional coefficients can be found in Appendix B.4.4 and Appendix C.4.4.

4.3 Landau parameters

4.3.1 Introduction

Landau parameters are interesting quantities to compute for different reasons.

– It exists two sum rules that Landau parameters have to fulfill in order for the Pauli principle to be valid [110]. These sum rules have never been used to constrain EDF to be self-interaction free. It might thus be of interest to constrain parameters of the EDF, when the latter does not strictly derive from a pseudo-potential, to respect those two sum rules. In the present case where the EDF does derive from a pseudo-potential the two sum rules have to be analytically respected.

Sum rules can also be derived from the antisymmetry property of the scattering amplitude, which is calculated from the residual interaction. The antisymmetry of the residual interaction, to which Landau parameters are related, does not however ensure the antisymmetry of the observable scattering amplitude [111].

– Four of the Landau parameters, F_0, F_0', G_0 and G_0' are also related to the stiffness, i.e. second derivatives of the EOS with respect to density, isospin, spin and spin-isospin fluctuations around the saturation point [107]

$$K_\infty = 6\frac{\hbar^2 k_F^2}{2m_0^*}(1+F_0) \quad , \quad a_\tau = \frac{1}{3}\frac{\hbar^2 k_F^2}{2m_0^*}(1+F_0') \ , \tag{4.31a}$$

$$a_\sigma = \frac{1}{3}\frac{\hbar^2 k_F^2}{2m_0^*}(1+G_0) \quad , \quad a_{\sigma\tau} = \frac{1}{3}\frac{\hbar^2 k_F^2}{2m_0^*}(1+G_0') \ . \tag{4.31b}$$

For the EOS of SNM to have a stable minimum, all such second derivatives have to be greater than zero, such that F_0, F_0', G_0 and G_0' have to be greater than -1. Similarly the four others Landau parameters, F_1, F_1', G_1 and G_1' are related to the four effective masses characterizing nucleons in the four possible spin-isospin states

$$m_0^* = m(1+\frac{1}{3}F_1) \quad , \quad m_\tau^* = m(1+\frac{1}{3}F_1') \ , \tag{4.32a}$$

$$m_\sigma^* = m(1+\frac{1}{3}G_1) \quad , \quad m_{\sigma\tau}^* = m(1+\frac{1}{3}G_1') \ . \tag{4.32b}$$

Again, F_1, F_1', G_1 and G_1' have to be greater than -3 in order to forbid negative effective masses. Eventually, stability conditions exist for all Landau parameters that read

$$F_l > -(2l+1) \ , \ F_l' > -(2l+1) \ , \ G_l > -(2l+1) \ , \ G_l' > -(2l+1) \ . \tag{4.33}$$

4.3.2 Definition

Landau parameters are calculated via the spin-isospin parts of the residual interaction in infinite nuclear matter. The residual particle-hole interaction is defined in general through

$$V_{ij}^{\rm res} = \langle \vec{r}_i'\sigma_i' q_i, \vec{r}_j'\sigma_j' q_j | V^{\rm res} | \vec{r}_i\sigma_i q_i, \vec{r}_j\sigma_j q_j \rangle \equiv \frac{\partial^2 \mathcal{E}}{\partial\rho_{q_j}(\vec{r}_j'\sigma_j', \vec{r}_j\sigma_j)\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} \ , \tag{4.34}$$

and can be written in infinite nuclear matter, for momenta lying on the Fermi surface, as

$$V_{ij}^{\rm res} = N_0^{-1}\sum_l \left[F_l + F_l' \ \tau_i\circ\tau_j + G_l \ \vec{\sigma}_i\cdot\vec{\sigma}_j + G_l' \ \vec{\sigma}_i\cdot\vec{\sigma}_j \ \tau_i\circ\tau_j\right] P_l(\cos\theta) \ , \tag{4.35}$$

where coefficients F_l, F_l', G_l and G_l' are Landau parameters, $N_0 \equiv \dfrac{2m_0^*}{\pi^2\hbar^2}k_F$ is a normalization factor and θ is an angle defined using the incoming $\vec{p}$ and outcoming $\vec{p}'$ momenta of the two interacting particles. Those momenta are re-expressed using transfer momentum $\vec{q}$ coming from incoming and outcoming relative momenta

$$\vec{k} = \frac{1}{2}(\vec{p}_i - \vec{p}_j) \quad , \quad \vec{k}' = \frac{1}{2}(\vec{p}_i' - \vec{p}_j') \ , \tag{4.36}$$

thanks to $\vec{q} = \vec{k}' - \vec{k}$. Thus,

$$\vec{p}_i = \vec{q}_1 \quad , \quad \vec{p}_j = \vec{q}_2 + \vec{q} \ , \tag{4.37a}$$

$$\vec{p}_j' = \vec{q}_2 \quad , \quad \vec{p}_i' = \vec{q}_1 + \vec{q} \ , \tag{4.37b}$$

and eventually $\vec{q}_1\cdot\vec{q}_2 = q_1\,q_2\cos\theta$. All momenta have magnitude k_F.

4.3.3 Residual interaction

To make explicit the separation of the residual interaction in its four spin-isospin parts one has to use the following chain rule

$$\frac{\partial^2\mathcal{E}}{\partial\rho_{q_j}(\vec{r}'_j\sigma'_j,\vec{r}_j\sigma_j)\partial\rho_{q_i}(\vec{r}'_i\sigma'_i,\vec{r}_i\sigma_i)} = \sum_{\mathcal{Q}_a}\sum_{\mathcal{Q}_b}\frac{\partial^2\mathcal{E}}{\partial\mathcal{Q}_a\partial\mathcal{Q}_b}\frac{\partial\mathcal{Q}_a}{\partial\rho_{q_j}(\vec{r}'_j\sigma'_j,\vec{r}_j\sigma_j)}\frac{\partial\mathcal{Q}_b}{\partial\rho_{q_i}(\vec{r}'_i\sigma'_i,\vec{r}_i\sigma_i)} \quad , \tag{4.38}$$

where $\mathcal{Q}_i$ represents any quasi-local spin-isospin density and their derivatives

$$\mathcal{Q}_i = \left\{\rho_0,\rho_1,\vec{s}_0,\vec{s}_1,\vec{\nabla}\rho_0,\vec{\nabla}\rho_1,\nabla_\mu s_{0,\nu},\nabla_\mu s_{1,\nu},\tau_0,\tau_1,\vec{T}_0,\vec{T}_1,\vec{j}_0,\vec{j}_1,J_{0,\mu\nu},J_{1,\mu\nu}\right\} \quad , \tag{4.39}$$

such that the sums run over all possible pairs of them.

4.3.4 Infinite nuclear matter

The number of derivatives to perform in Eq. 4.38 is large and equal to the binomial coefficient $\binom{16}{2}$. For the bilinear functional, most of them cancel because each term of the functional is scalar-isoscalar and contains up to two gradients, e.g. the bilinear functional term $\rho_0\vec{s}_0$ does not exist such that the second derivative of the functional with respect to ρ_0 and $\vec{s}_0$ is zero. As for the trilinear functional the presence of a third density allows for many more non-zero second derivatives. However, knowing that the residual interaction will be used in SNM to obtain the Landau parameters, one can anticipate that many second-order derivatives will be zero. Indeed, in infinite nuclear matter the only two non-zero densities are ρ_0 and τ_0, such that second derivatives depending on any other density is eventually zero. As a result, non-zero second derivatives are the same for both bilinear and trilinear functionals

$$V_0^{\rho\rho} \equiv \frac{\partial^2\mathcal{E}}{\partial\rho_0\partial\rho_0} \quad , \quad V_1^{\rho\rho} \equiv \frac{\partial^2\mathcal{E}}{\partial\rho_1\partial\rho_1} \quad , \tag{4.40a}$$

$$V_0^{ss} \equiv \frac{\partial^2\mathcal{E}}{\partial s_0\partial s_0} \quad , \quad V_1^{ss} \equiv \frac{\partial^2\mathcal{E}}{\partial s_1\partial s_1} \quad , \tag{4.40b}$$

$$V_0^{\tau\rho} \equiv \frac{\partial^2\mathcal{E}}{\partial\tau_0\partial\rho_0} \quad , \quad V_1^{\tau\rho} \equiv \frac{\partial^2\mathcal{E}}{\partial\tau_1\partial\rho_1} \quad , \tag{4.40c}$$

$$V_0^{Ts} \equiv \frac{\partial^2\mathcal{E}}{\partial T_0\partial s_0} \quad , \quad V_1^{Ts} \equiv \frac{\partial^2\mathcal{E}}{\partial T_1\partial s_1} \quad , \tag{4.40d}$$

$$V_0^{jj} \equiv \frac{\partial^2\mathcal{E}}{\partial j_0\partial j_0} \quad , \quad V_1^{jj} \equiv \frac{\partial^2\mathcal{E}}{\partial j_1\partial j_1} \quad , \tag{4.40e}$$

$$V_0^{JJ} \equiv \frac{\partial^2\mathcal{E}}{\partial J_0\partial J_0} \quad , \quad V_1^{JJ} \equiv \frac{\partial^2\mathcal{E}}{\partial J_1\partial J_1} \quad , \tag{4.40f}$$

$$V_0^{\nabla\rho\nabla\rho} \equiv \frac{\partial^2\mathcal{E}}{\partial\nabla\rho_0\partial\nabla\rho_0} \quad , \quad V_1^{\nabla\rho\nabla\rho} \equiv \frac{\partial^2\mathcal{E}}{\partial\nabla\rho_1\partial\nabla\rho_1} \quad , \tag{4.40g}$$

$$V_0^{\nabla s\nabla s} \equiv \frac{\partial^2\mathcal{E}}{\partial\nabla s_0\partial\nabla s_0} \quad , \quad V_1^{\nabla s\nabla s} \equiv \frac{\partial^2\mathcal{E}}{\partial\nabla s_1\partial\nabla s_1} \quad . \tag{4.40h}$$

These quantities are provided by the code in Appendix B.4.5 and Appendix C.4.5. The next step is to compute the derivatives of the quasi-local densities with respect to the non local density

$\rho_q(\vec{r}'\sigma', \vec{r}\,\sigma)$. First let us define

$$V_{ij}^{\mathcal{Q}_a\mathcal{Q}_a} \equiv \frac{\partial^2\mathcal{E}}{\partial\mathcal{Q}_a\partial\mathcal{Q}_a}\frac{\partial\mathcal{Q}_a}{\partial\rho_{q_j}(\vec{r}_j'\sigma_j', \vec{r}_j\sigma_j)}\frac{\partial\mathcal{Q}_a}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} \quad , \tag{4.41a}$$

$$\begin{aligned} V_{ij}^{\mathcal{Q}_a\mathcal{Q}_b} \equiv & \frac{\partial^2\mathcal{E}}{\partial\mathcal{Q}_a\partial\mathcal{Q}_b}\frac{\partial\mathcal{Q}_a}{\partial\rho_{q_j}(\vec{r}_j'\sigma_j', \vec{r}_j\sigma_j)}\frac{\partial\mathcal{Q}_b}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} \\ & + \frac{\partial^2\mathcal{E}}{\partial\mathcal{Q}_a\partial\mathcal{Q}_b}\frac{\partial\mathcal{Q}_b}{\partial\rho_{q_j}(\vec{r}_j'\sigma_j', \vec{r}_j\sigma_j)}\frac{\partial\mathcal{Q}_a}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} \quad , \end{aligned} \tag{4.41b}$$

to re-expressed the residual interaction in infinite nuclear matter as

$$\begin{aligned} V_{ij}^{\text{res}} = & \sum_{\mathcal{Q}_a} V_{ij}^{\mathcal{Q}_a\mathcal{Q}_a} + \sum_{\mathcal{Q}_a}\sum_{\mathcal{Q}_b\neq\mathcal{Q}_a} V_{ij}^{\mathcal{Q}_a\mathcal{Q}_b} \\ = & + V_{ij}^{\rho_0\rho_0} + V_{ij}^{\rho_1\rho_1} + V_{ij}^{s_0s_0} + V_{ij}^{s_1s_1} \\ & + V_{ij}^{\rho_0\tau_0} + V_{ij}^{\rho_1\tau_1} + V_{ij}^{s_0T_0} + V_{ij}^{s_1T_1} \\ & + V_{ij}^{j_0j_0} + V_{ij}^{j_1j_1} + V_{ij}^{J_0J_0} + V_{ij}^{J_1J_1} \\ & + V_{ij}^{\nabla\rho_0\nabla\rho_0} + V_{ij}^{\nabla\rho_1\nabla\rho_1} + V_{ij}^{\nabla s_0\nabla s_0} + V_{ij}^{\nabla s_1\nabla s_1} \quad , \end{aligned} \tag{4.42}$$

where each line of Eq. 4.42 corresponds to a different gradient structure and each column to a different spin-isospin structure. Using Eq. 3.14, one has

$$\frac{\partial\rho_0}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = 1 \quad , \quad \frac{\partial\rho_1}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = \tau_i \tag{4.43a}$$

$$\frac{\partial\vec{s}_0}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = \vec{\sigma}_i \quad , \quad \frac{\partial\vec{s}_1}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = \vec{\sigma}_i\tau_i \tag{4.43b}$$

$$\frac{\partial\tau_0}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = \vec{\nabla}_i'\cdot\vec{\nabla}_i \quad , \quad \frac{\partial\tau_1}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = \vec{\nabla}_i'\cdot\vec{\nabla}_i\,\tau_i \tag{4.43c}$$

$$\frac{\partial\vec{T}_0}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = \vec{\nabla}_i'\cdot\vec{\nabla}_i\,\vec{\sigma}_i \quad , \quad \frac{\partial\vec{T}_1}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = \vec{\nabla}_i'\cdot\vec{\nabla}_i\,\vec{\sigma}_i\tau_i \tag{4.43d}$$

$$\frac{\partial\vec{j}_0}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = \frac{i}{2}\left(\vec{\nabla}_i' - \vec{\nabla}_i\right) \quad , \quad \frac{\partial\vec{j}_1}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = \frac{i}{2}\left(\vec{\nabla}_i' - \vec{\nabla}_i\right)\tau_i \tag{4.43e}$$

$$\frac{\partial J_{0,\mu\nu}}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = \frac{i}{2}\left(\vec{\nabla}_i' - \vec{\nabla}_i\right)\vec{\sigma}_i \quad , \quad \frac{\partial J_{1,\mu\nu}}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = \frac{i}{2}\left(\vec{\nabla}_i' - \vec{\nabla}_i\right)\vec{\sigma}_i\tau_i \tag{4.43f}$$

$$\frac{\partial\vec{\nabla}\rho_0}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = \left(\vec{\nabla}_i' + \vec{\nabla}_i\right) \quad , \quad \frac{\partial\vec{\nabla}\rho_1}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = \left(\vec{\nabla}_i' + \vec{\nabla}_i\right)\tau_i \tag{4.43g}$$

$$\frac{\partial\nabla_\mu s_{0,\nu}}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = \left(\vec{\nabla}_i' + \vec{\nabla}_i\right)\vec{\sigma}_i \quad , \quad \frac{\partial\nabla_\mu s_{1,\nu}}{\partial\rho_{q_i}(\vec{r}_i'\sigma_i', \vec{r}_i\sigma_i)} = \left(\vec{\nabla}_i' + \vec{\nabla}_i\right)\vec{\sigma}_i\tau_i \quad . \tag{4.43h}$$

Eventually, contributions to Eq. 4.42 are

$$V_{ij}^{\rho_0\rho_0} = V_0^{\rho\rho} \quad , \tag{4.44a}$$

$$V_{ij}^{\rho_1\rho_1} = V_1^{\rho\rho}\;\tau_i\circ\tau_j \quad , \tag{4.44b}$$

$$V_{ij}^{s_0s_0} = V_0^{ss}\;\vec{\sigma}_i\cdot\vec{\sigma}_j \quad , \tag{4.44c}$$

$$V_{ij}^{s_1s_1} = V_1^{ss}\;\tau_i\circ\tau_j\,\vec{\sigma}_i\cdot\vec{\sigma}_j \quad , \tag{4.44d}$$

$$V_{ij}^{\rho_0\tau_0} = V_0^{\rho\tau}\left(\vec{\nabla}_i'\cdot\vec{\nabla}_i + \vec{\nabla}_j'\cdot\vec{\nabla}_j\right) \quad , \tag{4.44e}$$

$$V_{ij}^{\rho_1\tau_1} = V_1^{\rho\tau}\;\tau_i\circ\tau_j\left(\vec{\nabla}_i'\cdot\vec{\nabla}_i + \vec{\nabla}_j'\cdot\vec{\nabla}_j\right) \quad , \tag{4.44f}$$

$$V_{ij}^{s_0T_0} = V_0^{sT}\ \vec{\sigma}_i\cdot\vec{\sigma}_j\Big(\vec{\nabla}_i'\cdot\vec{\nabla}_i+\vec{\nabla}_j'\cdot\vec{\nabla}_j\Big)\ , \tag{4.44g}$$

$$V_{ij}^{s_1T_1} = V_1^{sT}\ \tau_i\circ\tau_j\,\vec{\sigma}_i\cdot\vec{\sigma}_j\Big(\vec{\nabla}_i'\cdot\vec{\nabla}_i+\vec{\nabla}_j'\cdot\vec{\nabla}_j\Big)\ , \tag{4.44h}$$

$$V_{ij}^{j_0j_0} = V_0^{jj}\ \frac{-1}{4}\Big(\vec{\nabla}_i'-\vec{\nabla}_i\Big)\cdot\Big(\vec{\nabla}_j'-\vec{\nabla}_j\Big)\ , \tag{4.44i}$$

$$V_{ij}^{j_1j_1} = V_1^{jj}\ \tau_i\circ\tau_j\frac{-1}{4}\Big(\vec{\nabla}_i'-\vec{\nabla}_i\Big)\cdot\Big(\vec{\nabla}_j'-\vec{\nabla}_j\Big)\ , \tag{4.44j}$$

$$V_{ij}^{J_0J_0} = V_0^{JJ}\ \vec{\sigma}_i\cdot\vec{\sigma}_j\frac{-1}{4}\Big(\vec{\nabla}_i'-\vec{\nabla}_i\Big)\cdot\Big(\vec{\nabla}_j'-\vec{\nabla}_j\Big)\ , \tag{4.44k}$$

$$V_{ij}^{J_1J_1} = V_1^{JJ}\ \tau_i\circ\tau_j\,\vec{\sigma}_i\cdot\vec{\sigma}_j\frac{-1}{4}\Big(\vec{\nabla}_i'-\vec{\nabla}_i\Big)\cdot\Big(\vec{\nabla}_j'-\vec{\nabla}_j\Big)\ , \tag{4.44l}$$

$$V_{ij}^{\nabla\rho_0\nabla\rho_0} = V_0^{\nabla\rho\nabla\rho}\ \Big(\vec{\nabla}_i'+\vec{\nabla}_i\Big)\cdot\Big(\vec{\nabla}_j'+\vec{\nabla}_j\Big)\ , \tag{4.44m}$$

$$V_{ij}^{\nabla\rho_1\nabla\rho_1} = V_1^{\nabla\rho\nabla\rho}\ \tau_i\circ\tau_j\Big(\vec{\nabla}_i'+\vec{\nabla}_i\Big)\cdot\Big(\vec{\nabla}_j'+\vec{\nabla}_j\Big)\ , \tag{4.44n}$$

$$V_{ij}^{\nabla s_0\nabla s_0} = V_0^{\nabla s\nabla s}\ \vec{\sigma}_i\cdot\vec{\sigma}_j\Big(\vec{\nabla}_i'+\vec{\nabla}_i\Big)\cdot\Big(\vec{\nabla}_j'+\vec{\nabla}_j\Big)\ , \tag{4.44o}$$

$$V_{ij}^{\nabla s_1\nabla s_1} = V_1^{\nabla s\nabla s}\ \tau_i\circ\tau_j\,\vec{\sigma}_i\cdot\vec{\sigma}_j\Big(\vec{\nabla}_i'+\vec{\nabla}_i\Big)\cdot\Big(\vec{\nabla}_j'+\vec{\nabla}_j\Big)\ , \tag{4.44p}$$

4.3.5 Landau parameters

To evaluate the relation between gradients in Eq. 4.44 and angle θ in Eq. 4.35 one has to express gradients in terms of momenta (Eq. 4.37) using

$$\vec{k}_j = -i\vec{\nabla}_j \quad , \quad \vec{k}_j' = i\vec{\nabla}_j' \quad , \quad i\vec{k}_j = \vec{\nabla}_j \quad , \quad -i\vec{k}_j' = \vec{\nabla}_j'\ . \tag{4.45}$$

The various gradient structures read thus

$$\begin{aligned}\Big(\vec{\nabla}_i'\cdot\vec{\nabla}_i+\vec{\nabla}_j'\cdot\vec{\nabla}_j\Big) &= \Big(\vec{k}_i'\cdot\vec{k}_i+\vec{k}_j'\cdot\vec{k}_j\Big)\\ &= \Big(\vec{q}_1^{\,2}+\vec{q}\cdot\vec{q}_1+\vec{q}_2^{\,2}+\vec{q}\cdot\vec{q}_2\Big)\ , \qquad (4.46a)\\ \Big(\vec{\nabla}_i'-\vec{\nabla}_i\Big)\cdot\Big(\vec{\nabla}_j'-\vec{\nabla}_j\Big) &= -\Big(\vec{k}_i'+\vec{k}_i\Big)\cdot\Big(\vec{k}_j'+\vec{k}_j\Big)\\ &= -2\Big(2\vec{q}_1\cdot\vec{q}_2+\frac{1}{2}\vec{q}^{\,2}+\vec{q}_1\cdot\vec{q}+\vec{q}_2\cdot\vec{q}\Big)\ , \qquad (4.46b)\\ \Big(\vec{\nabla}_i'+\vec{\nabla}_i\Big)\cdot\Big(\vec{\nabla}_j'+\vec{\nabla}_j\Big) &= -\Big(\vec{k}_i'-\vec{k}_i\Big)\cdot\Big(\vec{k}_j'-\vec{k}_j\Big)\\ &= \vec{q}^{\,2}\ . \qquad (4.46c)\end{aligned}$$

Landau parameters are obtained taking the limit $q\to 0$ where the interaction only acts at the Fermi surface. In this limit $q_1 = q_2 = k_F$, $\vec{q}_1\cdot\vec{q}_2 = k_F^2\cos\theta$, and

$$\Big(\vec{\nabla}_i'\cdot\vec{\nabla}_i+\vec{\nabla}_j'\cdot\vec{\nabla}_j\Big) = 2k_F^2\ , \tag{4.47a}$$

$$\Big(\vec{\nabla}_i'-\vec{\nabla}_i\Big)\cdot\Big(\vec{\nabla}_j'-\vec{\nabla}_j\Big) = -4k_F^2\cos\theta\ , \tag{4.47b}$$

$$\Big(\vec{\nabla}_i'+\vec{\nabla}_i\Big)\cdot\Big(\vec{\nabla}_j'+\vec{\nabla}_j\Big) = 0\ , \tag{4.47c}$$

such that using Eq. 4.35 one finds contributions to $l = 0$ and $l = 1$ only according to

$$\begin{aligned}
F_0 =& N_0\Big(V_0^{\rho\rho} + 2k_F^2 V_0^{\rho\tau}\Big) \\
=& N_0\Big(2A_0^\rho \ + 2A_0^\tau \ k_F^2 + 6B_0^\rho \ \rho_0 + 2B_0^\tau \ \tau_0 + 4B_0^\tau \ k_F^2\rho_0\Big) \ , && \text{(4.48a)} \\
F_0' =& N_0\Big(V_1^{\rho\rho} + 2k_F^2 V_1^{\rho\tau}\Big) \\
=& N_0\Big(2A_1^\rho \ + 2A_1^\tau \ k_F^2 + 2B_1^\rho \ \rho_0 + 2B_{10}^\tau \ \tau_0 + 2B_1^\tau \ k_F^2\rho_0\Big) \ , && \text{(4.48b)} \\
G_0 =& N_0\Big(V_0^{ss} + 2k_F^2 V_0^{sT}\Big) \\
=& N_0\Big(2A_0^s \ + 2A_0^T \ k_F^2 + 2B_0^s \ \rho_0 + 2B_0^{\tau s} \ \tau_0 + 2B_0^T \ k_F^2\rho_0\Big) \ , && \text{(4.48c)} \\
G_0' =& N_0\Big(V_1^{ss} + 2k_F^2 V_1^{sT}\Big) \\
=& N_0\Big(2A_1^s \ + 2A_1^T \ k_F^2 + 2B_1^s \ \rho_0 + 2B_{10}^{\tau s} \ \tau_0 + 2B_1^T \ k_F^2\rho_0\Big) \ , && \text{(4.48d)} \\
F_1 =& N_0\Big(k_F^2 V_0^{jj}\Big) \\
=& N_0\Big(2A_0^j \ k_F^2 + 2B_0^j \ k_F^2\rho_0\Big) \ , && \text{(4.48e)} \\
F_1' =& N_0\Big(k_F^2 V_1^{jj}\Big) \\
=& N_0\Big(2A_1^j \ k_F^2 + 2B_1^j \ k_F^2\rho_0\Big) \ , && \text{(4.48f)} \\
G_1 =& N_0\Big(k_F^2 V_0^{JJ}\Big) \\
=& N_0\Big(2A_0^J \ k_F^2 + 2B_0^J \ k_F^2\rho_0\Big) \ , && \text{(4.48g)} \\
G_1' =& N_0\Big(k_F^2 V_1^{JJ}\Big) \\
=& N_0\Big(2A_1^J \ k_F^2 + 2B_1^J \ k_F^2\rho_0\Big) \ . && \text{(4.48h)}
\end{aligned}$$

The final result is reproduced in terms of Skyrme parameters in Tab. {4.1}, after having used Eq. 4.11b to replace τ_0 in terms of ρ_0.

4.3.6 Sum rules on Landau parameters

The EDF from which the residual interaction derives, has been constructed from an anti-symmetrized vertex, such that all particle permutations have been taken into account to ensure Pauli-principle. In case the antisymmetrized vertex is a two-body pseudo-potential multiplied by the two-body antisymmetrizer, taking two derivatives of the EDF with respect to non-local densities gives back the original antisymmetrized vertex. In case a two- plus three-body antisymmetrized pseudo-potential has been used, the residual interaction remains a two-body antisymmetrized vertex. Consequently, the exclusion principle demands that residual interaction 4.35 is antisymmetric under the exchange of incoming or outgoing particles, which is similar to asking the two-body state to respect Eq. 3.33. Using Eq. 4.35 with $\vec{p}_i = \vec{p}_j$, such that in INM $\theta = 0$, and requiring the latter property to hold for each spin-isospin channel, one obtains two sum rules

$$\begin{aligned}
\sum_l F_l + F_l' + G_l + G_l' =& 0 && \text{(4.49a)} \\
\sum_l F_l - 3F_l' - 3G_l + 9G_l' =& 0 \ , && \text{(4.49b)}
\end{aligned}$$

	f_0	f'_0	g_0	g'_0	f_1	f'_1	g_1	g'_1
t_0	$\frac{3}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$+0$	$+0$	$+0$	$+0$
t_0x_0	$+0$	$-\frac{1}{2}$	$\frac{1}{2}$	$+0$	$+0$	$+0$	$+0$	$+0$
$t_1k_F^2$	$\frac{3}{8}$	$-\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{3}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$
$t_1x_1k_F^2$	$+0$	$-\frac{1}{4}$	$\frac{1}{4}$	$+0$	$+0$	$\frac{1}{4}$	$-\frac{1}{4}$	$+0$
$t_2k_F^2$	$\frac{5}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$-\frac{5}{8}$	$-\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{1}{8}$
$t_2x_2k_F^2$	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{8}$	$-\frac{1}{2}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{8}$
$u_0\rho_0$	$\frac{9}{8}$	$-\frac{3}{8}$	$-\frac{3}{8}$	$-\frac{3}{8}$	$+0$	$+0$	$+0$	$+0$
$u_1\rho_0k_F^2$	$\frac{39}{80}$	$-\frac{13}{80}$	$-\frac{13}{80}$	$-\frac{13}{80}$	$-\frac{3}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$
$u_1y_1\rho_0k_F^2$	$+0$	$-\frac{1}{40}$	$\frac{1}{40}$	$+0$	$+0$	$\frac{1}{8}$	$-\frac{1}{8}$	$+0$
$u_2\rho_0k_F^2$	$\frac{39}{32}$	$-\frac{1}{32}$	$-\frac{1}{32}$	$-\frac{1}{32}$	$-\frac{15}{32}$	$-\frac{7}{32}$	$-\frac{7}{32}$	$-\frac{7}{32}$
$u_2y_{21}\rho_0k_F^2$	$\frac{39}{40}$	$\frac{1}{20}$	$\frac{1}{20}$	$-\frac{3}{40}$	$-\frac{3}{8}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{8}$
$u_2y_{22}\rho_0k_F^2$	$\frac{39}{80}$	$-\frac{31}{80}$	$\frac{35}{80}$	$-\frac{3}{80}$	$-\frac{3}{16}$	$-\frac{5}{16}$	$\frac{1}{16}$	$-\frac{1}{16}$

Table 4.1: Landau parameters expressed in terms of Skyrme parameters. Coefficients f_l, f'_l, g_l and g'_l are nothing but Landau parameters F_l, F'_l, G_l and G'_l divided by the normalization factor N_0.

where we have used that $P_l(1) = 1$. Eq. 4.49a stands for the two-body spin and isospin-triplet $S = T = 1$, for which $\vec{\sigma}_i \cdot \vec{\sigma}_j = \tau_i \circ \tau_j = 1$, while Eq. 4.49b stands for the two-body spin and isospin-singlet $S = T = 0$, for which $\vec{\sigma}_i \cdot \vec{\sigma}_j = \tau_i \circ \tau_j = -3$. In both cases the relative orbital angular-momentum of the two-body state is odd to fulfill the exclusion principle as the contribution for $\vec{p}_i = \vec{p}_j$ to this channel vanishes.

Sum rules 4.49 are fulfilled for Landau parameters derived from the two- plus three-body pseudo-potential, see Tab. {4.1}. It is a check that the derivations of the EDF and of the residual interaction are correct. In case the EDF derives from a two-body density-dependent pseudo-potential, such that antisymmetry is not respected, sum rules 4.49 are not necessarily fulfilled. This can be understood by separating the trilinear functional according to Eq. 3.93. Looking at Tab. {4.2}, one can see that Eq. 4.49 are not respected if using $\mathcal{E}^{\rho\rho[\rho_0]}$ alone. The conclusion drawn in Sec. 3.4.4.2 stands, i.e. the Pauli principle is fulfilled not only thanks to the interdependence of the functional coefficients entering $\mathcal{E}^{\rho\rho[\rho_0]}$, but also thanks to the presence of $\mathcal{E}^{\rho\rho\rho}_{\text{extra}}$.

4.3.7 Sum rules on particle-hole scattering amplitude

The residual interaction, also called particle-hole interaction, is not a physically observable object in contrast to the scattering amplitude associated to the motion of a particle-hole pair [111]. The latter is related to the former through an integral equation, such that the particle-hole interaction can be seen as the irreducible vertex and the scattering amplitude as the total vertex. In a perturbative approach the scattering amplitude has by definition the property of antisymmetry with respect to the exchange of the two incoming our outgoing fermions [111, 112]. However, the antisymmetrized character of the residual interaction does not guarantee the antisymmetry of the scattering amplitude, frequently broken in practice. In the iteration process of the integral equation, reducible diagrams might appear without their Pauli principle counterparts [111, 113]. It is due to the lack of complexity of the irreducible residual interaction deriving, e.g. from the EDF. Inserting density dependencies in the pseudo-potential has allowed

	f_0	f'_0	g_0	g'_0	f_1	f'_1	g_1	g'_1
	$\mathcal{E}^{\rho\rho[\rho_0]}$							
$u_0\rho_0$	$\frac{9}{8}$	$-\frac{3}{8}$	$-\frac{3}{8}$	$-\frac{3}{8}$	$+0$	$+0$	$+0$	$+0$
$u_1\rho_0 k_F^2$	$\frac{39}{80}$	$-\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{3}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$
$u_1y_1\rho_0 k_F^2$	$+0$	$-\frac{1}{16}$	$\frac{1}{16}$	$+0$	$+0$	$\frac{1}{8}$	$-\frac{1}{8}$	$+0$
$u_2\rho_0 k_F^2$	$\frac{39}{32}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$-\frac{15}{32}$	$-\frac{7}{32}$	$-\frac{7}{32}$	$-\frac{7}{32}$
$u_2y_{21}\rho_0 k_F^2$	$\frac{39}{40}$	$\frac{1}{8}$	$\frac{1}{8}$	$+0$	$-\frac{3}{8}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{8}$
$u_2y_{22}\rho_0 k_F^2$	$\frac{39}{80}$	$-\frac{1}{8}$	$\frac{1}{4}$	$+0$	$-\frac{3}{16}$	$-\frac{5}{16}$	$\frac{1}{16}$	$-\frac{1}{16}$
	$\mathcal{E}^{\rho\rho\rho}_{\text{extra}}$							
$u_1\rho_0 k_F^2$	$+0$	$-\frac{3}{80}$	$-\frac{3}{80}$	$-\frac{3}{80}$	$+0$	$+0$	$+0$	$+0$
$u_1y_1\rho_0 k_F^2$	$+0$	$\frac{3}{80}$	$-\frac{3}{80}$	$+0$	$+0$	$+0$	$+0$	$+0$
$u_2\rho_0 k_F^2$	$+0$	$-\frac{3}{32}$	$-\frac{3}{32}$	$-\frac{3}{32}$	$+0$	$+0$	$+0$	$+0$
$u_2y_{21}\rho_0 k_F^2$	$+0$	$-\frac{3}{40}$	$-\frac{3}{40}$	$-\frac{3}{40}$	$+0$	$+0$	$+0$	$+0$
$u_2y_{22}\rho_0 k_F^2$	$+0$	$-\frac{21}{80}$	$\frac{15}{80}$	$-\frac{3}{80}$	$+0$	$+0$	$+0$	$+0$

Table 4.2: Landau parameters expressed in terms of three-body Skyrme parameters. Results are separated into the contribution derived from $\mathcal{E}^{\rho\rho[\rho_0]}$, i.e. the part of the trilinear functional obtainable from a two-body density-dependent pseudo-potential, and the contribution derived from the remaining part $\mathcal{E}^{\rho\rho\rho}_{\text{extra}}$ (see Eq. 3.93).

in some case to better account for such Pauli principle counterparts [111]. In this case however, the residual interaction in itself is not antisymmetric anymore, necessarily implying that the energy suffers from self-interaction.
Analog sum-rules to Eq. 4.49 are easily derived to verify the antisymmetry of the scattering amplitude. First, the expansion in Legendre polynomials of the scattering amplitude is given by

$$\Gamma_{ij} \equiv N_0^{-1} \sum_l \left[B_l + C_l\ \tau_i \circ \tau_j + D_l\ \vec{\sigma}_i \cdot \vec{\sigma}_j + E_l\ \vec{\sigma}_i \cdot \vec{\sigma}_j\ \tau_i \circ \tau_j\right] P_l(\cos\theta)\ . \tag{4.50}$$

Knowing the integral equation that relates the scattering amplitude to residual interaction 4.35, one obtains, in abscence of tensor terms, [111, 112, 114]

$$B_l = \frac{F_l}{1+\frac{F_l}{2l+1}}\quad,\quad C_l = \frac{F'_l}{1+\frac{F'_l}{2l+1}}\quad,\quad D_l = \frac{G_l}{1+\frac{G_l}{2l+1}}\quad,\quad E_l = \frac{G'_l}{1+\frac{G'_l}{2l+1}}\ . \tag{4.51}$$

The same reasoning as used in Sec. 4.3.6 provides sum rules for expansion coefficients of the scattering amplitude

$$\sum_l B_l + C_l + D_l + E_l = 0\ , \tag{4.52a}$$

$$\sum_l B_l - 3C_l - 3D_l + 9E_l = 0\ , \tag{4.52b}$$

which can be rearranged as [114]

$$\sum_l B_l + 3E_l = 0 \ , \tag{4.53a}$$

$$\sum_l \frac{2}{3} B_l + C_l + D_l = 0 \ . \tag{4.53b}$$

In a Born approximation, i.e. when the magnitude of Landau parameters entering Eq. 4.51 are negligible compared to $2l + 1$, Eq. 4.52 gives back Eq. 4.49. However, Landau parameters are not small in nuclear matter, such that physically speaking sum rule 4.49 cannot really be justified starting from the scattering amplitude.

Chapter 5

Optimization procedure

Abstract: The present chapter deals with the optimization procedure of free parameters. First, a study of infinite nuclear matter properties from the newly derived trilinear EDF is performed to significantly constrain the parameter space. The result of this preliminary study is taken into account to establish the actual optimization procedure. In such a procedure, free parameters are adjusted on both infinite nuclear matter and finite nuclei properties.

Contents

5.1 Introduction

In Chap. 3 the analytical form of the Skyrme pseudo-potential has been determined and the energy functional arising from it derived. Such a pseudo-potential depends on a set of parameters that need to be optimized. Traditionally, the quality of the resulting parameterization significantly depends on the fitting procedure, i.e. on the choice of fitted nuclear observables or properties. One can of course greatly benefit from the experience acquired through past studies.

5.1.1 Fitting protocol

The parameters optimization starts with the choice of nuclear properties that you expect to be imperative for your EDF to reproduce, and of those that should play a significant but less crucial role. In other words, one has to determine the weights of each considered property. The fit can in fact be seen as an adjustment of parameters on an infinite number of nuclear properties with weights varying from 0 to infinity. This underlines the first difficulty associated with the determination of quantitative weights based on qualitative arguments, knowing that changing such weights can change significantly the quality of the resulting parameterization. Additionally, the adjustment is a time consuming operation whose cost increases with the number of properties to be adjusted.

The question is thus, which nuclear properties our nuclear pseudo-potential has to be adjusted to, and with which weights, in order to reproduce and predict as many nuclear data as possible? Two types of problem occur.

- First, the number of parameters could be small compared to the number of indispensable properties the EDF should reproduce. The pseudo-potential is likely to be over-constrained in this case such that requiring to better reproduce a given property inevitably deteriorates other features. After years of study it appears that it has been the case for usual quasi bilinear EDFs developed in the past, such that EDF parameterization fitted with a bias towards a particular set of observables have to be used with great care when predicting other types of properties.
- Second, the number of parameters could be large [94]. The main problem may then comes from the time consuming character of the adjustment as well as from the difficulty to find experimental data that can meaningfully constrain all parameters. Usually, one takes into account analytical constraints on the parameters to reduce the size of the allowed space. Such analytical constraints mostly come from infinite nuclear matter properties but are in a limited number, see Chap. 4. Increasing the number of parameters requires the use of more non-analytical constraints such as nuclear masses and radii obtained using time-consuming SR- or MR-EDF codes.

The optimization of the parameters might be more difficult at first for a new form of Skyrme EDF, such as the one used here, given that terms might be correlated with each others through some of the chosen fitted properties. Obtaining the best fit protocol, i.e. the best weights, necessitates to perform extensive trial and error studies in order to understand how terms behave. The present work displays the first step in that direction for the newly developped EDF form.

5.1.2 Least square method

Having selected the properties parameters should be fitted to, a method for the actual optimization is to be chosen. In the present study, the optimization is performed using an analog of the least square method that we briefly explain in the following.
First, consider a model describing a set of nuclear properties e_i, themselves expressed in terms of a set of parameters $\vec{x} = \{x_k\}$ through

$$e_i = f_i(\vec{x}) \ , \tag{5.1}$$

where e_i typically denote actual observables such as ground-state energies and charge radii of a set of nuclei but may also denote a series of infinite nuclear matter properties. In the present study the model is the Skyrme EDF developped in Chap. 3, i.e. parameters $\vec{x}$ are those of the corresponding pseudo-potential.
Parameters $\vec{x}$ are determined by means of a fit of the $f_i(\vec{x})$ on experimental observables or known

infinite nuclear matter properties e_i. For this purpose, the least-square method minimizes a χ^2 deviation measuring the quality of the model, i.e.

$$\chi^2 = \sum_{i=1}^{n_{obs}} \chi_i^2 \qquad \text{with} \qquad \chi_i^2 = \left(\frac{f_i(\vec{x}) - e_i}{\Delta_i} \right)^2 , \tag{5.2}$$

where n_{obs} is the number of selected nuclear properties. The weights Δ_i^{-1} are those discussed above, such that the smaller the weight Δ_i^{-1} the smaller the impact of the associated e_i on the χ^2 minimization, i.e. the larger $f_i(\vec{x}) - e_i$ can be without impacting the χ^2 value.
For potentially accurate models, Δ_i is to be taken as Δe_i defined as the experimental uncertainty associated with the measure of e_i. Otherwise, as in our case, models are not accurate enough and Δ_i is larger than Δe_i and chosen according to our intuition and expertise regarding the accuracy expected from the model. If χ_i^2 is lesser than 1, it means that our model reproduces the experimental value e_i with an uncertainty smaller than Δ_i.
In the present case, the actual χ^2 minimization is performed using a simplex algorithm called Nelder-Mead method [115]. Eventually, the fitting procedure provides us with parameter values $\vec{x}_0$ that minimize the χ^2 deviation, see FIG. 5.1 for a schematic representation. In the example

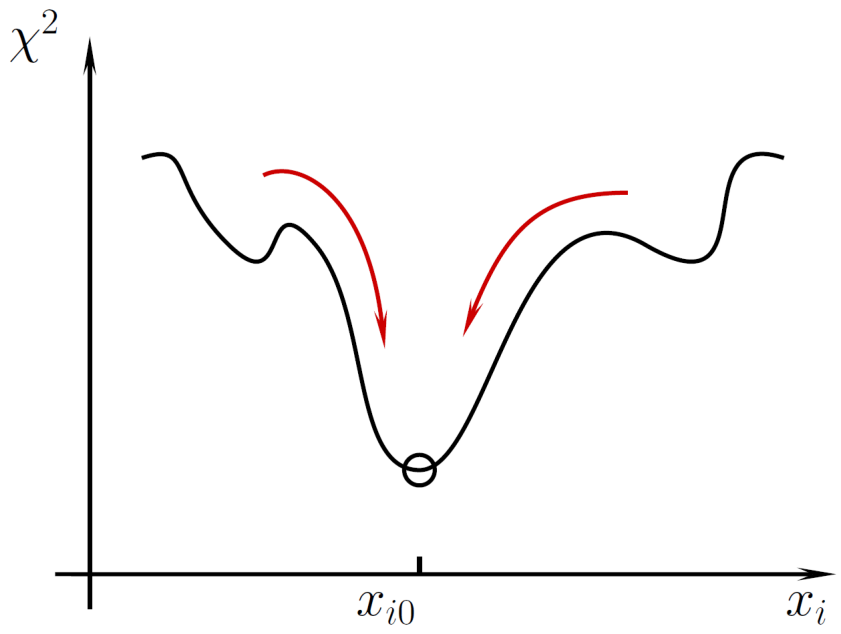

Figure 5.1: Minimization of χ_i^2 deviation represented schematically. For simplification, the χ^2 deviation is shown as a function of one parameter only.

of FIG. 5.1, the χ^2 deviation is minimized for a unique value of the parameter x_i. For severals observables f_i, the minimum of each contribution to χ^2 is likely to be obtained for different values of that particular parameter, see FIG. 5.2. In such a case, the final value x_{i0} is the one that minimizes the sum of all χ_i^2. The reasoning can be trivially extended to several parameters $\vec{x} = \{x_k\}$.

The χ^2 deviation of the least-square method traditionally has a statistical meaning. Presently, we prefer to refer to the function to be minimized as the merit function although it does ressemble a χ^2 deviation (EQ. 5.2).

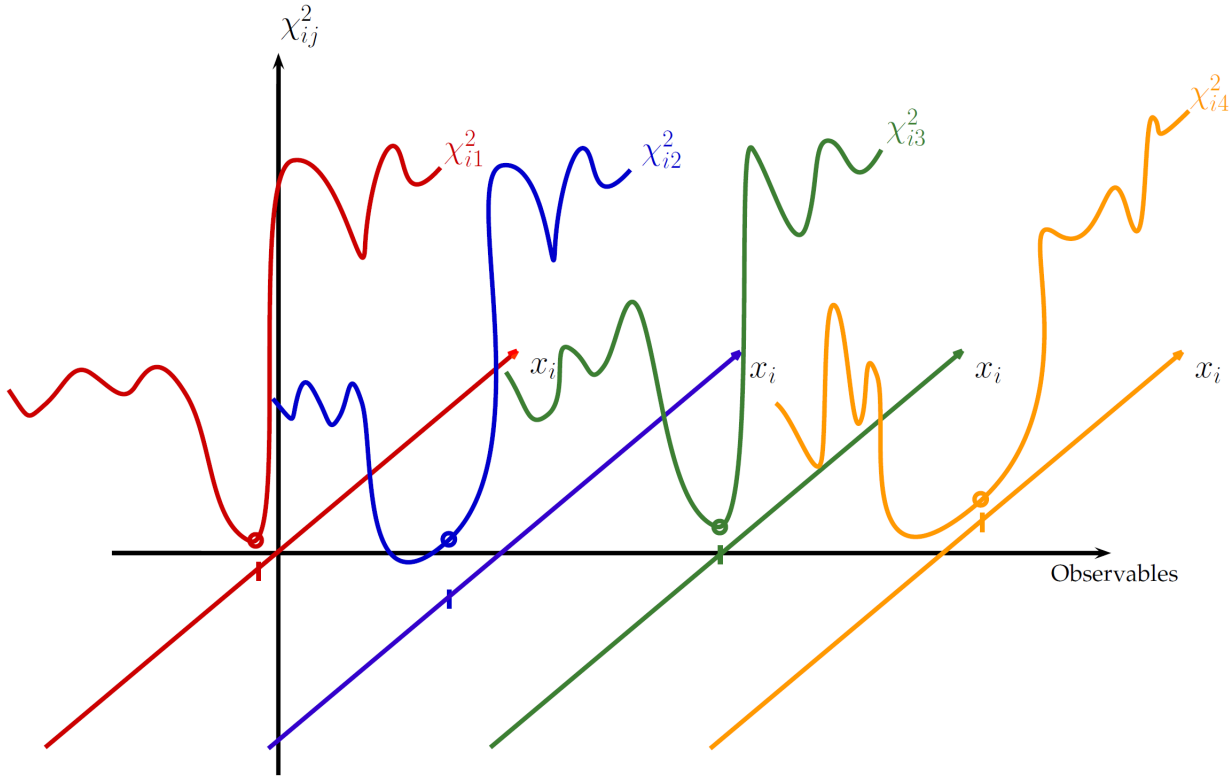

Figure 5.2: χ^2_i deviation for severals observables f_i as a function of a single parameter x_i.

5.1.3 Proposed fit strategy

In the present document, which represents a first step in a long term project direction, the fitting procedure will not differ significantly from the traditional Saclay-Lyon protocol, from which SLyX parameterization have been constructed [108].

In such an approach, INM properties are first used to provide analytical constraints on several linear combinations of parameters. Ideally, one could analytically determine as many linear combinations that there are pseudo-potential parameters. However, the situation is far from the ideal one, essentially because several INM properties are not primordial to reproduce. As a result, some of them are only used to give a zeroth-order determination of the parameters. The latter are then re-adjusted on nuclear masses and radii. Parameters that cannot be predetermined through INM properties are entirely adjusted on finite nuclei properties. It is significantly more time consuming to adjust such parameters as there is no first guess for their value.

Adding a three-body pseudo-potential to a two-body one enhances the number of parameters compared to usual (quasi) bilinear EDFs deriving from a density-dependent two-body potential. It seems to imply that an enhancement of the Saclay-Lyon fit strategy is necessary. The three-body pseudo-potential, Eqs. (3.87,3.88), has six parameters and the two-body one, Eq. 3.52, has seven, for a total of thirteen parameters. Usual (quasi) bilinear EDF parameterization, have

nine parameters[1]. As a result, only four parameters are added to the usual parameter space.

It has been remarked that a large parameter space increases the difficulty of the fit and that the optimal $\vec{x}_0$ can eventually lead to an EDF displaying instabilities in Hartree-Fock calculations [94, 116, 117]. Adding four parameters might seem sufficient enough to enrich the EDF without bringing unavoidable instabilities. In particular, a thorough study of our pseudo-potential in infinite nuclear matter may allow us to avoid many instabilities. Last but not least, let us stress again that the main objective of the presently developped pseudo-potential is not to provide a better reproduction of nuclear properties at the SR level than provided by existing EDF parameterizations, but rather to be safe for MR-EDF calculations.

5.2 Infinite nuclear matter

The present section is dedicated to performing a preliminary study that aims at constraining pseudo-potential parameters by focusing on infinite nuclear matter properties. It allow us to narrow down the size of the parameter space to be eventually explored.

5.2.1 Symmetric nuclear matter properties

The four main empirical properties of symmetric nuclear matter properties are

- the saturation density $\rho_{\rm sat} = 0,16 \pm 0,002\text{fm}^{-3}$ corresponding to the density of the nuclear matter in its equilibrium state. Its value has been obtained through electron elastic scattering on heavy nuclei, which gives access to the charge distribution and thus to the matter density of the system. The total density at the center of heavy nuclei is essentially independent of the system, giving credit to the infinite nuclear matter concept and yielding the value of $\rho_{\rm sat}$.
- the energy per particle at saturation point. It corresponds to the leading term of Bethe-Weizsäcker semi-empirical mass formula. Its value, $\frac{E}{A}(\rho_{\rm sat}) = -16,0 \pm 0,2$ MeV has been extracted using such a mass formula to reproduce a large set of experimental nuclear masses [118, 119].
- the incompressibility coefficient K_∞ at saturation. Its value is $K_\infty \simeq 230 \pm 20$ MeV. For a detailed discussion on how to access K_∞ through the Isoscalar Giant Monopole Resonance in doubly-magic nuclei, see [120–122].
- the isoscalar effective mass at saturation density that drives the density of states near the Fermi energy and that is related to Quadrupolar Isoscalar Giant Gesonance energy. The value thusextracted is $m_0^* \simeq 0.85 \pm 0.05\, m$ [123, 124].

Eventually, the typical values for these four properties are

$$\rho_{\rm sat} = 0.16 \pm 0.002 \text{ fm}^{-3} \ , \tag{5.3a}$$

$$\frac{E}{A}(\rho_{\rm sat}) = -16.0 \pm 0.2 \text{ MeV} \ , \tag{5.3b}$$

$$m_0^*/m = 0.85 \pm 0.05 \ , \tag{5.3c}$$

$$K_\infty = 230 \pm 20 \text{ MeV} \ . \tag{5.3d}$$

Empirical values Eq. 5.3 allow the analytical determination of four linear combinations of parameters appearing in the SNM equation of state.

1. We are omitting tensor terms in the pseudo-potential altogether in the present study.

5.2.2 Density-dependence and three-body potential

In the past, gradient-less three-body pseudo-potential have already been used to reproduce nuclear properties and in particular SNM properties. As a matter of fact, Skyrme introduced in combination with the two-body pseudo-potential [100]. It appeared at that time that three-body contributions are essential to reproduce nuclear properties. Indeed, it provides a repulsive effect canceling attractive two-body contributions at high densities, allowing the nuclear fluid to have an equilibrium point at finite density. Eventually, results were in satisfactory agreement with experimental data thanks to the SIII parameterization [92].
However, a gradient-less three-body pseudo-potential gives opposite contributions to time even and time odd terms, see the first line of Tabs. {C.1-C.2}. As a result, repulsive spin-independent contributions imply attractive spin-dependent contributions and lead to a spin instabilities of nuclear matter [125, 126]. This is the reason why it was proposed to replace the gradient-less three-body pseudo-potential by a two-body on depending linearly on the scalar matter density.
For such a (quasi) bilinear EDF deriving from a density-dependent two-body pseudo-potential,

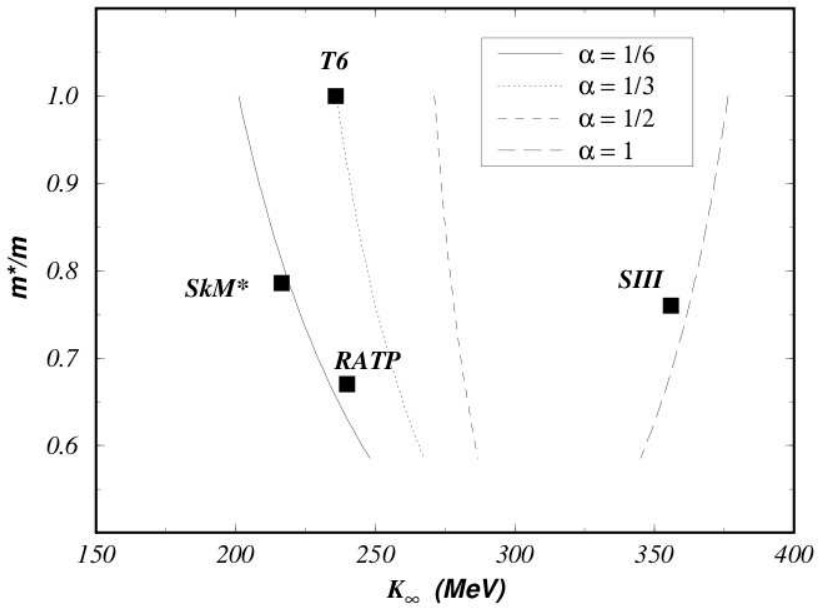

Figure 5.3: Correlation between the compressibility K_∞ and the isoscalar effective mass m_0^*/m as a function of the α parameter which governs the density dependence of the potential. Reprinted with permission from Chabanat *et al.* [Nucl. Phys. A **627**, 710 (1997)].

the parameters entering the SNM equation of state are t_0, Θ_s and t_3, where t_3 is the parameter in front of the density dependence. Three parameters are not enough to reproduce the four properties 5.3. Considering the energy per particle and the density at saturation as key properties to reproduce, two linear combinations out of three are fixed. The last one determines the value of the isoscalar effective mass and the incompressibility, such that choosing a value for the first property determines the second. Possible values taken by K_∞ and m_0^* are given by a set of correlation curves in Fig. 5.3 that vary with the exponent α of the density dependent factor. It can be seen that K_∞ is always overestimated if using a linear density dependence as coming from a gradient-less three-body potential. As a matter of fact, accessing correct values for both K_∞ and m_0^* required a lowering of the exponent of the density-dependent factor, e.g. $\alpha = 1/6$

for SLyX [108], which we know now to be unsafe in MR-EDF calculations. It will be one of the main objective below to see whether using a major general three-body pseudo-potential allows us to overcome the two historical limitations of a gradient-less one, i.e. avoiding spin instabilities and reaching empirically determined values of both m_0^* and K_∞.

5.2.3 Critical density and inflection point

Using a complete central two- plus three-body pseudo-potential four linear combinations of parameters appear in the SNM equation of state (Eq. 4.19), i.e. t_0, u_0, Θ_s and Θ_{3s}, defined in Eq. 4.18. As a result, empirical values 5.3 can all be exactly reproduced if required. Such an analytical determination of the four (combinations of) parameters leads to

$$t_0 = -1266.602 \text{ MeV fm}^3 , \tag{5.4a}$$
$$u_0 = 7080.677 \text{ MeV fm}^6 , \tag{5.4b}$$
$$\Theta_s = 1605.779 \text{ MeV fm}^3 , \tag{5.4c}$$
$$\Theta_{3s} = -7749.113 \text{ MeV fm}^6 . \tag{5.4d}$$

However, difficulties appear when looking at the corresponding equation of state and the effective mass as a function of density, see Fig. 5.4.

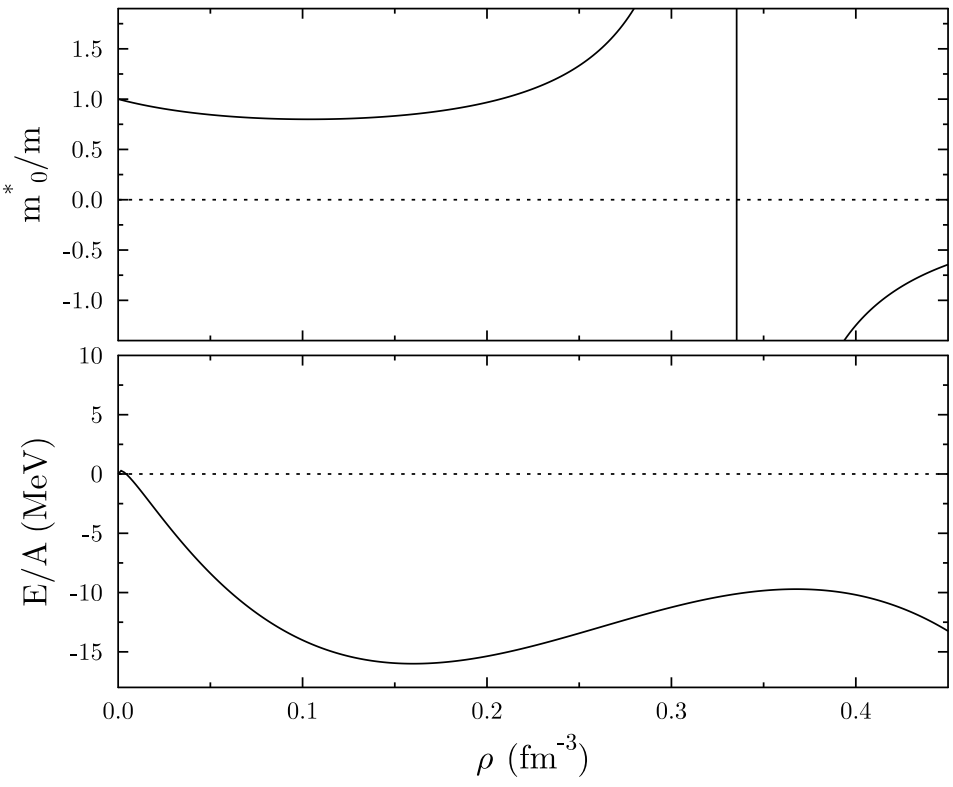

Figure 5.4: Binding energy per nucleon (lower panel) and effective mass (upper panel) in symmetric nuclear matter as a function of the density. At $\rho = 0.3\text{fm}^{-3}$ the equation of state begins to collapse such that the nuclear matter is not stable anymore and a pole occurs for the effective mass.

– the equation of state is not stable with respect to an increase of the density, i.e. it is energetically favorable for SNM to have an infinite density. Such an issue can be understood

by looking at Eq. 4.19. The term corresponding to the highest power of ρ is negative when using Eq. 5.4, as Θ_{3s} is negative. The position of the inflection point of the equation of state is now denoted as ρ_{infl}.

– a pole appears, for a critical value of the density hereafter denoted as ρ_{cr}, in the isoscalar effective mass. Again, such a pole comes from the fact that Θ_{3s} is negative such that the denominator in Eq. 4.24 can be null.

Let us first remark that those patterns relates to the fact that we are adjusting parameters on saturation properties and not on the behaviour of the equation of state at higher densities. Of course it is impossible to adjust the parameters on the entire equation of state while keeping acceptable incompressibility and an effective mass without pole. Looking at Eqs. (4.21,4.24) it becomes clear that the two unwanted features relate to the correlation that exists between the incompressibility and the effective mass. Indeed, taking Θ_s and Θ_{3s} positive to a specific value in Eq. 4.24 would imply a too large value of the incompressibility 4.21. The problem cannot be avoided entirely, without deteriorating the density and energy per particle of the saturation point. As a result, one has to take a negative value for Θ_{3s}. However, the position of the singularity ρ_{cr} can be obtained solving

$$\Theta_{3s}\rho_{\text{cr}}^2 + \Theta_s\rho_{\text{cr}} + 16\,\frac{\hbar^2}{2m} = 0 \ , \tag{5.5}$$

such that one can choose the position of the singularity in the effective mass by setting a relation between Θ_s and Θ_{3s}. Having one parameter less, the four empirical values Eq. 5.3 can not be reproduced exactly anymore. The approach used to study the impact of ρ_{cr} is to build a merit function from SNM properties and minimize it, allowing such properties to differ slightly from the empirical value 5.3. Fig. 5.5 shows the results when the value of ρ_{cr} is varied. Increasing ρ_{cr} generates an increase of K_∞ and a decrease of m_0^*/m. Rejecting ρ_{cr} and ρ_{infl} to large enough value eventually returns parameterizations that are safe for the computation of nuclei. Indeed, the part of the equation of state that actually impacts properties of finite nuclei is located near the saturation point. Hopefully, it is possible to reject both ρ_{cr} and ρ_{infl} to two or three time saturation density, see Fig. 5.5.

Choosing $\rho_{\text{cr}} = 0.48$, SNM properties become

$$\rho_{\text{sat}} = 0.1606 \text{ fm}^{-3} \ , \tag{5.6a}$$
$$\frac{E}{A}(\rho_{\text{sat}}) = -15.901 \text{ MeV} \ , \tag{5.6b}$$
$$m_0^*/m = 0.7045 \ , \tag{5.6c}$$
$$K_\infty = 255.496 \text{ MeV} \ , \tag{5.6d}$$
$$\rho_{\text{cr}} = 0.48 \text{ fm}^{-3} \ , \tag{5.6e}$$
$$\rho_{\text{infl}} = 0.363 \text{ fm}^{-3} \ , \tag{5.6f}$$

with the corresponding values for the parameters

$$t_0 = -1209.835 \text{ MeV fm}^3 \ , \tag{5.7a}$$
$$u_0 = 5273.114 \text{ MeV fm}^6 \ , \tag{5.7b}$$
$$\Theta_s = 1649.865 \text{ MeV fm}^3 \ , \tag{5.7c}$$
$$\Theta_{3s} = -4877.187 \text{ MeV fm}^6 \ . \tag{5.7d}$$

The equation of state and the effective mass obtained with parameterization 5.7 are more satisfying than in Fig. 5.4 as is shown in Fig. 5.6.

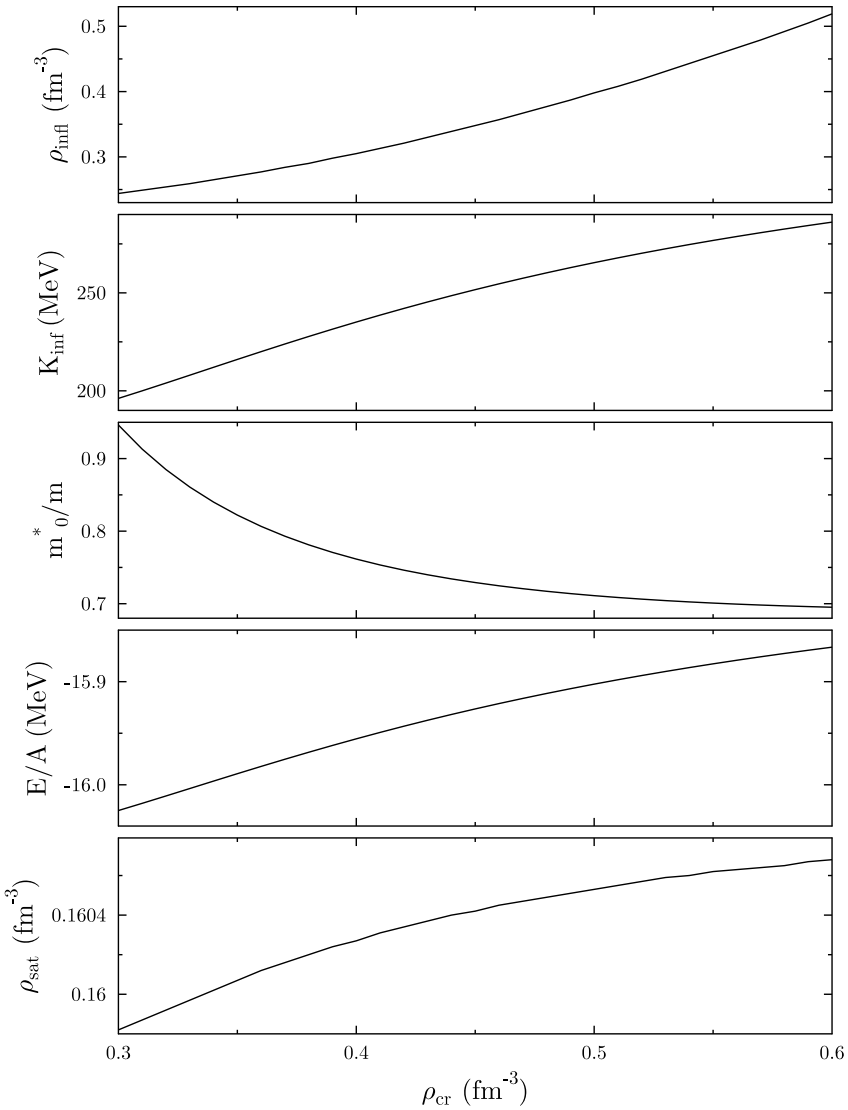

Figure 5.5: Saturation density, binding energy per nucleon at equilibrium, isoscalar effective mass, incompressibility and position of the inflection point as functions of the critical density.

5.2.4 Asymmetric nuclear matter and pure neutron matter

Thanks to symmetric matter properties 5.3, one has determined four among the thirteen (combinations of) parameters of the two- plus three-body pseudo-potential. Linear combinations of parameters, x_0, Θ_v, Θ_{3v} and $\Theta_{3v'}$, given in Eq. 4.18, can also be constrained using asymmetric and pure neutron matter properties. Neutron matter equation of state, Eq. 4.29, is used to adjust x_0, Θ_v and Θ_{3v}, thanks to a set of eighteen points from [127], such that

$$x_0 = 0.342224 \ , \tag{5.8a}$$
$$\Theta_v = 1267.587 \text{ MeV fm}^3 \ , \tag{5.8b}$$
$$\Theta_{3v} = -5052.235 \text{ MeV fm}^6 \ . \tag{5.8c}$$

The result is shown in Fig. 5.7 where it can be seen that the obtained parameterization reproduces in a better way the equation of state compared to SLy4 parameterization. The additional

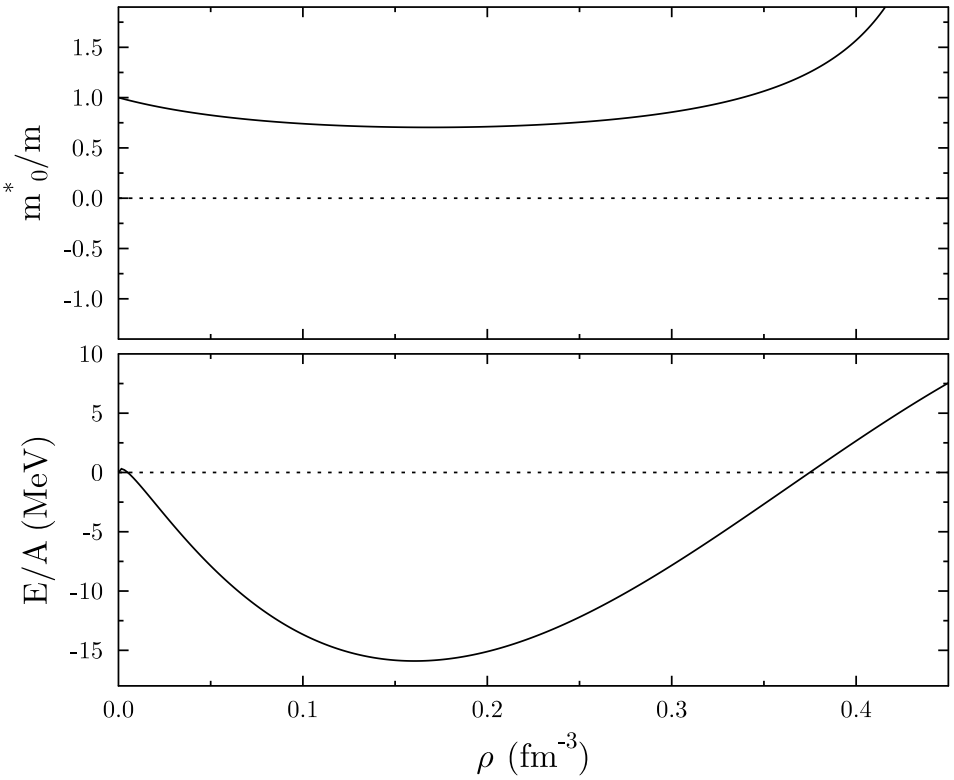

Figure 5.6: Binding energy per nucleon (lower panel) and effective mass (upper panel) in symmetric nuclear matter as a function of the density.

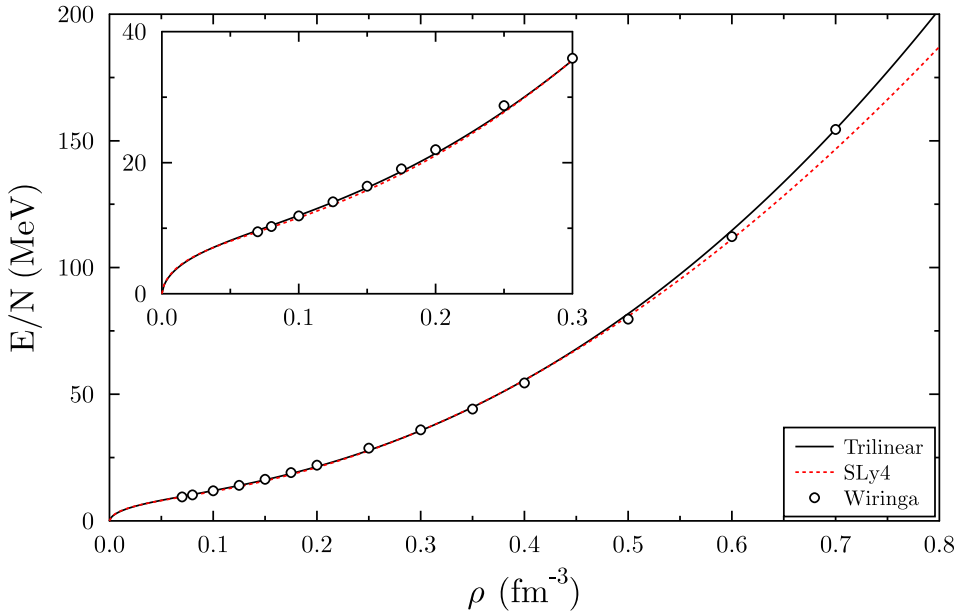

Figure 5.7: Binding energy per nucleon in pure neutron matter with two different scales.

parameter Θ'_{3v} can then be determined through the symmetry energy coefficient, Eq. 4.26, using the empirical value

$$a_\tau = 32 \text{ MeV} \ , \tag{5.9}$$

such that one obtains

$$\Theta'_{3v} = 56.228 \text{ MeV fm}^6 \, . \tag{5.10}$$

Parameters t_0, x_0, u_0, Θ_s, Θ_v, Θ_{3s}, Θ_{3v} and Θ'_{3v} being determined, one can now check the evolution of neutron and proton effective masses (Eq. 4.30) in pure neutron matter, see Fig. 5.8. The evolution of the effective masses with the density is not linear, contrarily to traditional

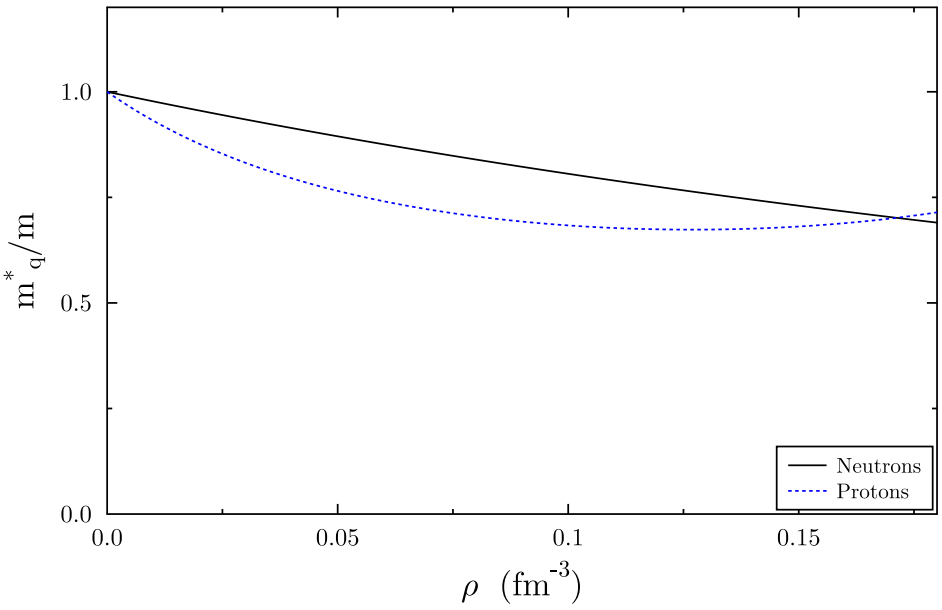

Figure 5.8: Neutron and proton effective masses in pure neutron matter.

functionals like SLy4. Furthermore, one observes that the sign of the neutron-proton effective mass splitting is the one predicted by BHF and DBHF calculations below saturation density, as opposed to many modern Skyrme EDF parameterizations [117].

5.2.5 Landau parameters

Thanks to symmetric, isospin asymmetric and pure neutron matter, eight out of thirteen (combinations of) parameters have been tightly constrained analytically. The remaining ones contributes to Landau parameters Tab. {4.1} for which experimental data are difficult to extract. For instance looking at Eq. 4.31, one can relate F_0 Landau parameter to the nuclear incompressibility whose value is not easily deducible from measurements [121, 122]. On the other hand, there exists ab-initio theoretical data on which parameters could also be fitted [128]. Unfortunately, the present used pseudo-potential is not rich enough to allow for a fine adjustment on such ab-initio data, which anyway have yet to be improved. Consequently we presently constrain Landau parameters in a loose way, simply requiring the EDF to be stable against infinite wavelength spin and isospin fluctuations, i.e. to fulfill conditions 4.33.

Fig. 5.9 shows the eight active Landau parameters as a function of density using parameterization Eqs. (5.7,5.8,5.10) and taking all remaining linear combinations to zero. First, a

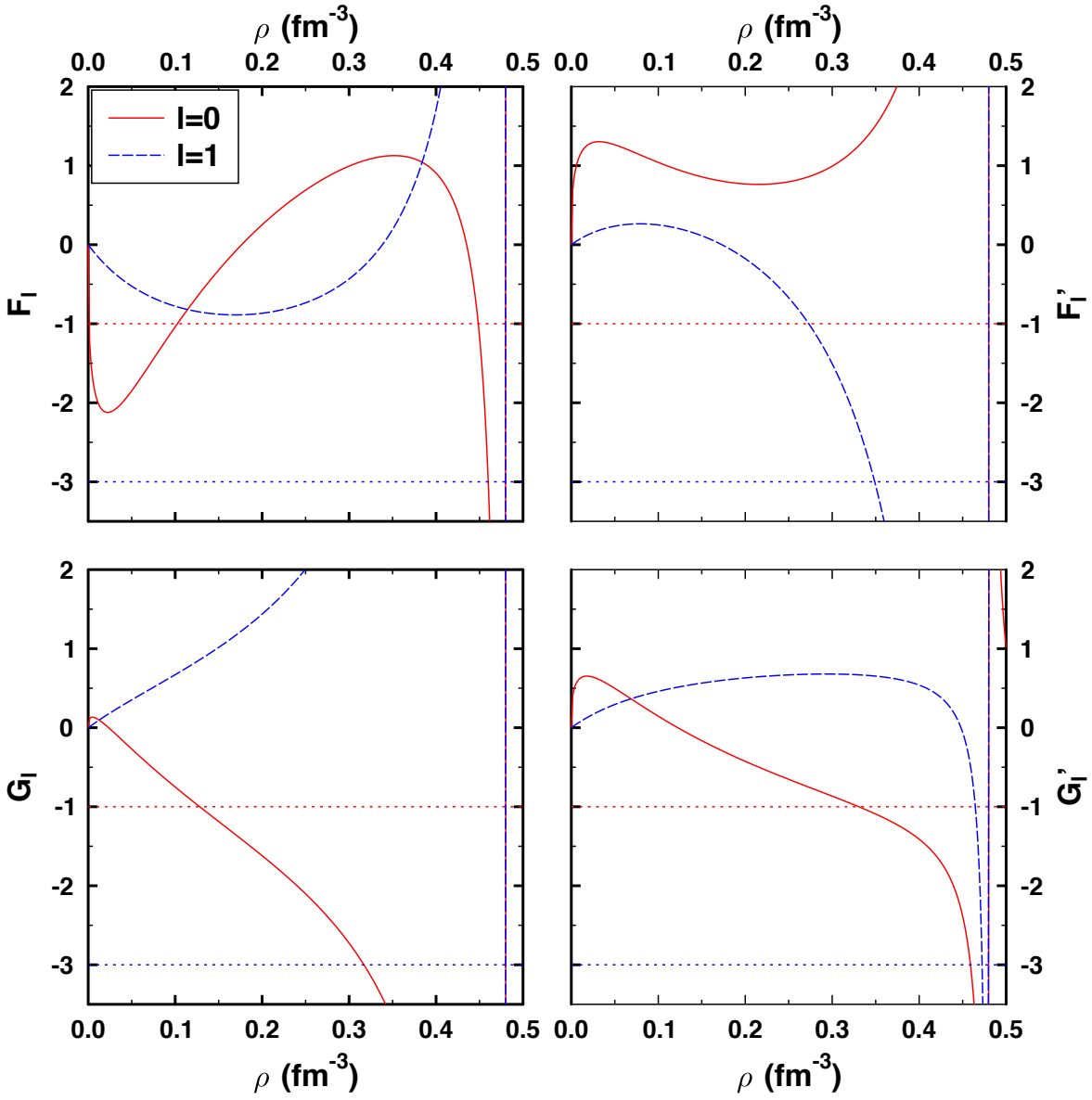

Figure 5.9: Landau parameters as a function of the density. The two dashed lines represents the upper limits not to cross for $l = 0$ and $l = 1$ Landau parameters, in order to avoid an instabilities area (Eq. 4.33)

pole appears for each Landau parameter at $\rho_{\rm cr}$ and comes from the normalization factor N_0 in Eq. 4.48 which is a function of the isoscalar effective mass. For such a parametrization $l = 1$ Landau parameters are rather safe with respect to instability condition 4.33, except for G_1 that enters the instability area at twice saturation density. F_0' and G_0' follows the same behaviour. Again it is not straightforward to decide if two times saturation density is sufficient to provide safe parameterizations with respect to instabilities. The instability with respect to density fluctuations and associated with $F_0 < -1$ is physical and known as the spinodal instability. It relates to the density interval where K_∞ is negative [129, 130]. The spin instability associated with $G_0 < -1$ was discussed above and was expected to be hard to fulfill. It is due to the attractive contribution of spin-dependent EDF terms deriving from a pure contact three-body pseudo-potential [125]. One was hoping that adding gradient three-body terms would allow us to avoid such instabilities. It appears to be difficult but can be improved upon in the final determination of the parameters, see Chap. 6.

5.2.6 Conclusion

The main result of the preliminary study is that our pseudo-potential cannot reproduce saturation properties without displaying a singularity in the effective mass and a collapse of the equation of state in symmetric nuclear matter. However, it was shown possible to control those two features and determine or at least strongly constrain eight of the thirteen potential parameters using a set of infinite nuclear matter properties and eventually obtain a decent description of all essential properties of INM. Starting from such results, we now proceed to the actual adjustment of new parameterization.

5.3 Adjustment based on nuclei and INM properties

The complete parameter optimization is performed via the minimization of the merit function

$$\chi^2_{\rm tot} = \chi^2_{\rm INM} + \chi^2_{\rm Nuclei} \ . \tag{5.11}$$

The minimum of $\chi^2_{\rm tot}$ is found through multiple SR-EDF calculations of semi-magic nuclei and using a simplex algorithm.

5.3.1 Constrains from infinite nuclear matter properties

To find the best parameterization, it is convenient to reduce the size of the parameter space in which the best parameterization should be. For this purpose, analytical infinite nuclear matter constrains were used. The parameterization obtained in Eqs. (5.7,5.8,5.10) or using the same method but varying $\rho_{\rm cr}$, $\rho_{\rm infl}$, m_0^* and K_∞, are thus used as initial points for the complete adjustment procedure. Obviously, INM constrains do not just provide the starting parameterization but are also included in the merit function 5.11 to be minimized, following

$$\chi^2_{\rm INM} = \chi^2_{\rm SNM} + \chi^2_{\rm ANM} + \chi^2_{\rm PNM} + \chi^2_{\rm Landau} \ , \tag{5.12}$$

where each component of $\chi^2_{\rm INM}$ separates into N merit functions according to

$$\chi^2 = \sum_{i=1}^{N} \chi_i^2 \ , \tag{5.13}$$

N being the number of properties used in SNM, ANM, the number of points in the PNM EOS or the number of Landau parameters.

5.3.1.1 Symmetric and asymmetric nuclear matter

Merit functions related to SNM or ANM properties are expressed under the form

$$\chi^2_{\rm NM} = \left(\frac{f_{\rm NM}(\vec{x}) - e_{\rm NM}}{\Delta_{\rm NM}} \right)^2 \tag{5.14}$$

$$, \tag{5.15}$$

such that errors $\Delta_{\rm NM}$ have to be given to the code for each of the properties.
For SNM, $e_{\rm NM}$ values for E/A and $\rho_{\rm sat}$ are given in Eq. 5.3. Contrarily K_∞ and m_0^*/m are varied over a range of possible values. Indeed, choosing K_∞ and m_0^*/m determines $\rho_{\rm cr}$ and $\rho_{\rm infl}$. A systematic study thus needs to be accomplished. A set of parameterizations is thus generated for which

$$e_{E/A} = -16.0 \text{ MeV} \ , \tag{5.16a}$$
$$e_{\rho_{\rm sat}} = 0.16 \text{ fm}^{-3} \ , \tag{5.16b}$$
$$e_{m_0^*/m} = \{0.70\,,\ 0.71\,,\ 0.72\,,\ 0.73\,,\ 0.74\,,\ 0.75\,,\ 0.76\,,\ 0.77\,,\ 0.78\,,\ 0.79\,,\ 0.80\,,\ 0.81\} \ , \tag{5.16c}$$
$$e_{K_\infty} = \{230\,,\ 240\,,\ 250\,,\ 260\,,\ 270\} \text{ MeV} \ , \tag{5.16d}$$

where all the combinations of $e_{m_0^*/m}$ and e_{K_∞} have been tried out. Corresponding parameterizations will be denoted as

$$\mathrm{S_3Ly}_{e_{K_\infty}}^{10*e_{m_0^*/m}} \ . \tag{5.17}$$

Values for the associated errors are

$$\Delta_{E/A} = 0.16 \text{ MeV} \quad , \quad \Delta_{\rho_{\rm sat}} = 0.003 \text{ fm}^{-3} \quad , \quad \Delta_{m_0^*/m} = 0.001 \quad , \quad \Delta_{K_\infty} = 3 \text{ MeV} \ . \tag{5.18}$$

For ANM, the property on which the pseudo-potential is adjusted is the symmetry energy coefficient Eq. 4.26 whose value and error are

$$e_{a_\tau} = 32 \text{ MeV} \quad \text{and} \quad \Delta_{a_\tau} = 1 \text{ MeV} \ . \tag{5.19}$$

5.3.1.2 Pure neutron matter

For the eighteen points of the PNM EOS the merit function takes the form

$$\chi^2_{\rm PNM} = \sum_{i=1}^{18} \left(\frac{\frac{E}{N}(\vec{x}, \rho_i) - \frac{E^{\rm Wir}}{N}(\rho_i)}{\Delta_{\rm PNM}} \right)^2 \ , \tag{5.20}$$

where $E^{\rm Wir}$ denotes the Wiringa EOS, see [127]. The chosen values for $\Delta_{\rm PNM}$ are

$$\Delta_{\rm PNM} = 0.1 \, \frac{E^{\rm Wir}}{N}(\rho_i) \text{ MeV for } \rho_i \leq 0.5 fm^{-3} \tag{5.21a}$$
$$\Delta_{\rm PNM} = 0.2 \, \frac{E^{\rm Wir}}{N}(\rho_i) \text{ MeV for } \rho_i > 0.5 fm^{-3} \ . \tag{5.21b}$$

5.3.1.3 Landau parameters

A constrain on Landau parameters is used to avoid instabilities (Eq. 4.33). For each Landau parameters $X_l \equiv \{F_l, F'_l, G_l, G'_L\}$ and $l = \{0, 1\}$, the following expression $\chi^2_{X_l}$ contributes to the merit function $\chi^2_{\rm Landau}$

$$\begin{cases} \chi^2_{X_l} = \left(\dfrac{X_l(\vec{x}) + (2l+1)}{\Delta_{X_l}} \right)^2 & \text{if} \quad X_l(\vec{x}) \leq (2l+1) \\ \chi^2_{X_l} = 0 \quad \text{if} \quad X_l(\vec{x}) > -(2l+1) \end{cases} \ , \tag{5.22}$$

where Δ_{X_l} is chosen to be

$$\Delta_{X_l} = 10^{-3} \ . \tag{5.23}$$

5.3.2 Nuclei observable

The second part of the merit function χ^2_{Nuclei} comes from nuclei observables. To chose the best set of nuclei on which parameters are optimized, one has to ask two questions

- Which observables are practically accessible? Unlike INM properties, finite nuclei observables are not obtained as analytical expressions but through numerical means. It implies that each evaluation of nuclei observables is time-consuming. However some of them are faster to compute. For instance spherical, i.e. semi-magic or doubly magic, nuclei take only a few seconds to evaluate, whereas deformed, i.e. open shell, nuclei are more numerically demanding.
- Which observables the pseudo-potential should reproduce? SR-EDF method can only safely address bulk properties of either spherical or well deformed nuclei, while MR-EDF method gives natural access to properties significantly impacted by dynamical correlations. Using only SR-EDF method for the optimization as we do here imposes to use bulk properties only. An alternative consists of performing the optimization on pseudo-data, i.e. data from which theoretically computed dynamical correlations have been subtracted. Whereas only one such fit has been performed so far [131], including MR correlations at the level of the fit is part of our long term strategy but is not done here.

As a result of such considerations, the set of nuclei used in the present study is

$$^{40}\text{Ca},\ ^{48}\text{Ca},\ ^{56}\text{Ni},\ ^{100}\text{Sn},\ ^{132}\text{Sn},\ ^{208}\text{Pb} \ , \tag{5.24}$$

such that χ^2_{Nuclei} is decomposed into

$$\chi^2_{\text{Nuclei}} = \chi^2_{^{40}\text{Ca}} + \chi^2_{^{48}\text{Ca}} + \chi^2_{^{56}\text{Ni}} + \chi^2_{^{100}\text{Sn}} + \chi^2_{^{132}\text{Sn}} + \chi^2_{^{208}\text{Pb}} \ . \tag{5.25}$$

Observables used are binding energies and charge radii such that

$$\chi^2_{^A\text{X}} = \frac{1}{6}\left(\frac{E^{^A\text{X}}_{\vec{x}} - E^{^A\text{X}}_{exp}}{\Delta_E^{^A\text{X}}}\right)^2 + \frac{1}{5}\left(\frac{r^{^A\text{X}}_{\vec{x}} - r^{^A\text{X}}_{exp}}{\Delta_r^{^A\text{X}}}\right)^2 \ , \tag{5.26}$$

where $^A\text{X} = \{^{40}\text{Ca},\ ^{48}\text{Ca},\ ^{56}\text{Ni},\ ^{132}\text{Sn}\}$, E_{exp} and r_{exp} are experimental binding energies and charge radii, whereas $E_{\vec{x}}$ and $r_{\vec{x}}$ are the theoretical counterpart obtained from SR-EDF calculations. The factors $\frac{1}{6}$ and $\frac{1}{5}$ are normalization factors with 6 the number of binding energies and 5 the number of charge radii used in the protocol. The charge radius of ^{100}Sn is unkown such that only its energy contributes

$$\chi^2_{^{100}\text{Sn}} = \frac{1}{6}\left(\frac{E^{^{100}\text{Sn}}_{\vec{x}} - E^{^{100}\text{Sn}}_{exp}}{\Delta_E^{^{100}\text{Sn}}}\right)^2 \ . \tag{5.27}$$

For ^{208}Pb, neutron spin-orbit splitting

$$\epsilon_{3p} \equiv \epsilon_{\nu 3p_{1/2}} - \epsilon_{\nu 3p_{3/2}} \ , \tag{5.28}$$

is added to the binding energy and the charge radius such that

$$\chi^2_{^{208}\text{Pb}} = \frac{1}{6}\left(\frac{E^{^{208}\text{Pb}}_{\vec{x}} - E^{^{208}\text{Pb}}_{exp}}{\Delta_E^{^{208}\text{Pb}}}\right)^2 + \frac{1}{5}\left(\frac{r^{^{208}\text{Pb}}_{\vec{x}} - r^{^{208}\text{Pb}}_{exp}}{\Delta_r^{^{208}\text{Pb}}}\right)^2 + \left(\frac{\epsilon^{^{208}\text{Pb}}_{3p,\vec{x}} - \epsilon^{^{208}\text{Pb}}_{3p,exp}}{\Delta_{\epsilon_{3p}}^{^{208}\text{Pb}}}\right)^2 \ . \tag{5.29}$$

Experimental values have been taken from [132] while associated errors are

$$\Delta_E^{^{40}\mathrm{Ca}} = 0.800 \text{ MeV} \quad , \quad \Delta_r^{^{40}\mathrm{Ca}} = 0.020 \text{ fm}^{-3} \quad , \tag{5.30a}$$
$$\Delta_E^{^{48}\mathrm{Ca}} = 0.200 \text{ MeV} \quad , \quad \Delta_r^{^{48}\mathrm{Ca}} = 0.020 \text{ fm}^{-3} \quad , \tag{5.30b}$$
$$\Delta_E^{^{56}\mathrm{Ni}} = 0.800 \text{ MeV} \quad , \quad \Delta_r^{^{56}\mathrm{Ni}} = 0.020 \text{ fm}^{-3} \quad , \tag{5.30c}$$
$$\Delta_E^{^{100}\mathrm{Sn}} = 0.800 \text{ MeV} \quad , \tag{5.30d}$$
$$\Delta_E^{^{132}\mathrm{Sn}} = 0.200 \text{ MeV} \quad , \quad \Delta_r^{^{132}\mathrm{Sn}} = 0.020 \text{ fm}^{-3} \quad , \tag{5.30e}$$
$$\Delta_E^{^{208}\mathrm{Pb}} = 0.200 \text{ MeV} \quad , \quad \Delta_r^{^{208}\mathrm{Pb}} = 0.020 \text{ fm}^{-3} \quad , \quad \Delta_{\epsilon_{3p}}^{^{208}\mathrm{Pb}} = 0.1 \text{ MeV} \ . \tag{5.30f}$$

A remark has to be added about doubly-magic $N = Z$ nuclei such as ^{40}Ca, ^{56}Ni and ^{100}Sn. One knows that Wigner energy contributes to their binding. For that reason $N = Z$ nuclei binding energies have smaller weights than $N \neq Z$ nuclei in the adjustment procedure. It would of course be better to design pseudo-data subtracting Wigner energy to those binding energies. However, such a strategy is not used here and necessitates a specific study of Wigner energy.

5.3.3 SNM properties and χ^2 merit function

The χ^2 merit function has now been introduced. As a first test, a preliminary set of parameterizations has been obtained fixing SNM properties, i.e. taking

$$\Delta_{E/A} = 0 \text{ MeV} \quad , \quad \Delta_{\rho_{\mathrm{sat}}} = 0 \text{ fm}^{-3} \quad , \quad \Delta_{m_0^*/m} = 0 \quad , \quad \Delta_{K_\infty} = 0 \text{ MeV} \ , \tag{5.31}$$

instead of using Eq. 5.18. Values obtained for the merit function at the end of the optimization following such a strategy are high and a good reproduction of nuclei is also impossible. Allowing SNM properties to vary slightly improves those results tremendously as can be seen from thanks Fig. 5.10. As a result, allowing SNM properties to vary is essential even if the range of allowed variation is small.

5.3.4 Final parameterizations

For this preliminary work, four of the parameterizations obtained following the protocol presented in this section have been selected. Their χ^2 merit function are not too high and their ρ_{cr} not too low, see Fig. 5.10. Characteristics of the chosen parameterizations are given in Tab. {5.1}. Furthermore, the (quasi) bilinear EDF parameterization SLy4 [108] will be used in the following to perform comparison. SLy4 has been adjusted using a fitting procedure close to the one presently used and is thus an appropriate reference point to assess the performance of the new parameterizations.

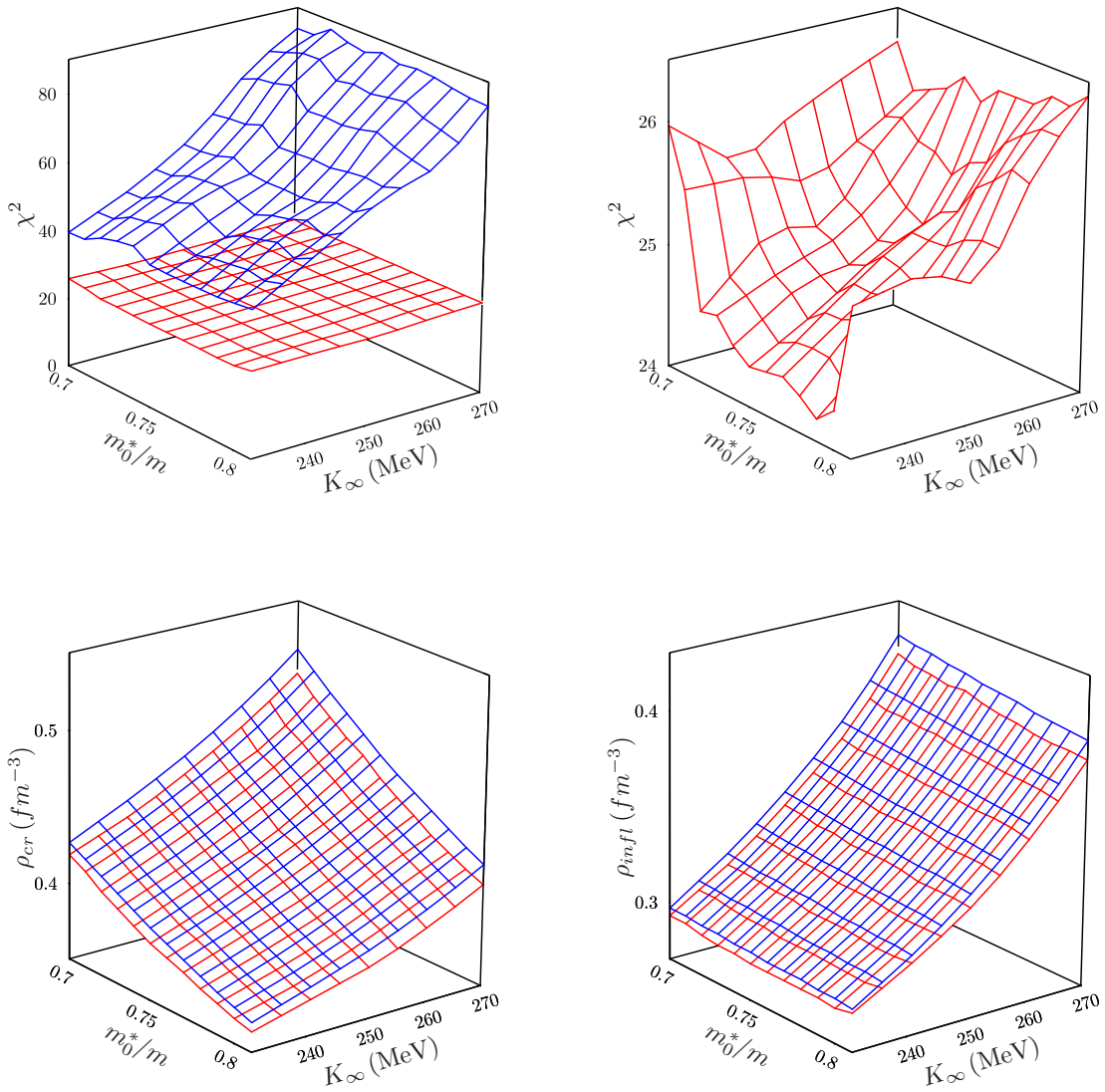

Figure 5.10: χ^2 merit function (upper panel), ρ_{cr} (lower left panel) and ρ_{infl} (lower right panel) for different parameterizations. Blue curves corresponds to parameterizations with strictly fixed value of SNM properties whereas red curves correspond to allowing SNM properties to vary slightly.

$S_3Ly_{K_\infty}^{10\,m_0^*/m}$	$S_3Ly_{260}^{71}$	$S_3Ly_{250}^{73}$	$S_3Ly_{230}^{76}$	$S_3Ly_{250}^{81}$
$\rho_{\rm cr}$	0.464	0.431	0.383	0.383
$\rho_{\rm infl}$	0.362	0.333	0.289	0.327
χ^2	25.5642	24.9810	24.3528	25.1409
t_0	-1234.26	-1241.74	-1265.03	-1235.57
t_1	623.21	632.87	669.63	593.02
t_2	-217.33	-234.08	-271.87	-377.94
x_0	0.48484	0.47435	0.44137	0.43802
x_1	0.66198	0.63208	0.54432	0.57900
x_2	-1.01933	-1.00591	-0.99620	-1.02459
u_0	5589.27	5867.27	6422.56	6430.14
u_1	-2544.53	-2929.78	-3751.15	-3237.15
y_1	1.35482	1.36726	1.37316	1.65119
u_2	587.17	486.50	473.80	469.10
y_{21}	-1.55804	-1.61876	-1.61303	-1.61148
y_{22}	-0.87820	-0.99543	-0.89831	-0.91245
W_0	114.04	113.55	115.91	107.63

Table 5.1: Parameterizations used in the present study.

Chapter 6

Results and outlooks

Abstract: A set of parameterizations obtained through the fitting procedure described in Chap. 5 is used to compute INM and nuclei properties. Results provide information on the quality of the fitting procedure and on the relevance of the pseudo-potential introduced in Chap. 3. Thanks to such a post-fit analysis, a hierarchy of possible improvements are proposed.

Contents

6.1 Introduction

The parameterizations generated by the adjustment procedure are the best suited to reproduced a set of fitted observables, given a set of allowed errors. Hopefully, other nuclear observables are also well reproduced. The result of such a post fit analysis is a measure of the quality of the pseudo-potential. Obviously it will strongly depends on the fitting procedure used, i.e. the observables and the weights chosen. It is thus better to use various parameterizations, obtained by slightly varying the fit procedure, to compute nuclear observables such that one can eventually select the best one.

For this preliminary work we have chosen a small set of parameterizations, Tab. {5.1}. Nuclear properties tested here are limited to semi-magic spherical nuclei within SR-EDF approach. The reproduction of deformed nuclei and the inclusion of dynamical correlations is postponed to later; the latter being the main motivation behind the present use of a three-body pseudo-potential, see Chap. 2.

6.2 Infinite nuclear matter properties

6.2.1 Symmetric nuclear matter

In symmetric nuclear matter the adjustment focused on properties of the saturation point keeping control of the pole in the effective mass and the inflection point in the equation of state. Saturation densities (Tab. {6.1}) of our trilinear EDF tend to be systematically lower than the

$S_3Ly_{e_{K_\infty}}^{10\, e_{m_0^*/m}}$	$S_3Ly_{260}^{71}$	$S_3Ly_{250}^{73}$	$S_3Ly_{230}^{76}$	$S_3Ly_{250}^{81}$	SLy4
E/A	-16.088	-16.087	-16.062	-16.079	-15.972
$\rho_{\rm sat}$	0.157	0.157	0.157	0.157	0.160
m_0^*/m	0.710	0.730	0.760	0.810	0.695
K_∞	259.829	250.208	230.049	249.894	229.901
$\rho_{\rm cr}$	0.464	0.431	0.383	0.383	*
$\rho_{\rm infl}$	0.362	0.333	0.289	0.327	*
κ_0	0.408	0.370	0.316	0.235	0.440

Table 6.1: Saturation properties for different parameterizations.

empirical one 5.3a. Indeed, corresponding values always correspond to the targeted $e_{\rho_{\rm sat}}$ minus the accepted error $\Delta_{\rho_{\rm sat}}$ given in Eq. 5.18. This error has thus to be chosen not to large if one wants to obtain an acceptable saturation density. Other SNM properties do not show such tendency to reach the border of the allowed interval.
The energy per particle for our parameterizations is greater than the empirical starting point while it is smaller for SLy4. This enhancement with respect to empirical value 5.3b might be advantageous to reproduce a correct mass systematic. At least this happened to be necessary for (quasi) bilinear EDFs [133, 134].
Symmetric nuclear matter EOS are shown in Fig. 6.1 for the four test parameterizations as well as for SLy4. Tested parameterizations only differ at high densities such that they should be used with care to compute compact objects, e.g. neutron stars. On the other hand, we recall that densities beyond about 2 $\rho_{\rm sat}$ should be irrelevant for finite nuclei. Nevertheless, remedying such a pathological high-density behavior might be accomplished by adding a repulsive gradient-less four-body pseudo-potential. Indeed, such a pseudo-potential will provide the leading contribution to the high-density EOS, Eq. 4.19.
It is of interest to extract the contributions to the four (effective) two-body spin-isospin channels [117] and compare then to recent ab-initio calculations based on chiral two- plus three-body interactions [135]. However, the definition of such effective two-body channels is not straightforward when starting from three-body pseudo potentials and is postponed to a future work.

The isoscalar effective mass is shown in Fig. 6.2. Eliminating its pole is not straightforward. A gradient-less four-body pseudo-potential will not change such a behavior while higher-order density gradients will increase the number of such poles. The four test parameterizations display a pole beyond 2.5 $\rho_{\rm sat}$, which should be safe. However, the existence of such a pole influences the density profile of the isoscalar effective mass at lower densities, i.e. for $\rho \leq \rho_{\rm sat}$. How much this impacts properties of finite nuclei remains to be characterized. The use of Skyrme pseudo-potential requires to reject the associated critical density to high enough density.

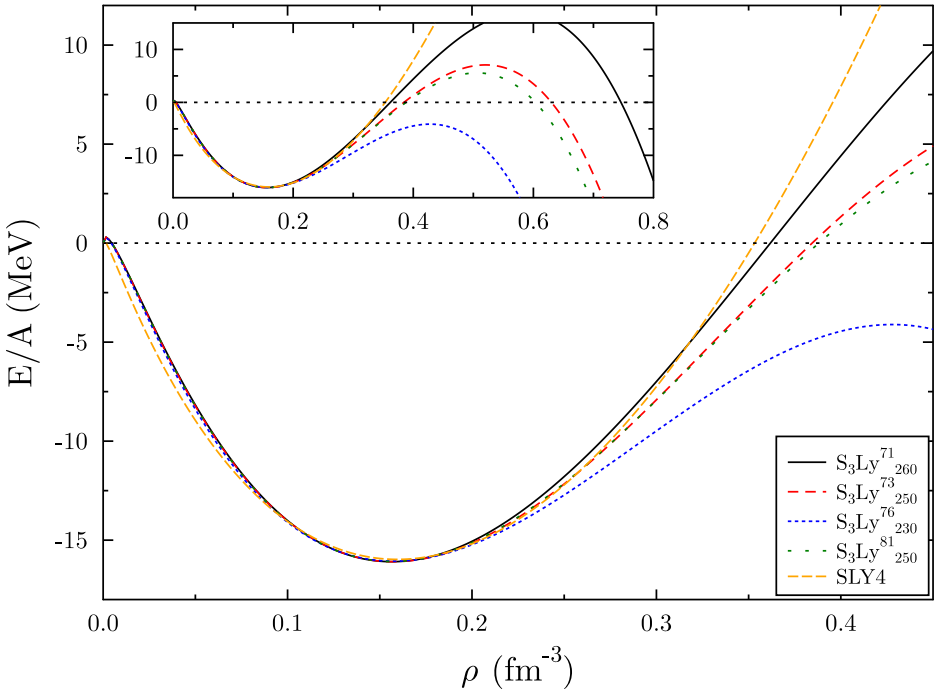

Figure 6.1: Symmetric nuclear matter equation of state for various Skyrme parameterizations. The range for the density axis is the one in which our methods is approximately valid. However, high densities values of the energy per particles are also given in the smaller window.

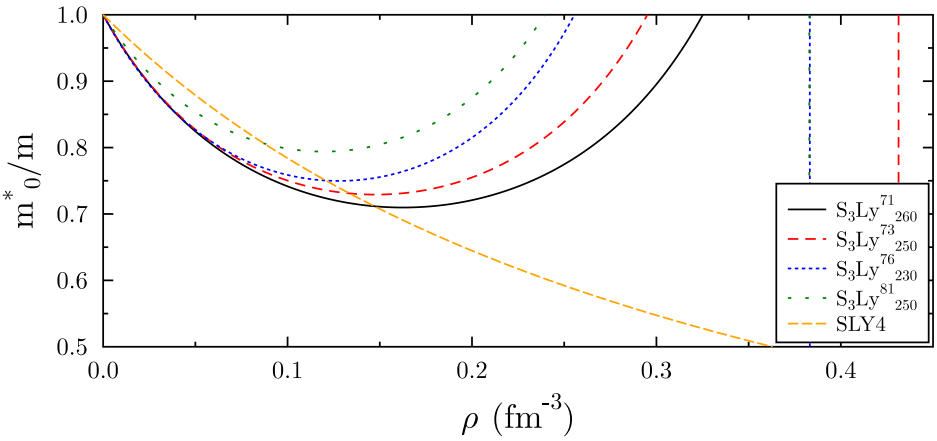

Figure 6.2: Isoscalar effective mass as a function of density.

6.2.2 Asymmetric and pure neutron matter

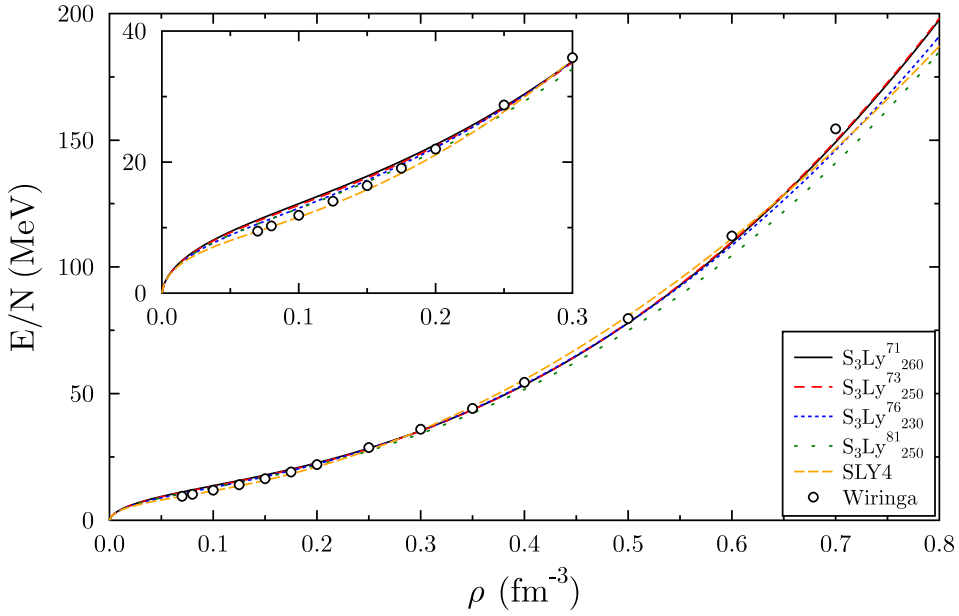

Figure 6.3: Pure neutron matter equation of state.

Ab-initio pure neutron matter EOS is well reproduced with all the four parameterizations, see FIG. 6.3. In the present study the ab-initio EOS from [127] is used to be consistent with SLy4 that is used as a benchmark. More recent ab-initio EOS exist [136] and will be used in the near future to further optimize our parameterizations.

The splitting of neutron and proton effective masses in PNM is shown in FIG. 6.4 while its

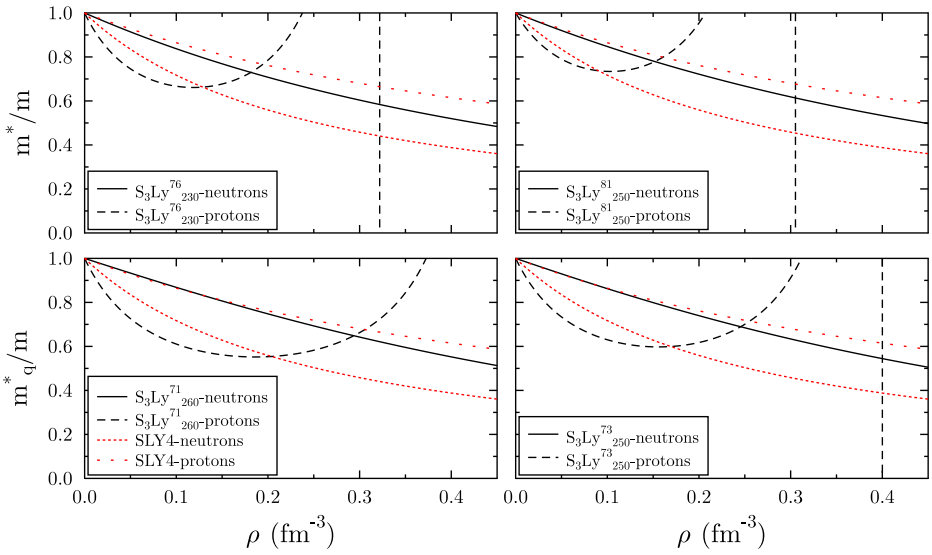

Figure 6.4: Neutron and proton effective masses.

value at saturation density is listed in TAB. {6.2}. The sign of the splitting is in agreement with ab-initio-calculations [137], contrary to modern (quasi) bilinear EDFs. The magnitude of the splitting is inversely proportional to the isoscalar effective mass, knowing that best ab-initio

$S_3Ly_{K_\infty}^{10\,m_0^*/m}$	$S_3Ly_{260}^{71}$	$S_3Ly_{250}^{73}$	$S_3Ly_{230}^{76}$	$S_3Ly_{250}^{81}$	SLy4
a_τ	31.623	31.746	31.998	32.240	32.004
m_τ^*/m	0.558	0.598	0.686	0.790	0.800
$\Delta m^*/m$	0.417	0.340	0.167	0.042	-0.186

Table 6.2: Symmetry energy coefficient, isovector effective mass and neutron-proton effective mass splitting in PNM.

calculations predict a value of the order 0.3. Nevertheless, the pole in the proton effective mass appears close to saturation density, in particular for parameterizations with the largest values of the isoscalar effective mass.
The value of the symmetry energy coefficient a_τ, Eq. 5.9 is given in Tab. {6.2} for our four parameterizations of interest. It seems that there is no strong constrains that prevent the parameterizations to get a reasonable value of this coefficient.

6.2.3 Landau parameters

Landau parameters are shown in Fig. 6.5 and their value at saturation density are listed in Tab. {6.3}. Let us remind that Landau parameters at saturation density contribute to χ^2 merit

$S_3Ly_{K_\infty}^{10\,m_0^*/m}$	$S_3Ly_{260}^{71}$	$S_3Ly_{250}^{73}$	$S_3Ly_{230}^{76}$	$S_3Ly_{250}^{81}$	SLy4
F_0	-0.153	-0.164	-0.200	-0.072	-0.276
F_0'	0.855	0.909	1.002	1.155	0.814
G_0	-0.986	-0.998	-0.998	-0.998	1.385
G_0'	-0.326	-0.365	-0.417	-0.636	0.902
F_1	-0.870	-0.810	-0.720	-0.570	-0.916
F_1'	0.815	0.664	0.325	0.077	-0.395
G_1	-0.002	0.074	0.284	0.194	0.0
G_1'	0.667	0.690	0.724	0.851	0.0

Table 6.3: Landau parameters at saturation density.

function and are constrained to respect conditions 4.33. The latter has been designed mainly to fulfill the spin instability condition, i.e. $G_0 > -1$, which was expected to be problematic for EDF deriving from a three-body pseudo-potential, see Sec. 5.2.5 and [125]. It is obvious from Tab. {6.3} that the spin instability condition would not be fulfilled without a constrain in the fit. Eventually, the instability occurs to close to saturation density and, contrary to our original hope, three-body gradient terms do not really improve the situation compared to used a simple gradient-less term. Adding a four-body gradient-less pseudo-potential might help and is postponed to the near future.
Conclusions regarding other Landau parameters are the same as in Sec. 5.2.5. Eventually, the adjustment on nuclei data does not change the qualitative behavior of Landau parameters as a function of density, compare Figs. (5.9,6.5).

Scattering amplitude sum rules presented in Sec. 4.3.7, can also be checked at saturation density. As for the first writing of those sum rules, see Eq. 4.52 test parameterizations are far to

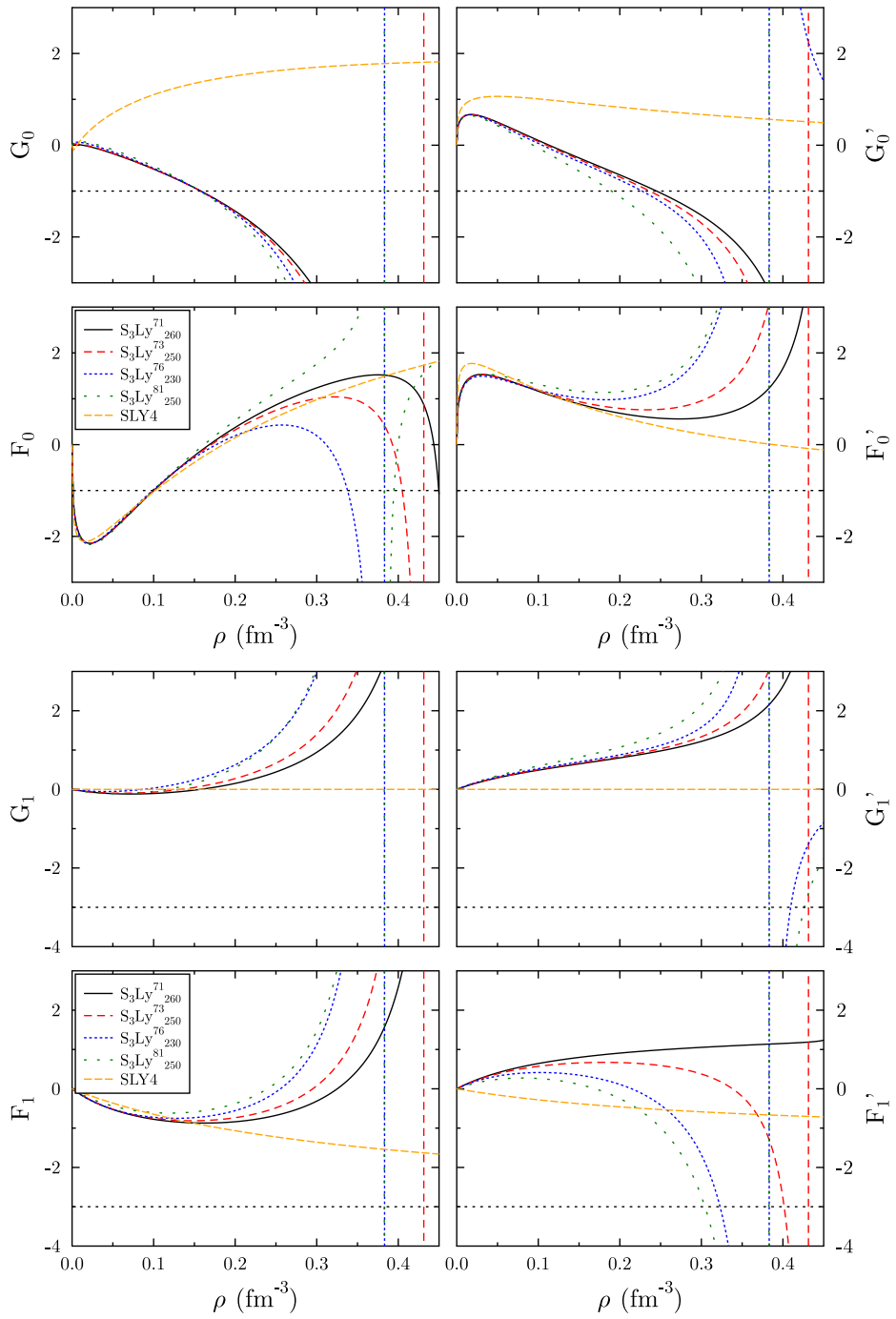

Figure 6.5: Landau parameters for different parameterizations.

$S_3Ly_{K_\infty}^{10\,m_0^*/m}$	$S_3Ly_{260}^{71}$	$S_3Ly_{250}^{73}$	$S_3Ly_{230}^{76}$	$S_3Ly_{250}^{81}$	SLy4
Eq. 4.52a	-71.630	-499.143	-500.334	-501.239	-0.652
Eq. 4.52b	-210.003	-1492.031	-1494.618	-1487.533	0.845
Eq. 4.53a	-1.222	-1.349	-1.596	-4.046	-0.278
Eq. 4.53b	-71.223	-458.693	-499.802	-499.891	-0.560

Table 6.4: Scattering amplitude sum rules Eqs. (4.52,4.53).

the physical value as a result of the spin-instability. Indeed, $G'_0 = -1$ is a pole of the scattering amplitude E_0, which is why our parameterizations send back anomalously large values for the sum rule. The first sum rule of the second writing, see Eq. 4.53a, is the only one where E_0 does not appear. As a result, the value obtained for our parameterizations, at least those with low isoscalar effective mass, are rather good compared to others given in [111] but is still not as satisfactory as for SLy4 parameterizations.

6.3 Nuclei properties

6.3.1 Pairing EDF

To compute semi-magic nuclei, a pairing functional need to be added to normal functional, Eqs. (3.40,3.53,3.54,3.91,3.92). The pairing functional coming from the two- plus three-body pseudo-potential designed in Chap. 3 has not been derived yet. As a matter of fact, it is mandatory to derive it in order to obtain a safe parameterization for MR-EDF calculations without the need for the regularization method developed in [47–49]. For this preliminary work, a simple gradient-less bilinear surface pairing EDF is used that derives from the pseudo-potential

$$v^{\kappa\kappa[\rho]} = t_{\text{pair}}\,\hat{\delta}_{r_1 r_2}\left(1 - \frac{\rho(\vec{R})}{\rho_{\text{sat}}}\right) \quad . \tag{6.1}$$

The smooth cut-off [138] is used for the active pairing space, such that it includes roughly one major shell, from 5 MeV above to 5 MeV below the Fermi level.

6.3.2 Fields and densities

Fields and densities obtained in ^{132}Sn are reproduced in Figs. (6.6,6.7) and do not display strong differences compared to those obtained from traditional (quasi) bilinear functionals. It appears that trilinear functionals lead to smoother central fields and densities as well as to spin-orbit fields and densities that are very slightly shifted towards the interior of the surface.

6.3.3 Binding energies

A systematic of binding energies is displayed in Fig. 6.8. The binding energy differences between theory and experiment is shown as a function of mass number and isospin asymmetry. Generally speaking, arches are greater for newly developed parameterizations. However the wrong trend that tends to overbind small-A nuclei and underbind large-A nuclei is attenuated for trilinear parameterizations thanks to the larger volume energy coefficient compared to SLy4 [134], which is a tendency of the trilinear parameterizations as previously discussed. However the value of the energy per particle for trilinear parameterizations is larger than the one advocated by Bertsch or Niksic [133, 134]. It seems that the ideal value for such functional is thus higher

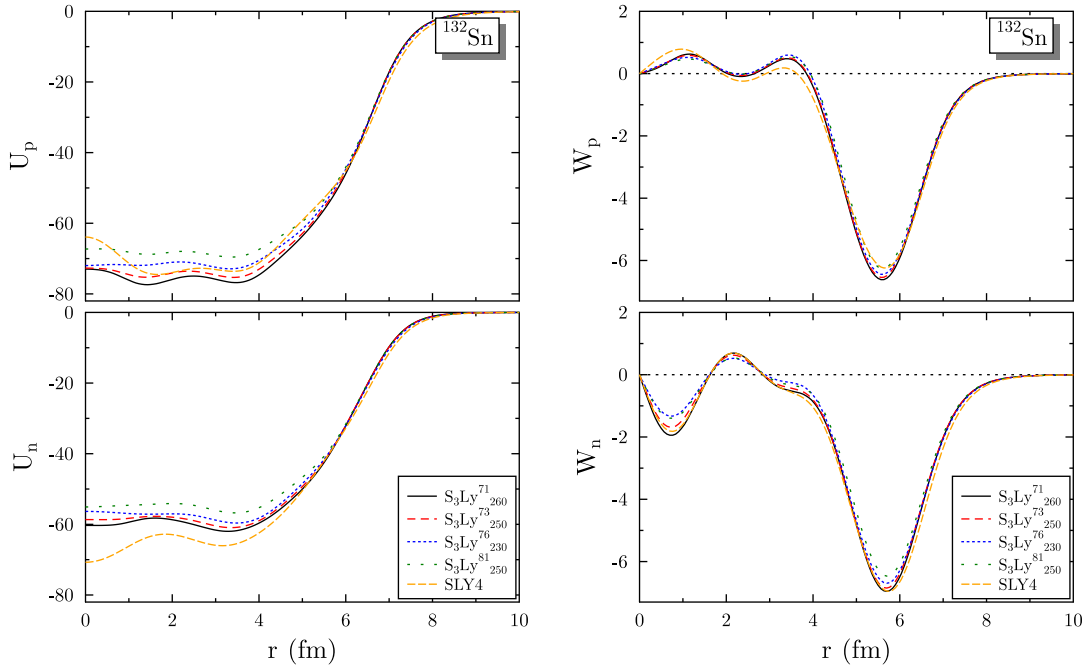

Figure 6.6: Neutron and proton, central and spin-orbit field.

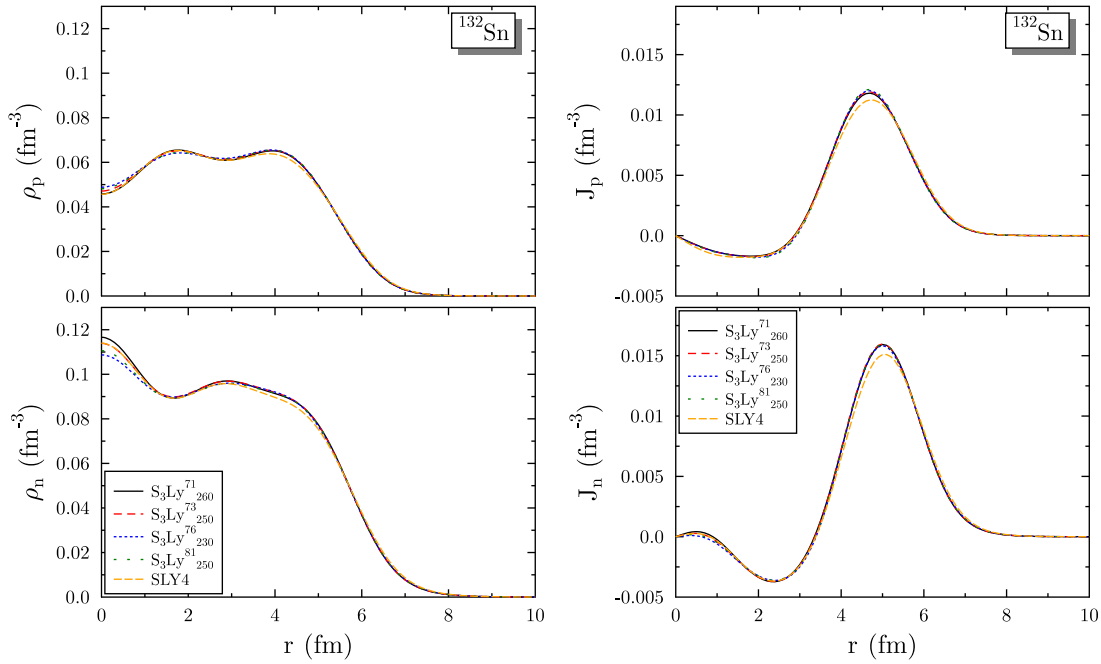

Figure 6.7: Neutron and proton, matter and spin-orbit density.

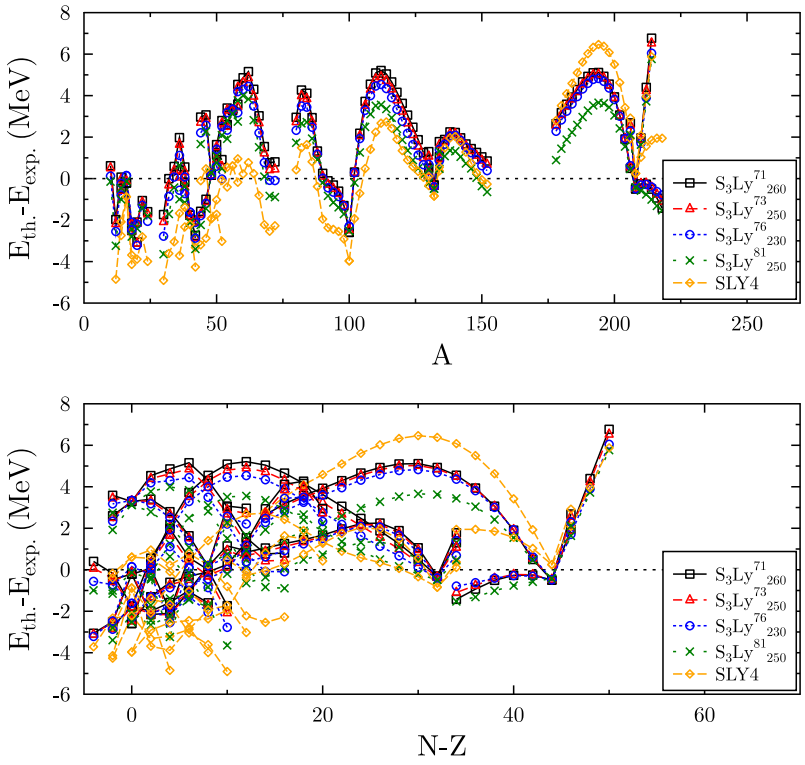

Figure 6.8: Energy differences between theory and experiment as a function of A and $N - Z$. Isotonic and isotopic chains are joined by lines.

$S_3Ly^{10\,m_0^*/m}_{K_\infty}$	$S_3Ly^{71}_{260}$	$S_3Ly^{73}_{250}$	$S_3Ly^{76}_{230}$	$S_3Ly^{81}_{250}$	SLy4
	Isotopic chains				
$\bar{\Delta}_E$ (MeV)	2.18	2.02	1.79	1.19	0.75
$\bar{\Delta}_{\|E\|}$ (MeV)	2.74	2.61	2.42	2.01	2.63
σ_E (MeV)	2.40	2.36	2.28	2.05	3.12
	Isotonic chains				
$\bar{\Delta}_E$ (MeV)	0.73	0.63	0.47	0.05	-0.54
$\bar{\Delta}_{\|E\|}$ (MeV)	1.63	1.56	1.46	1.38	1.67
σ_E (MeV)	1.87	1.82	1.76	1.70	2.03

Table 6.5: Average of the theoretical and experimental energy differences and of their absolute values, as well as rms deviations, for isotopic and isotonic chains.

than for traditional (quasi) bilinear EDFs. Similarly, nuclei with large isospin asymmetry are now as underbound as nuclei with small isospin asymmetry. Also the parameterization with the largest value of the isoscalar effective mass $S_3Ly^{81}_{250}$ reproduces the best experimental masses with the smallest. This follows the trend seen with (quasi) bilinear parameterizations [139]. More quantitative comparisons can be performed by computing [140, 141] the average of errors

$$\bar{\Delta}_E = \langle E_{\text{th.}} - E_{\text{exp.}} \rangle \ , \tag{6.2}$$

as well as of the errors absolute value $\bar{\Delta}_{|E|}$ as well as the rms deviation

$$\sigma_E = \sqrt{\langle \left(\Delta_E - \bar{\Delta}_E\right)^2 \rangle} \ , \tag{6.3}$$

for each parameterization, see TAB. {6.5}. The average error is smaller for SLy4 parameterization than for trilinear EDF ones as a result of compensation effects induced by the wrong mass trend mentioned above. On the other hand, $\bar{\Delta}_{|E|}$ and rms deviation are larger for SLy4. Trilinear parameterizations are thus better to reproduce experimental binding energies, and $S_3Ly^{81}_{250}$ is the best of all. It also appears that isotonic chains are better reproduced for all four parameterizations compared to SLy4.

6.3.4 Radii

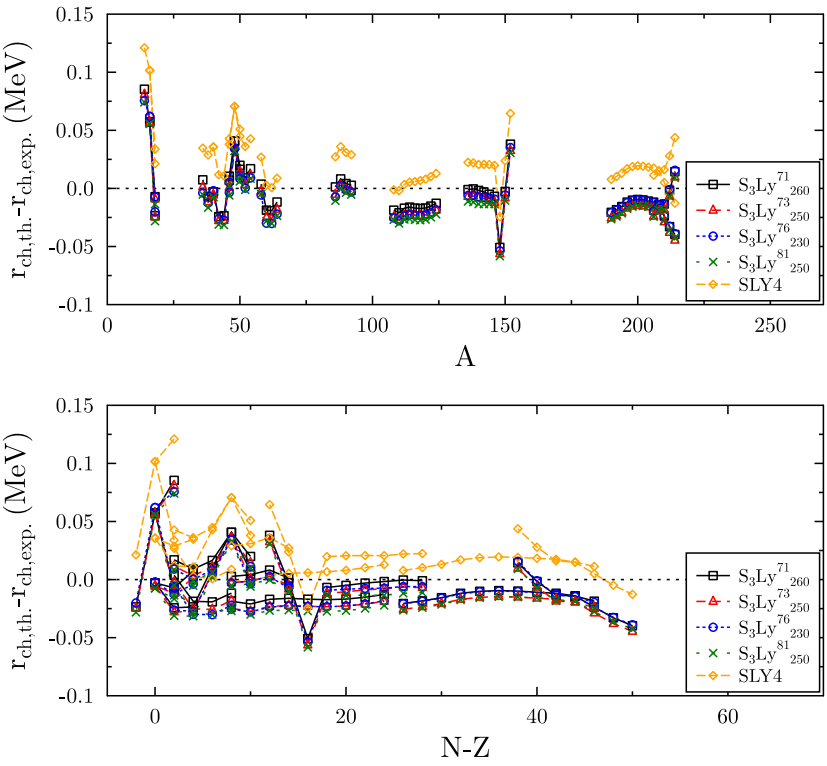

Figure 6.9: Difference of theoretical and experimental charge radius differences as a function of A and $N - Z$.

The difference between theoretical and experimental charge radii is displayed in FIG. 6.9 as a function of mass number and isospin asymmetry. In this case there is no difference between small and large mass number or isospin asymmetry. However it can be seen that SLy4 systematically

$S_3Ly_{K_\infty}^{10\,m_0^*/m}$	$S_3Ly_{260}^{71}$	$S_3Ly_{250}^{73}$	$S_3Ly_{230}^{76}$	$S_3Ly_{250}^{81}$	SLy4
	Isotopic chains				
$\bar{\Delta}_{r_c}$ (10^{-2} fm)	-1.0	-1.6	-1.4	-1.8	1.7
$\bar{\Delta}_{\lvert r_c\rvert}$ (10^{-2} fm)	1.8	2.2	2.0	2.4	1.9
σ_{r_c} (10^{-2} fm)	1.8	1.9	1.9	1.8	2.2
	Isotonic chains				
$\bar{\Delta}_{r_c}$ (10^{-2} fm)	0.5	0.0	0.1	-0.3	3.5
$\bar{\Delta}_{\lvert r_c\rvert}$ (10^{-2} fm)	1.6	1.7	1.5	1.8	3.6
σ_{r_c} (10^{-2} fm)	2.5	2.5	2.4	2.5	2.7

Table 6.6: Average of the theoretical and experimental charge radius differences and of their absolute values, as well as rms deviations, for isotopic and isotonic chains.

over-estimates charge radii, while trilinear ones under-estimate them. Even if adding dynamical correlations will increase charge radii overall, it will not be sufficient in most cases to agree well with experimental data [142]. Still it is more comfortable to underestimate experimental data at the SR-EDF level.
Overall, all four trilinear parameterizations give rather similar results for charge radii. On a more detailed level, $S_3Ly_{250}^{81}$ appears to be the worst parameterization and $S_3Ly_{260}^{71}$ the best. It can be seen from the average of the errors and the rms deviation given in Tab. {6.6}. Trilinear parameterizations are slightly better than Sly4. All three parameterizations behave very similarly with no significant trend among them, i.e. the variation among the set is negligible compared to the difference with SLy4.

6.3.5 Two-nucleon separation energies

Two-neutron and two-proton separation energies

$$S_{2n}(N,Z) = E(N-2,Z) - E(N,Z) \ , \tag{6.4a}$$
$$S_{2p}(N,Z) = E(N,Z-2) - E(N,Z) \ , \tag{6.4b}$$

are presented in Figs. (6.10,6.11). Differences between parameterizations are insignificant compared to differences with data. Theoretical and experimental separation energies differ the most in tin and lead isotopes around magic shell gaps, showing that level density around Fermi level is not large enough as a result of small effective masses and missing correlations [142]. Trilinear functional parameterizations enhance slightly such a feature.

6.3.6 Pairing gaps

A measure of pairing correlations can be assessed through the extraction of pairing gaps. The connection between finite difference mass formulae employed to extract the odd-even mass staggering and theoretical gaps presently used is not straightforward [143–145]. A zeroth-order

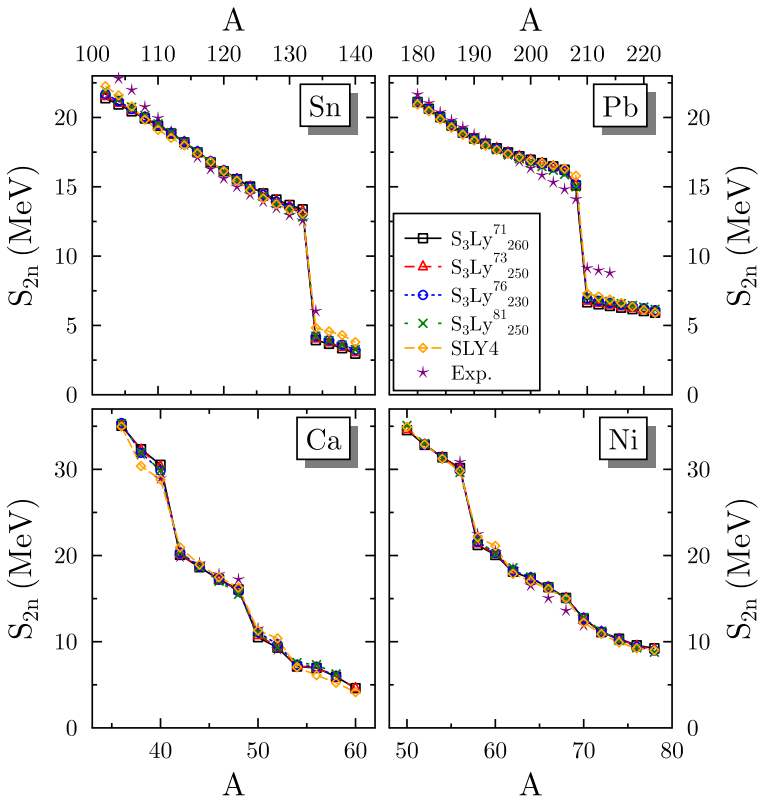

Figure 6.10: Isotopic chains separation energies.

comparison is obtained by displaying experimental three-point mass difference formula,

$$\Delta_n^{(3)}(N) \equiv \frac{(-1)^N}{2}\Big[E(N-1,Z) - 2E(N,Z) + E(N+1,Z)\Big] \ , \tag{6.5a}$$

$$\Delta_p^{(3)}(Z) \equiv \frac{(-1)^Z}{2}\Big[E(N,Z-1) - 2E(N,Z) + E(N,Z+1)\Big] \ , \tag{6.5b}$$

against theoretical spectral gaps at the Fermi energy calculated in even-even nuclei. Such a comparison is shown in Figs. (6.12,6.13). Furthermore theoretical gaps presented in this study do not take into account (i) time reversal symmetry breaking effects in odd nuclei, (ii) self consistent blocking effects as well as (iii) dynamical pairing fluctuations, such that it is difficult at this level to assess which parameterizations are performing best.

Trilinear parameterizations tend to generate smaller gaps, reflecting a smaller density spectrum around the Fermi level. It has to be determined if this scattered spectrum is systematic and global, even for parameterizations with large m_0^*, or a local effect due to levels rearrangement. Anti-pairing Coulomb effect is known to reduce proton pairing gaps with respect to neutrons ones [146]. But theoretically proton gaps are also under-estimating experimental odd-even mass staggering, due to the pairing functional structure. As a result of the neutron skin in heavy nuclei, an isoscalar density dependence in the pairing functional, generates smaller proton gaps than neutron ones. Adding an isovector density dependence to the pairing functional corrects for this unwanted effect that is usually compensated for by using a stronger proton pairing strength [147].

Eventually, the pairing functional we aim to develop will not be derived from a density-dependent pseudo-potential but rather from the two- plus three-body pseudo-potential used for the particle-

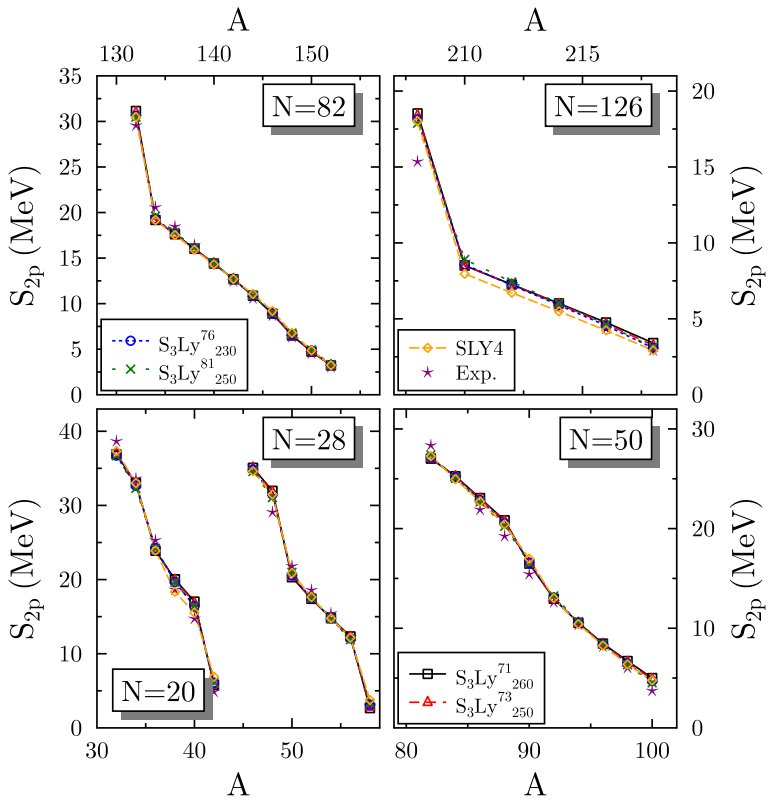

Figure 6.11: Isotonic chains separation energies.

hole part. This is necessary to avoid self-pairing effects and thus to perform safe MR-EDF calculations [47–49].

6.3.7 Effective single-particle energies

Difficulties also arise regarding the definition and interpretation of single-particle energies. Experimentally one accesses one-nucleon separation energies from two neighboring nuclei. In EDF models, however, it is customary to discuss the shell structure in terms of the eigen-spectrum of the one-body field h (Eq. 3.103). In case of magic nuclei and assuming a magic core neither subject to rearrangement or polarization effects nor to any collective excitation following the addition or removal of a nucleon, separation energies with eigen-states of the odd-mass neighbors are equal to single-particle energies, Koopmans' theorem is fulfilled [148]. This highly idealized situation is modified by static and dynamic correlations, e.g. core polarization and particle-vibration coupling, that fragment the single-particle strength, and thus alter one-nucleon separation energies. When the fragmentation is significant, the naive comparison between calculated single-particle energies and experimental separation energies is not meaningful anymore [149]. It is however possible to extract *a posteriori* from a strongly correlated system an effective single-particle shell structure, from which correlations are to a large extent screened out, as centroids of separation energies [150–152]. Such centroids are shown, within SR-EDF method, to precisely correspond to eigenvalues of the one-body field h [153].
As a result, one should compared both experimental and theoretical separation energies, which is difficult to compute for the theoretical part, or both experimental and theoretical centroids of separation energies, i.e. effective single-particle energies, which is hard to assess from experi-

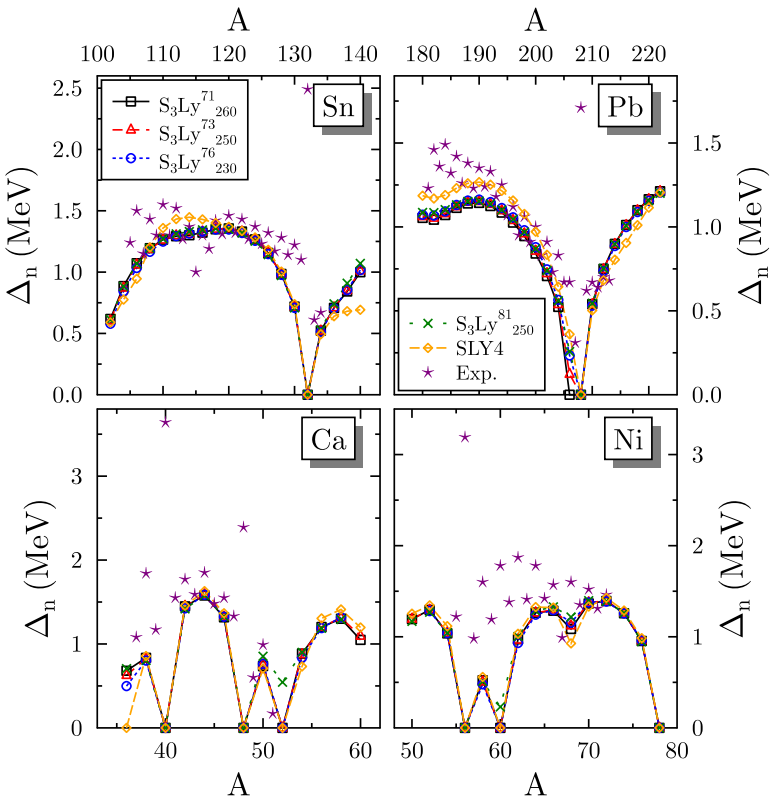

Figure 6.12: Neutron theoretical spectral gaps against experimental evaluation of odd-even mass staggering extracted through three-point mass formulas, for isotopic chains.

ments. For the present discussion, experimental separation energies are compared to theoretical single-particle energies. The effective single-particle shell structure of selected doubly-magic nuclei is discussed at the SR-EDF level, i.e. omitting core polarization effects. The single-particle spectrum of tin isotopes is reproduced in FIG. 6.14, while selected spin-orbit splittings, defined through [154]

$$\Delta\epsilon_l \equiv \frac{1}{2l+1}\Big(\epsilon_{j=l-1/2} - \epsilon_{j=l+1/2}\Big) \ , \tag{6.6}$$

and spin-orbit centroids, defined thanks to

$$\epsilon_l^{\rm cent} = \frac{l+1}{2l+1}\epsilon_{j=l+1/2} + \frac{l}{2l+1}\epsilon_{j=l-1/2} \ , \tag{6.7}$$

are shown in FIG. 6.15 and FIG. 6.16, respectively. One observes that

- Spin-orbit splitting of pairs of levels located on opposite sides of the Fermi energy are not safe at the SR-EDF level. The level that is below Fermi level, for such pairs, is the so-called intruder state. Polarization effects entering in the core state energies affect significantly such splittings [149]. Such pairs of single-particle states are indicated in red in FIGS. (6.15,6.16).
- Pairs of single-particle energies that are far from the Fermi energy are likely to relate to a strongly fragmented strength, such that they are likely to have lost their single-particle nature. Those pairs are indicated in blue in FIGS. (6.15,6.16).

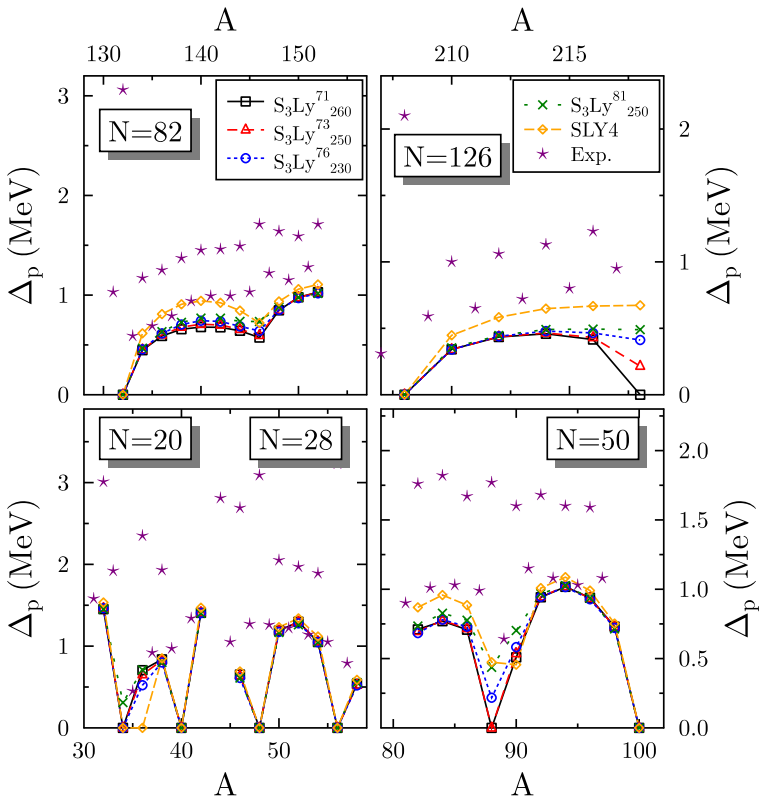

Figure 6.13: Proton theoretical spectral gaps against experimental evaluation of odd-even mass staggering extracted through three-point mass formulas, for isotonic chains.

As a consequence, EDF calculations should overestimate empirical spin-orbit splittings for red pairs, that are expect to be decreased by polarization effects. Looking at Fig. 6.15 we observe, however, that all parameterizations give values that are already close to experimental ones, or even smaller for trilinear parameterizations. On the other hand, spin-orbit splittings of blue pairs, that are not expecting to be changed adding polarization effects, are in general too large for all the parameterizations, but tend to be smaller for trilinear parameterizations compared to (quasi) bilinear one. Consequences of such wrong trend has been discussed in [155]. Trilinear parameterizations do not provide any improvement in that respect.
On this side, improvements might come from the inclusion of the spin-orbit three-body pseudo-potential that could be adjusted to improve those particular features.

Differences between parameterizations for spin-orbit centroids are small, there is thus no advantages or disadvantages to use trilinear or (quasi) bilinear parameterizations.

It appear that (Figs. (6.14,6.16))

- Spin-orbit centroids of high-l intruder states, such as $\pi 1g$, $\nu 1h$ for ^{132}Sn and $\pi 1h$, $\nu 1i$ for ^{208}Pb, are close to experiments
- Spin-orbit centroids of states that are both above the Fermi level, such as $\pi 2d$, $\nu 2f$ for ^{132}Sn and $\pi 2f$, $\nu 2g$ for ^{208}Pb, tend to be overestimated
- Spin-orbit centroids of states that are both below the Fermi level, such as $\nu 2d$ for ^{132}Sn and $\pi 2d$, $\nu 2f$ for ^{208}Pb, are strongly underestimated.

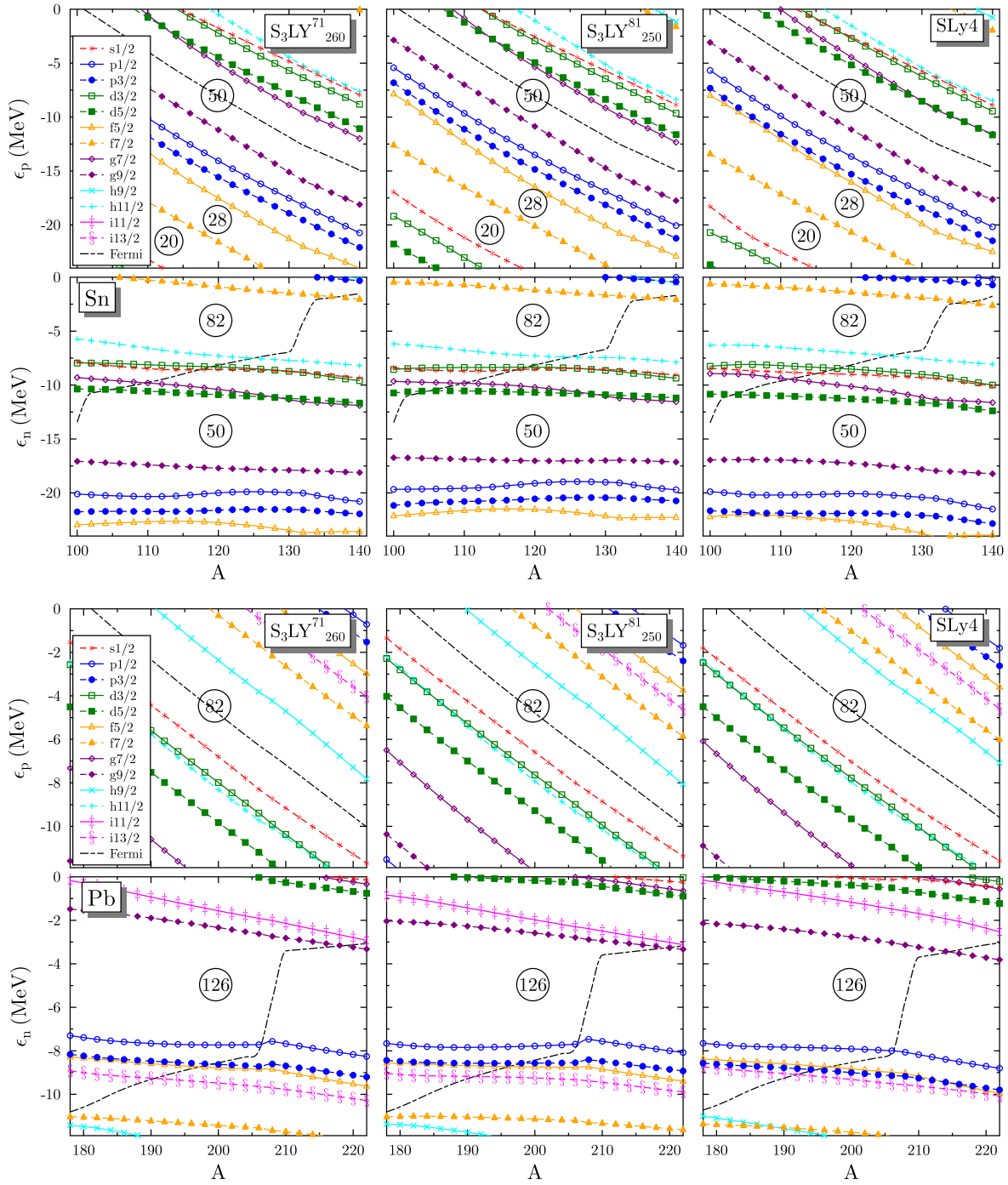

Figure 6.14: Effective single-particle energies of tin and lead isotopes around the Fermi level.

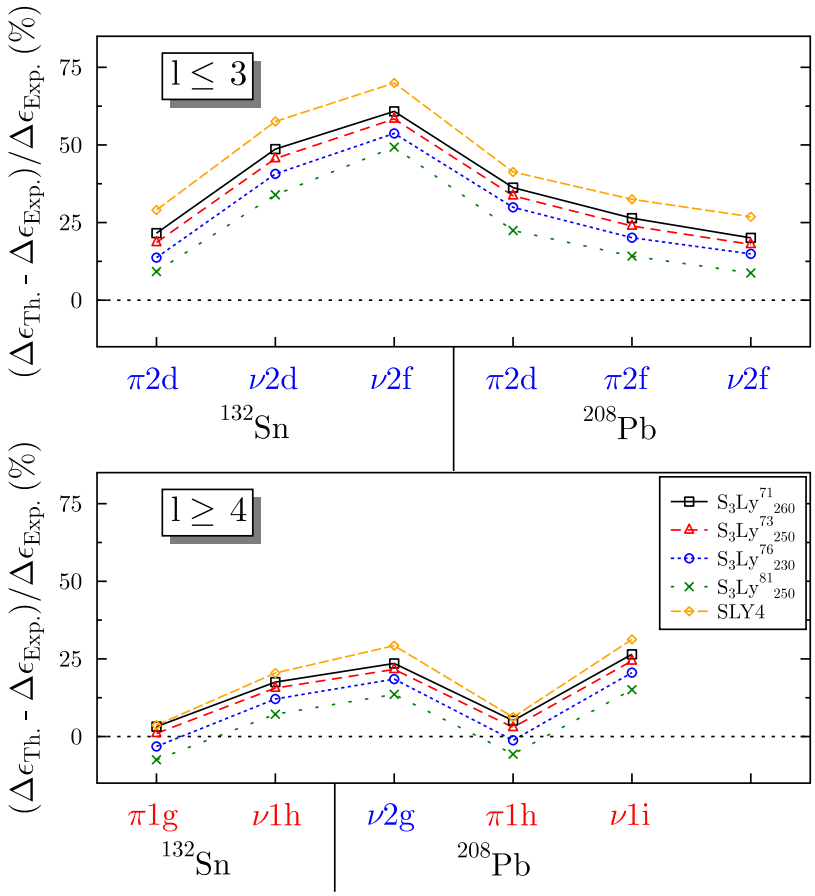

Figure 6.15: Relative theoretical-experimental differences of selected spin-orbit splittings. Red levels correspond to spin-orbit splitting that are on opposite side of the Fermi energy, and thus not safe at the SR-EDF. Blue levels correspond to spin-orbit splitting far from Fermi energy and thus do not have a clear single-particle nature.

As a consequence intruder states are sometimes wrongly put above states below the Fermi level, e.g. intruder state $\nu 1h_{11/2}$ is above $\nu 2d_{3/2}$ and $3s_{1/2}$ levels in tin isotopes, see FIG. 6.14. This problem is shared by all standard mean-fields methods [155], which compromises the description of entire mass regions.

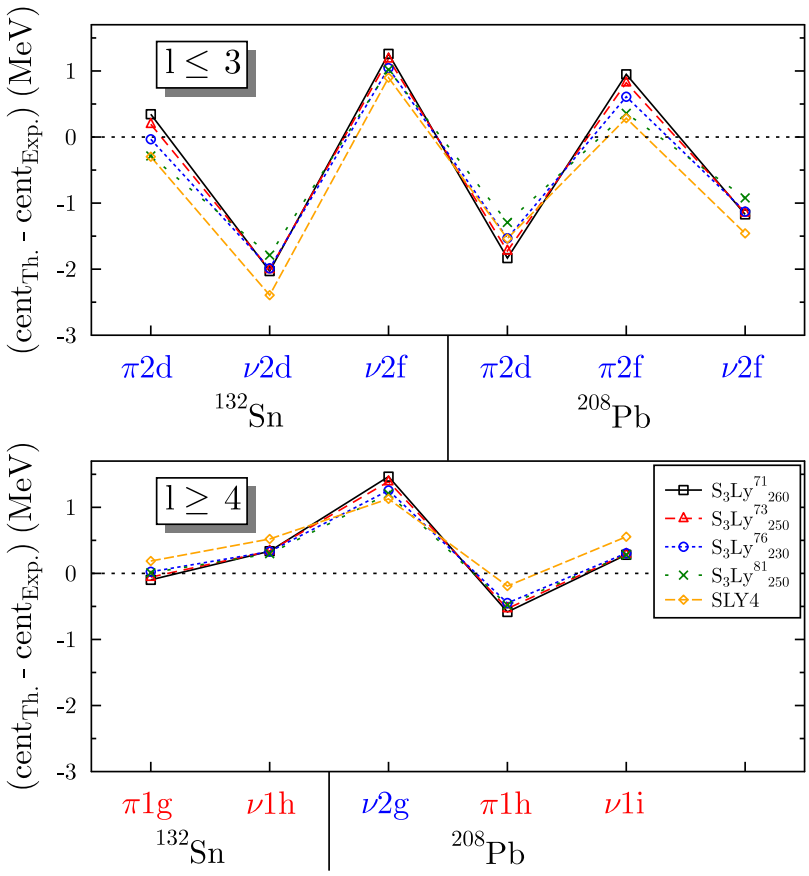

Figure 6.16: Theoretical-experimental differences of selected spin-orbit centroids. Red levels correspond to spin-orbit splitting that are on opposite side of the Fermi energy, and thus not safe at the SR-EDF. Blue levels correspond to spin-orbit splitting far from Fermi energy and thus do not have a clear single-particle nature.

Conslusions and outlook

Breaking and restoration of symmetries

The first part of the present document reviews the notion of symmetry breaking and restoration within the frame of the nuclear energy density functional (EDF) method (see Chaps. 1,2). Multi-reference (MR) EDF calculations are nowadays routinely applied with the aim of including long-range correlations associated with large-amplitude collective motions that are difficult to incorporate in a more traditional single-reference (SR), i.e. "mean-field", EDF formalism [45].

In the present work, we elaborate on key differences between pseudo-potential-based and more general implementations of the EDF method (see Chaps. 1,2). In particular, we point to difficulties encountered when formulating symmetry restoration within the EDF approach. The analysis performed in Ref. [48] to tackle problems encountered in Refs. [68–70] for particle number restoration serves as a baseline. Reaching out to angular-momentum restoration, we identify in a pseudo-potential-based framework a mathematical property of the energy density $\mathcal{E}^{LM}(\vec{R})$ associated with angular momentum restoration that could be used to constrain EDF kernels (see Chap. 2 and Appendix E). Consequently, possible future routes to better formulate symmetry restorations within the EDF method could encompass the following points.

- The fingerprints left on the energy density $\mathcal{E}^{LM}(\vec{R})$ by angular momentum conservation in a pseudo-potential-based method could be exploited to constrain the functional form of the energy kernel $E[\rho, \kappa, \kappa^*]$ when using a more general implementation of the EDF method.
- The regularization method proposed in Ref. [47] to deal with specific spurious features of MR-EDF calculations should be investigated as to what impact it has on properties of the energy density $\mathcal{E}^{LM}(\vec{R})$ in the case of angular momentum restoration.
- Similar mathematical properties extracted from a pseudo-potential-based method could be worked out for other symmetry groups of interest and used to constrain the form of the EDF kernel.

Efforts in those directions are currently being made [85]. An alternative consists of sticking to a well-defined pseudo-potential-based EDF method. However, there does not exist at this point in time such a parameterization of the EDF kernel that provides good enough phenomenology. The second part of the present thesis was dedicated to building such a parameterization.

Three-body Skyrme pseudo-potential

The second part of the present document deals with the development of a three-body Skyrme pseudo-potential added to the usual two-body one (see Chaps. 3,5,6).

First, the most general three-body Skyrme pseudo-potential was designed and the corresponding EDF kernel was derived (see Chap. 3). Second, the two- plus three-body pseudo-potential parameters were fitted to nuclear observables following a procedure close to the one used in the past to build Saclay-Lyon parameterizations of (quasi) bilinear functionals (see Chap. 5). Eventually, it seems possible to generate a parameterization that strictly derives from a pseudo-

potential and that provides as good results as state of the art (quasi) bilinear functionals (see Chap. 6). This is of great interest in view of performing safe MR-EDF calculations.
Outlooks of the present work are numerous and can be summarized as follows.

Functional form

The analytical derivation of the EDF from the central three-body pseudo-potential has constituted an important and non straightforward part of the present work. Further steps need to be accomplished in that respect.

- The derivation of the pairing functional corresponding to the pseudo-potential developed in Chap. 3 is the most crucial part, as it is needed to perform fully safe MR-EDF calculations. Such a derivation will follow similar steps as for the normal part of the EDF kernel, such that minor improvements of the formal computation code should be sufficient to perform this derivation.
- It is also necessary to derive the contributions of the three-body spin-orbit and tensor pseudo-potentials to the EDF kernel. This is of interest in view of improving the predictions of the one-nucleon shell structure. The formal computation code is expected to be more involved as one has to deal with the coupling between gradients and spin Pauli matrices that characterizes such pseudo-potentials.
- The derivation of the EDF from a four-body gradient-less pseudo-potential is straightforward and has already been performed.

Fit procedure

In this preliminary study, we have produced trilinear parameterizations using the standard Saclay-Lyon fitting procedure. In the future we aim at developing a more advanced fitting procedure.

- First, one needs to study if a gradient-less four-body pseudo-potential allows a better control of SNM critical and inflection densities, $\rho_{\rm cr}$ and $\rho_{\rm infl}$, as well as of spin instabilities, the latter being the weak point of the trilinear parameterizations developed in the present work.
- Modern INM EOS coming from ab-initio methods are also planned to be used, in particular for PNM. It would be also interesting to see if the adjustment of the parameterizations on effective two-body (S,T) channels and/or partial waves of the SNM EOS is possible. However, this necessitates the extraction of the effective two-body vertex from our three-body pseudo-potential.
- An analog study to the one performed in [117] on finite-size instabilities is necessary for our trilinear parameterizations. This is underway. Eventually, the aim is to couple the RPA code that accesses such instabilities to the adjustment procedure in order to reject unstable parameterizations.

Other improvements of the fitting procedure are kept for the long term, e.g.

- the adjustment on semi-magic nuclei, once the trilinear pairing functional has been derived
- the use of semi-infinite nuclear matter to constrain the surface energy coefficient
- the adjustment on pseudo-data, i.e. experimental data from which MR correlations have been subtracted.

Post-fit analysis

In the present document, the study of nuclear observables has been limited to a set of semi-magic nuclei. It has been sufficient to characterize the basic performance of the new parameterizations by benchmarking them against the results obtained with SLy4 [108]. In the near future, we aim at studying a wider range of observables, including

- properties of deformed nuclei
- those that are strongly impacted by dynamical correlations and for which MR-EDF calculations are mandatory.

Eventually, a more systematic post-fit analysis is needed. A large set of observables against which parameterizations have to be tested must be determined. Moreover, statistical analysis tools are planned to be used in the spirit of recent studies [156–158].

Appendix A

Skyrme functional calculations and complementary tools

Abstract: Complementary tools regarding the definition of the Skyrme pseudo potential are provided and the derivation of the corresponding Skyrme EDF is performed.

Contents

A.1 Computation of the energy

The aim of this section is to prove Eq. 3.3 that provides the energy resulting from the pseudo Hamiltonian Eq. 3.1 in terms of normal and anomalous density matrices Eq. 3.4. The matrix

element of the kinetic part of the Hamiltonian is easily obtained using Eq. 3.4a and reads

$$E^{\rho}_{kin} \equiv \sum_{ij} \langle i|\hat{t}|j\rangle \rho_{ji} \ . \tag{A.1}$$

Eq. A.1 shows that the kinetic energy density is linear in the normal density matrix. The pseudo two-body part of the energy is obtained using Wick theorem [87], that expresses the matrix element of two creation and two annihilation operators in terms of normal and anomalous one-body density matrices

$$\langle \Phi|a^{\dagger}_i a^{\dagger}_j a_l a_k|\Phi\rangle \quad = \quad \rho_{ki}\rho_{lj} - \rho_{kj}\rho_{li} + \kappa^{*}_{ij}\kappa_{kl} \ . \tag{A.2}$$

Knowing that $\kappa_{kl} = \frac{1}{2}\kappa_{kl} - \frac{1}{2}\kappa_{lk}$, owing to the skew symmetric nature of the anomalous density matrix, the two-body energy reads

$$E^{\rho\rho}_{Sk} \equiv \frac{1}{2}\sum_{ijkl} \tilde{v}^{2Sk}_{ijkl}\ \rho_{ki}\,\rho_{lj} + \frac{1}{4}\sum_{ijkl} \tilde{v}^{2Sk}_{ijkl}\ \kappa^{*}_{ij}\,\kappa_{kl} \ , \tag{A.3}$$

where $\tilde{v}^{2Sk}_{ijkl}$ denotes antisymmetrized matrix elements

$$\tilde{v}^{2Sk}_{ijkl} \equiv \langle ij|v^{2Sk}\mathcal{A}_{12}|kl\rangle = v^{2Sk}_{ijkl} - v^{2Sk}_{ijlk} \ . \tag{A.4}$$

Eq. A.3 shows that the energy density deriving from the two-body part of the pseudo potential is bilinear in the density matrices. The pseudo three-body part works equivalently. First, let us write only the part involving normal contractions, i.e.

$$\begin{aligned}\langle \Phi|a^{\dagger}_i a^{\dagger}_j a^{\dagger}_k a_n a_m a_l|\Phi\rangle_{\rho\rho\rho} = {} & \rho_{li}\rho_{mj}\rho_{nk} - \rho_{mi}\rho_{lj}\rho_{nk} - \rho_{ni}\rho_{mj}\rho_{lk} \\ & -\rho_{li}\rho_{nj}\rho_{mk} + \rho_{ni}\rho_{lj}\rho_{mk} + \rho_{mi}\rho_{nj}\rho_{lk} \ ,\end{aligned} \tag{A.5}$$

which after renaming indices, reads

$$\frac{1}{6}\sum_{ijklmn} v^{3Sk}_{ijklmn}\langle \Phi|a^{\dagger}_i a^{\dagger}_j a^{\dagger}_k a_n a_m a_l|\Phi\rangle_{\rho\rho\rho} \quad = \quad \frac{1}{6}\sum_{ijklmn} \tilde{v}^{3Sk}_{ijklmn}\rho_{li}\rho_{mj}\rho_{nk} \ , \tag{A.6}$$

where $\tilde{v}^{3Sk}_{ijklmn}$ denotes antisymmetrized matrix elements

$$\tilde{v}^{3Sk}_{ijklmn} \equiv \langle ijk|v^{3Sk}\mathcal{A}_{123}|lmn\rangle = v^{3Sk}_{ijklmn} - v^{3Sk}_{ijkmln} - v^{3Sk}_{ijknml} - v^{3Sk}_{ijklnm} + v^{3Sk}_{ijkmnl} + v^{3Sk}_{ijknlm} \ . \tag{A.7}$$

As to the part involving anomalous contractions, one finds

$$\begin{aligned}\langle \Phi|a^{\dagger}_i a^{\dagger}_j a^{\dagger}_k a_n a_m a_l|\Phi\rangle_{\kappa\kappa\rho} \quad = \quad & +\kappa^{*}_{ij}\kappa_{lm}\rho_{nk} - \kappa^{*}_{ij}\kappa_{ln}\rho_{mk} + \kappa^{*}_{ij}\kappa_{mn}\rho_{lk} \\ & -\kappa^{*}_{ik}\kappa_{lm}\rho_{nj} + \kappa^{*}_{ik}\kappa_{ln}\rho_{mj} - \kappa^{*}_{ik}\kappa_{mn}\rho_{lj} \\ & +\kappa^{*}_{jk}\kappa_{mn}\rho_{li} - \kappa^{*}_{jk}\kappa_{ln}\rho_{mi} + \kappa^{*}_{jk}\kappa_{lm}\rho_{ni} \ ,\end{aligned} \tag{A.8}$$

such that

$$\frac{1}{6}\sum_{ijklmn} v^{3Sk}_{ijklmn}\langle \Phi|a^{\dagger}_i a^{\dagger}_j a^{\dagger}_k a_n a_m a_l|\Phi\rangle_{\kappa\kappa\rho} = \frac{1}{2}\sum_{ijklmn} \Big[+ v^{3Sk}_{ijklmn} - v^{3Sk}_{ijklnm} - v^{3Sk}_{ijknml}\Big]\kappa^{*}_{ij}\kappa_{lm}\rho_{nk} \tag{A.9}$$

where we have used that $v^{3Sk}_{abcdef} = v^{3Sk}_{acbdfe} = v^{3Sk}_{bcaefd}$ and $\kappa_{ab} = -\kappa_{ba}$. To make antisymmetrized matrix elements appear, we further proceed as

$$\begin{aligned}
\frac{1}{6}\sum_{ijklmn} v^{3Sk}_{ijklmn}\langle\Phi|a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l|\Phi\rangle_{\kappa\kappa\rho} &= \frac{1}{2}\sum_{ijklmn}\frac{1}{2}\Big[+v^{3Sk}_{ijklmn}+v^{3Sk}_{ijklmn}-v^{3Sk}_{ijklnm} \\
&\qquad -v^{3Sk}_{ijklnm}-v^{3Sk}_{ijknml}-v^{3Sk}_{ijknml}\Big]\kappa^*_{ij}\kappa_{lm}\rho_{nk} \\
&= \frac{1}{4}\sum_{ijklmn}\Big[+v^{3Sk}_{ijklmn}-v^{3Sk}_{ijkmln}-v^{3Sk}_{ijklnm} \\
&\qquad +v^{3Sk}_{ijkmnl}-v^{3Sk}_{ijknml}+v^{3Sk}_{ijknlm}\Big]\kappa^*_{ij}\kappa_{lm}\rho_{nk} \\
&= \frac{1}{4}\sum_{ijklmn}\tilde{v}^{3Sk}_{ijklmn}\kappa^*_{ij}\kappa_{lm}\rho_{nk}\ .
\end{aligned} \tag{A.10}$$

Combining Eq. A.6 and Eq. A.10, the potential energy deriving from the three-body part of the pseudo potential finally reads

$$E_{\rho\rho\rho} \equiv \frac{1}{6}\sum_{ijklmn}\tilde{v}^{3Sk}_{ijklmn}\rho_{li}\rho_{mj}\rho_{nk} + \frac{1}{4}\sum_{ijklmn}\tilde{v}^{3Sk}_{ijklmn}\kappa^*_{ij}\kappa_{lm}\rho_{nk}\ , \tag{A.11}$$

such that the associated energy density is trilinear in the density matrices

A.2 Quasi-local densities rules

Rules used in Sec. 3.1.3.4 are now proven. Let us first rewrite them explicitly as

$$\nabla_{\vec{r},\mu}\,\rho_q(\vec{r},\vec{r}')\Big|_{\vec{r}=\vec{r}'} = \frac{1}{2}\nabla_\mu\rho_q(\vec{r}) + i\,j_{q,\mu}(\vec{r}) \tag{A.12a}$$

$$\nabla_{\vec{r}',\mu}\,\rho_q(\vec{r},\vec{r}')\Big|_{\vec{r}=\vec{r}'} = \frac{1}{2}\nabla_\mu\rho_q(\vec{r}) - i\,j_{q,\mu}(\vec{r}) \tag{A.12b}$$

$$\nabla_{\vec{r},\mu}\,s_{\nu,q}(\vec{r},\vec{r}')\Big|_{\vec{r}=\vec{r}'} = \frac{1}{2}\nabla_\mu s_{\nu,q}(\vec{r}) + i\,J_{q,\mu\nu}(\vec{r}) \tag{A.12c}$$

$$\nabla_{\vec{r}',\mu}\,s_{\nu,q}(\vec{r},\vec{r}')\Big|_{\vec{r}=\vec{r}'} = \frac{1}{2}\nabla_\mu s_{\nu,q}(\vec{r}) - i\,J_{q,\mu\nu}(\vec{r}) \tag{A.12d}$$

$$\vec{\nabla}_{\vec{r}}\cdot\vec{\nabla}_{\vec{r}}\,\rho_q(\vec{r},\vec{r}')\Big|_{\vec{r}=\vec{r}'} = \frac{1}{2}\vec{\nabla}^2\rho_q(\vec{r}) - \tau_q(\vec{r}) - \sum_\mu i\,\nabla_\mu j_{q,\mu}(\vec{r}) \tag{A.12e}$$

$$\vec{\nabla}_{\vec{r}'}\cdot\vec{\nabla}_{\vec{r}'}\,\rho_q(\vec{r},\vec{r}')\Big|_{\vec{r}=\vec{r}'} = \frac{1}{2}\vec{\nabla}^2\rho_q(\vec{r}) - \tau_q(\vec{r}) + \sum_\mu i\,\nabla_\mu j_{q,\mu}(\vec{r}) \tag{A.12f}$$

$$\vec{\nabla}_{\vec{r}}\cdot\vec{\nabla}_{\vec{r}}\,s_{q,\nu}(\vec{r},\vec{r}')\Big|_{\vec{r}=\vec{r}'} = \frac{1}{2}\vec{\nabla}^2 s_{q,\nu}(\vec{r}) - T_{q,\nu}(\vec{r}) - \sum_\mu i\,\nabla_\mu J_{q,\mu\nu}(\vec{r}) \tag{A.12g}$$

$$\vec{\nabla}_{\vec{r}'}\cdot\vec{\nabla}_{\vec{r}'}\,s_{q,\nu}(\vec{r},\vec{r}')\Big|_{\vec{r}=\vec{r}'} = \frac{1}{2}\vec{\nabla}^2 s_{q,\nu}(\vec{r}) - T_{q,\nu}(\vec{r}) + \sum_\mu i\,\nabla_\mu J_{q,\mu\nu}(\vec{r}) \tag{A.12h}$$

$$\sum_{\mu\nu\lambda}\epsilon_{\mu\nu\lambda}\nabla_{\vec{r}',\mu}\nabla_{\vec{r},\nu}\rho_q(\vec{r},\vec{r}')\Big|_{\vec{r}=\vec{r}'} = \sum_{\mu\nu\lambda}\epsilon_{\mu\nu\lambda}i\,\nabla_\mu j_{\nu,q}(\vec{r}) \tag{A.12i}$$

$$\sum_{\mu\nu\lambda}\epsilon_{\mu\nu\lambda}\nabla_{\vec{r}',\mu}\nabla_{\vec{r},\nu}s_{\lambda,q}(\vec{r},\vec{r}')\Big|_{\vec{r}=\vec{r}'} = \sum_{\mu\nu\lambda}\epsilon_{\mu\nu\lambda}i\,\nabla_\mu J_{\nu\lambda,q}(\vec{r})\ , \tag{A.12j}$$

where we refer to Eqs. (3.13a,3.13b) and Eq. 3.14 for the expression of the various local and non-local densities at play.

Rule Eq. A.12a:

$$
\begin{aligned}
&= \sum_{ij} \varphi_i^\dagger(\vec{r})\Big(\overrightarrow{\nabla}\varphi_j(\vec{r})\Big)\,\rho^q_{ji} \\
&= \sum_{ij} \Big[\frac{1}{2}\,\varphi_i^\dagger(\vec{r})\Big(\overrightarrow{\nabla}\varphi_j(\vec{r})\Big) + \frac{1}{2}\,\varphi_i^\dagger(\vec{r})\Big(\overrightarrow{\nabla}\varphi_j(\vec{r})\Big) + \frac{1}{2}\,\Big(\overrightarrow{\nabla}\varphi_i^\dagger(\vec{r})\Big)\varphi_j(\vec{r}) \\
&\qquad - \frac{1}{2}\,\Big(\overrightarrow{\nabla}\varphi_i^\dagger(\vec{r})\Big)\varphi_j(\vec{r})\Big]\,\rho^q_{ji} \\
&= \sum_{ij} \Big[\frac{1}{2}\,\varphi_i^\dagger(\vec{r})\Big(\overrightarrow{\nabla}\varphi_j(\vec{r})\Big) + \frac{1}{2}\,\Big(\overrightarrow{\nabla}\varphi_i^\dagger(\vec{r})\Big)\varphi_j(\vec{r}) + \frac{1}{2}\,\varphi_i^\dagger(\vec{r})\Big(\overrightarrow{\nabla}\varphi_j(\vec{r})\Big) \\
&\qquad - \frac{1}{2}\,\Big(\overrightarrow{\nabla}\varphi_i^\dagger(\vec{r})\Big)\varphi_j(\vec{r})\Big]\,\rho^q_{ji} \\
&= \frac{1}{2}\,\overrightarrow{\nabla}\rho_q(\vec{r}) + i\,\vec{j}_q(\vec{r})\ .
\end{aligned}
\tag{A.13}
$$

Rule Eq. A.12b:

$$
\begin{aligned}
&= \sum_{ij} \Big(\overrightarrow{\nabla}\varphi_i^\dagger(\vec{r})\Big)\varphi_j(\vec{r})\,\rho^q_{ji} \\
&= \sum_{ij} \Big[\frac{1}{2}\,\Big(\overrightarrow{\nabla}\varphi_i^\dagger(\vec{r})\Big)\varphi_j(\vec{r}) + \frac{1}{2}\,\Big(\overrightarrow{\nabla}\varphi_i^\dagger(\vec{r})\Big)\varphi_j(\vec{r}) + \frac{1}{2}\,\varphi_i^\dagger(\vec{r})\Big(\overrightarrow{\nabla}\varphi_j(\vec{r})\Big) \\
&\qquad - \frac{1}{2}\,\varphi_i^\dagger(\vec{r})\Big(\overrightarrow{\nabla}\varphi_j(\vec{r})\Big)\Big]\,\rho^q_{ji} \\
&= \sum_{ij} \Big[\frac{1}{2}\,\Big(\overrightarrow{\nabla}\varphi_i^\dagger(\vec{r})\Big)\varphi_j(\vec{r}) + \frac{1}{2}\,\varphi_i^\dagger(\vec{r})\Big(\overrightarrow{\nabla}\varphi_j(\vec{r})\Big) + \frac{1}{2}\,\Big(\overrightarrow{\nabla}\varphi_i^\dagger(\vec{r})\Big)\varphi_j(\vec{r}) \\
&\qquad - \frac{1}{2}\,\varphi_i^\dagger(\vec{r})\Big(\overrightarrow{\nabla}\varphi_j(\vec{r})\Big)\Big]\,\rho^q_{ji} \\
&= \frac{1}{2}\,\overrightarrow{\nabla}\rho_q(\vec{r}) - i\,\vec{j}_q(\vec{r})\ .
\end{aligned}
\tag{A.14}
$$

Rule Eq. A.12c:

$$
\begin{aligned}
&= \sum_{ij} \varphi_i^\dagger(\vec{r})\,\sigma_\nu\,\Big(\nabla_\mu\varphi_j(\vec{r})\Big)\,\rho^q_{ji} \\
&= \sum_{ij} \Big[\frac{1}{2}\,\varphi_i^\dagger(\vec{r})\,\sigma_\nu\,\Big(\nabla_\mu\varphi_j(\vec{r})\Big) + \frac{1}{2}\,\varphi_i^\dagger(\vec{r})\,\sigma_\nu\,\Big(\nabla_\mu\varphi_j(\vec{r})\Big) + \frac{1}{2}\,\Big(\nabla_\mu\varphi_i^\dagger(\vec{r})\Big)\,\sigma_\nu\,\varphi_j(\vec{r}) \\
&\qquad - \frac{1}{2}\,\Big(\nabla_\mu\varphi_i^\dagger(\vec{r})\Big)\,\sigma_\nu\,\varphi_j(\vec{r})\Big]\,\rho^q_{ji} \\
&= \sum_{ij} \Big[\frac{1}{2}\,\varphi_i^\dagger(\vec{r})\,\sigma_\nu\,\Big(\nabla_\mu\varphi_j(\vec{r})\Big) + \frac{1}{2}\,\Big(\nabla_\mu\varphi_i^\dagger(\vec{r})\Big)\,\sigma_\nu\,\varphi_j(\vec{r}) + \frac{1}{2}\,\varphi_i^\dagger(\vec{r})\,\sigma_\nu\,\Big(\nabla_\mu\varphi_j(\vec{r})\Big) \\
&\qquad - \frac{1}{2}\,\Big(\nabla_\mu\varphi_i^\dagger(\vec{r})\Big)\,\sigma_\nu\,\varphi_j(\vec{r})\Big]\,\rho^q_{ji} \\
&= \frac{1}{2}\,\nabla_\mu s_{\nu,q}(\vec{r}) + i\,J_{\mu\,\nu,q}(\vec{r})\ .
\end{aligned}
\tag{A.15}
$$

Rule Eq. A.12d:

$$
\begin{aligned}
&= \sum_{ij} \Big(\nabla_\mu \varphi_i^\dagger(\vec{r})\Big)\, \sigma_\nu\, \varphi_j(\vec{r})\, \rho^q_{ji} \\
&= \sum_{ij} \Big[\frac{1}{2}\Big(\nabla_\mu \varphi_i^\dagger(\vec{r})\Big)\, \sigma_\nu\, \varphi_j(\vec{r}) + \frac{1}{2}\Big(\nabla_\mu \varphi_i^\dagger(\vec{r})\Big)\, \sigma_\nu\, \varphi_j(\vec{r}) + \frac{1}{2}\, \varphi_i^\dagger(\vec{r})\, \sigma_\nu \Big(\nabla_\mu \varphi_j(\vec{r})\Big) \\
&\qquad - \frac{1}{2}\, \varphi_i^\dagger(\vec{r})\, \sigma_\nu \Big(\nabla_\mu \varphi_j(\vec{r})\Big)\Big]\, \rho^q_{ji} \\
&= \sum_{ij} \Big[\frac{1}{2}\Big(\nabla_\mu \varphi_i^\dagger(\vec{r})\Big)\, \sigma_\nu\, \varphi_j(\vec{r}) + \frac{1}{2}\, \varphi_i^\dagger(\vec{r})\, \sigma_\nu \Big(\nabla_\mu \varphi_j(\vec{r})\Big) + \frac{1}{2}\Big(\nabla_\mu \varphi_i^\dagger(\vec{r})\Big)\, \sigma_\nu\, \varphi_j(\vec{r}) \\
&\qquad - \frac{1}{2}\, \varphi_i^\dagger(\vec{r})\, \sigma_\nu \Big(\nabla_\mu \varphi_j(\vec{r})\Big)\Big]\, \rho^q_{ji} \\
&= \frac{1}{2}\, \nabla_\mu s_{\nu,q}(\vec{r}) + i\, J_{\mu\,\nu,q}(\vec{r}) \ . \qquad \text{(A.16)}
\end{aligned}
$$

Rule Eq. A.12e:

$$
\begin{aligned}
&= \sum_{ij} \varphi_i^\dagger(\vec{r}) \Big(\overrightarrow{\nabla}^2 \varphi_j(\vec{r})\Big)\, \rho^q_{ji} \\
&= \sum_{ij} \Big[\frac{1}{2}\varphi_i^\dagger(\vec{r}) \Big(\overrightarrow{\nabla}^2 \varphi_j(\vec{r})\Big) + \frac{1}{2}\Big(\overrightarrow{\nabla}^2 \varphi_i^\dagger(\vec{r})\Big)\varphi_j(\vec{r}) + \Big(\overrightarrow{\nabla} \varphi_i^\dagger(\vec{r})\Big)\Big(\overrightarrow{\nabla} \varphi_j(\vec{r})\Big) \\
&- \Big(\overrightarrow{\nabla} \varphi_i^\dagger(\vec{r})\Big)\Big(\overrightarrow{\nabla} \varphi_j(\vec{r})\Big) - \frac{1}{2}\Big(\overrightarrow{\nabla}^2 \varphi_i^\dagger(\vec{r})\Big)\varphi_j(\vec{r}) + \frac{1}{2}\varphi_i^\dagger(\vec{r}) \Big(\overrightarrow{\nabla}^2 \varphi_j(\vec{r})\Big)\Big]\, \rho^q_{ji} \\
&= \frac{1}{2}\overrightarrow{\nabla}^2 \rho_q(\vec{r}) - \tau_q(\vec{r}) - i\, \overrightarrow{\nabla} \vec{j}_q(\vec{r}) \ . \qquad \text{(A.17)}
\end{aligned}
$$

Rule Eq. A.12f:

$$
\begin{aligned}
&= \sum_{ij} \Big(\overrightarrow{\nabla}^2 \varphi_i^\dagger(\vec{r})\Big)\, \varphi_j(\vec{r})\, \rho^q_{ji} \\
&= \sum_{ij} \Big[\frac{1}{2}\Big(\overrightarrow{\nabla}^2 \varphi_i^\dagger(\vec{r})\Big)\varphi_j(\vec{r}) + \frac{1}{2}\varphi_i^\dagger(\vec{r}) \Big(\overrightarrow{\nabla}^2 \varphi_j(\vec{r})\Big) + \Big(\overrightarrow{\nabla} \varphi_i^\dagger(\vec{r})\Big)\Big(\overrightarrow{\nabla} \varphi_j(\vec{r})\Big) \\
&- \Big(\overrightarrow{\nabla} \varphi_i^\dagger(\vec{r})\Big)\Big(\overrightarrow{\nabla} \varphi_j(\vec{r})\Big) + \frac{1}{2}\Big(\overrightarrow{\nabla}^2 \varphi_i^\dagger(\vec{r})\Big)\varphi_j(\vec{r}) - \frac{1}{2}\varphi_i^\dagger(\vec{r}) \Big(\overrightarrow{\nabla}^2 \varphi_j(\vec{r})\Big)\Big]\, \rho^q_{ji} \\
&= \frac{1}{2}\overrightarrow{\nabla}^2 \rho_q(\vec{r}) - \tau_q(\vec{r}) + i\, \overrightarrow{\nabla} \vec{j}_q(\vec{r}) \ . \qquad \text{(A.18)}
\end{aligned}
$$

Rule Eq. A.12g:

$$
\begin{aligned}
&= \sum_{ij} \varphi_i^\dagger(\vec{r}) \vec{\sigma} \Big(\overrightarrow{\nabla}^2 \varphi_j(\vec{r})\Big)\, \rho^q_{ji} \\
&= \sum_{ij} \Big[\frac{1}{2}\varphi_i^\dagger(\vec{r}) \vec{\sigma} \Big(\overrightarrow{\nabla}^2 \varphi_j(\vec{r})\Big) + \frac{1}{2}\Big(\overrightarrow{\nabla}^2 \varphi_i^\dagger(\vec{r})\Big) \vec{\sigma} \varphi_j(\vec{r}) + \Big(\overrightarrow{\nabla} \varphi_i^\dagger(\vec{r})\Big) \vec{\sigma} \Big(\overrightarrow{\nabla} \varphi_j(\vec{r})\Big) \\
&- \Big(\overrightarrow{\nabla} \varphi_i^\dagger(\vec{r})\Big) \vec{\sigma} \Big(\overrightarrow{\nabla} \varphi_j(\vec{r})\Big) - \frac{1}{2}\Big(\overrightarrow{\nabla}^2 \varphi_i^\dagger(\vec{r})\Big) \vec{\sigma} \varphi_j(\vec{r}) + \frac{1}{2}\varphi_i^\dagger(\vec{r}) \vec{\sigma} \Big(\overrightarrow{\nabla}^2 \varphi_j(\vec{r})\Big)\Big]\, \rho^q_{ji} \\
&= \frac{1}{2}\sum_\mu \nabla_\mu \nabla_\mu s_{q,\nu}(\vec{r}) - T_{q,\nu}(\vec{r}) - \sum_\mu i\, \nabla_\mu J_{q,\mu\nu}(\vec{r}) \ . \qquad \text{(A.19)}
\end{aligned}
$$

Rule Eq. A.12h:

$$\begin{aligned}
&= \sum_{ij} \Big(\overrightarrow{\nabla}^2\varphi_i^\dagger(\vec{r})\Big)\vec{\sigma}\varphi_j(\vec{r})\,\rho^q_{ji} \\
&= \sum_{ij} \Big[\frac{1}{2}\Big(\overrightarrow{\nabla}^2\varphi_i^\dagger(\vec{r})\Big)\vec{\sigma}\varphi_j(\vec{r}) + \frac{1}{2}\varphi_i^\dagger(\vec{r})\vec{\sigma}\Big(\overrightarrow{\nabla}^2\varphi_j(\vec{r})\Big) + \Big(\overrightarrow{\nabla}\varphi_i^\dagger(\vec{r})\Big)\vec{\sigma}\Big(\overrightarrow{\nabla}\varphi_j(\vec{r})\Big) \\
&- \Big(\overrightarrow{\nabla}\varphi_i^\dagger(\vec{r})\Big)\vec{\sigma}\Big(\overrightarrow{\nabla}\varphi_j(\vec{r})\Big) + \frac{1}{2}\Big(\overrightarrow{\nabla}^2\varphi_i^\dagger(\vec{r})\Big)\vec{\sigma}\varphi_j(\vec{r}) - \frac{1}{2}\varphi_i^\dagger(\vec{r})\vec{\sigma}\Big(\overrightarrow{\nabla}^2\varphi_j(\vec{r})\Big)\Big]\rho^q_{ji} \\
&= \frac{1}{2}\sum_\mu \nabla_\mu\nabla_\mu s_{q,\nu}(\vec{r}) - T_{q,\nu}(\vec{r}) + \sum_\mu i\,\nabla_\mu J_{q,\mu\nu}(\vec{r})\ . \qquad \text{(A.20)}
\end{aligned}$$

Rule Eq. A.12i:

$$\begin{aligned}
&= \sum_{ij}\sum_{\mu\nu\lambda}\epsilon_{\mu\nu\lambda}\Big[\frac{1}{2}\nabla_\mu\varphi_i^\dagger\nabla_\nu\varphi_j + \frac{1}{2}\nabla_\mu\varphi_i^\dagger\nabla_\nu\varphi_j\Big]\rho^q_{ji} \\
&= \sum_{ij}\sum_{\mu\nu\lambda}\epsilon_{\mu\nu\lambda}\Big[\frac{1}{2}\nabla_\mu\varphi_i^\dagger\nabla_\nu\varphi_j - \frac{1}{2}\nabla_\nu\varphi_i^\dagger\nabla_\mu\varphi_j + \frac{1}{2}\varphi_i^\dagger\nabla_\mu\nabla_\nu\varphi_j - \frac{1}{2}\nabla_\mu\nabla_\nu\varphi_i^\dagger\varphi_j\Big]\rho^q_{ji} \\
&= \sum_{ij}\sum_{\mu\nu\lambda}\epsilon_{\mu\nu\lambda}\Big[\frac{1}{2}\nabla_\mu\Big(\varphi_i^\dagger\nabla_\nu\varphi_j\Big) - \frac{1}{2}\nabla_\mu\Big(\nabla_\nu\varphi_i^\dagger\varphi_j\Big)\Big]\rho^q_{ji} \\
&= \sum_{\mu\nu\lambda} i\,\epsilon_{\mu\nu\lambda}\nabla_\mu j_{\nu,q}(\vec{r})\ , \qquad \text{(A.21)}
\end{aligned}$$

where we have used that $\sum_{\mu\nu\lambda}\epsilon_{\mu\nu\lambda}\varphi_i^\dagger\nabla_\mu\nabla_\nu\varphi_j = -\sum_{\mu\nu\lambda}\epsilon_{\nu\mu\lambda}\varphi_i^\dagger\nabla_\mu\nabla_\nu\varphi_j = 0$ and $\sum_{\mu\nu\lambda}\epsilon_{\mu\nu\lambda}\nabla_\mu\nabla_\nu\varphi_i^\dagger\varphi_j = -\sum_{\mu\nu\lambda}\epsilon_{\nu\mu\lambda}\nabla_\mu\nabla_\nu\varphi_i^\dagger\varphi_j = 0$.
Rule Eq. A.12j:

$$\begin{aligned}
&= \sum_{ij}\sum_{\mu\nu\lambda}\epsilon_{\mu\nu\lambda}\Big[\frac{1}{2}\nabla_\mu\varphi_i^\dagger\,\sigma_\lambda\,\nabla_\nu\varphi_j + \frac{1}{2}\nabla_\mu\varphi_i^\dagger\,\sigma_\lambda\,\nabla_\nu\varphi_j\Big]\rho^q_{ji} \\
&= \sum_{ij}\sum_{\mu\nu\lambda}\epsilon_{\mu\nu\lambda}\Big[\frac{1}{2}\nabla_\mu\varphi_i^\dagger\,\sigma_\lambda\,\nabla_\nu\varphi_j - \frac{1}{2}\nabla_\nu\varphi_i^\dagger\,\sigma_\lambda\,\nabla_\mu\varphi_j + \frac{1}{2}\varphi_i^\dagger\,\sigma_\lambda\,\nabla_\mu\nabla_\nu\varphi_j - \frac{1}{2}\nabla_\mu\nabla_\nu\varphi_i^\dagger\,\sigma_\lambda\,\varphi_j\Big]\rho^q_{ji} \\
&= \sum_{ij}\sum_{\mu\nu\lambda}\epsilon_{\mu\nu\lambda}\Big[\frac{1}{2}\nabla_\mu\Big(\varphi_i^\dagger\,\sigma_\lambda\,\nabla_\nu\varphi_j\Big) - \frac{1}{2}\nabla_\mu\Big(\nabla_\nu\varphi_i^\dagger\,\sigma_\lambda\,\varphi_j\Big)\Big]\rho^q_{ji} \\
&= \sum_{\mu\nu\lambda} i\,\epsilon_{\mu\nu\lambda}\nabla_\mu J_{\nu\lambda,q}(\vec{r})\ . \qquad \text{(A.22)}
\end{aligned}$$

A.3 Coordinate exchange operators

The application of coordinate two-body exchange operators has already been discussed in Sec. 3.1.6, where it was recalled that for particular cases, e.g. when the interaction acts in an unique partial wave, the coordinate exchange operator can be replaced by ± 1. The present section aims at giving a direct mathematical proof for the specific case of central two- and three-body Skyrme interactions.

A.3.1 Two-body

The action of a coordinate exchange operator on a two-body state is given in Eq. 3.24a. The two-body Skyrme interaction depends on relative incoming and outcoming momenta operators

defined by Eqs. (3.43,3.44). One can see that

$$\langle\vec{r}_1'\vec{r}_2'|\hat{\vec{k}}_{12}P^r_{12}|\vec{r}_1\vec{r}_2\rangle = \langle\vec{r}_1'\vec{r}_2'|\hat{\vec{k}}_{12}|\vec{r}_2\vec{r}_1\rangle = \vec{k}_{\vec{r}_2\vec{r}_1}\delta_{r_1'r_2}\delta_{r_2'r_1} = -\vec{k}_{\vec{r}_1\vec{r}_2}\delta_{r_1'r_2}\delta_{r_2'r_1} \ , \quad \text{(A.23a)}$$

$$\langle\vec{r}_1'\vec{r}_2'|\hat{\vec{k}}'_{12}P^r_{12}|\vec{r}_1\vec{r}_2\rangle = \langle\vec{r}_1'\vec{r}_2'|\hat{\vec{k}}'_{12}|\vec{r}_2\vec{r}_1\rangle = \vec{k}_{\vec{r}_1'\vec{r}_2'}\delta_{r_1'r_2}\delta_{r_2'r_1} = \vec{k}_{\vec{r}_1'\vec{r}_2'}\delta_{r_1'r_2}\delta_{r_2'r_1} \ , \quad \text{(A.23b)}$$

and knowing that $\delta(\vec{r}_1'-\vec{r}_2)\delta(\vec{r}_2'-\vec{r}_1)\delta(\vec{r}_2-\vec{r}_1) = \delta(\vec{r}_1'-\vec{r}_1)\delta(\vec{r}_2'-\vec{r}_2)\delta(\vec{r}_2-\vec{r}_1)$, one deduces that

$$\langle\vec{r}_1'\vec{r}_2'|\hat{\vec{k}}_{12}\hat{\delta}_{r_{12}}P^r_{12}|\vec{r}_1\vec{r}_2\rangle = -\langle\vec{r}_1'\vec{r}_2'|\hat{\vec{k}}_{12}\hat{\delta}_{r_{12}}|\vec{r}_1\vec{r}_2\rangle \ , \quad \text{(A.24a)}$$

$$\langle\vec{r}_1'\vec{r}_2'|\hat{\vec{k}}'_{12}\hat{\delta}_{r_{12}}P^r_{12}|\vec{r}_1\vec{r}_2\rangle = +\langle\vec{r}_1'\vec{r}_2'|\hat{\vec{k}}'_{12}\hat{\delta}_{r_{12}}|\vec{r}_1\vec{r}_2\rangle \ . \quad \text{(A.24b)}$$

Similarly if one applies the coordinate exchange operator on the left

$$\langle\vec{r}_1'\vec{r}_2'|P^r_{12}\hat{\vec{k}}_{12}\hat{\delta}_{r_{12}}|\vec{r}_1\vec{r}_2\rangle = +\langle\vec{r}_1'\vec{r}_2'|\hat{\vec{k}}_{12}\hat{\delta}_{r_{12}}|\vec{r}_1\vec{r}_2\rangle \ , \quad \text{(A.25a)}$$

$$\langle\vec{r}_1'\vec{r}_2'|P^r_{12}\hat{\vec{k}}'_{12}\hat{\delta}_{r_{12}}|\vec{r}_1\vec{r}_2\rangle = -\langle\vec{r}_1'\vec{r}_2'|\hat{\vec{k}}'_{12}\hat{\delta}_{r_{12}}|\vec{r}_1\vec{r}_2\rangle \ , \quad \text{(A.25b)}$$

but this case never occurs in practice in two-body case because the antisymmetrizer is applied on the ket by convention. At least this is true if one uses directly the form of the interaction given in Eq. 3.52. Knowing such properties one easily deduce the impact of P^r_{12} for each term of the interaction (Eq. 3.52)

$$\langle\vec{r}_1'\vec{r}_2'|\hat{\delta}_{r_{12}}P^r_{12}|\vec{r}_1\vec{r}_2\rangle = \langle\vec{r}_1'\vec{r}_2'|\hat{\delta}_{r_{12}}|\vec{r}_1\vec{r}_2\rangle \ , \quad \text{(A.26a)}$$

$$\langle\vec{r}_1'\vec{r}_2'|\left(\hat{\vec{k}}'^2_{12}+\hat{\vec{k}}^2_{12}\right)\hat{\delta}_{r_{12}}P^r_{12}|\vec{r}_1\vec{r}_2\rangle = \langle\vec{r}_1'\vec{r}_2'|\left(\hat{\vec{k}}'^2_{12}+(-1)^2\hat{\vec{k}}^2_{12}\right)\hat{\delta}_{r_{12}}|\vec{r}_1\vec{r}_2\rangle \ , \quad \text{(A.26b)}$$

$$\langle\vec{r}_1'\vec{r}_2'|\hat{\vec{k}}'_{12}\cdot\hat{\vec{k}}_{12}\ \hat{\delta}_{r_{12}}P^r_{12}|\vec{r}_1\vec{r}_2\rangle = -\langle\vec{r}_1'\vec{r}_2'|\hat{\vec{k}}'_{12}\cdot\hat{\vec{k}}_{12}\ \hat{\delta}_{r_{12}}|\vec{r}_1\vec{r}_2\rangle \ , \quad \text{(A.26c)}$$

$$\langle\vec{r}_1'\vec{r}_2'|\hat{\vec{k}}'_{12}\wedge\hat{\vec{k}}_{12}\ \hat{\delta}_{r_{12}}P^r_{12}|\vec{r}_1\vec{r}_2\rangle = -\langle\vec{r}_1'\vec{r}_2'|\hat{\vec{k}}'_{12}\wedge\hat{\vec{k}}_{12}\ \hat{\delta}_{r_{12}}|\vec{r}_1\vec{r}_2\rangle \ , \quad \text{(A.26d)}$$

so that $P^r_{12}=1$ for terms (Eqs. (3.52a,3.52b)) and $P^r_{12}=-1$ for terms (Eqs. (3.52c,3.52d)).

A.3.2 Three-body

The situation is more complex in the three-body case because of the presence of the third particle. Indeed, there are three different two-body relative momenta and associated coordinate exchange operators. Coordinate exchange operators can eventually be replaced by ±1, only if the interaction is a sole function of the associated relative momenta.
The three coordinate exchange operators are defined through

$$P^r_{12}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle = |\vec{r}_2\vec{r}_1\vec{r}_3\rangle \ , \quad \text{(A.27a)}$$

$$P^r_{23}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle = |\vec{r}_1\vec{r}_3\vec{r}_2\rangle \ , \quad \text{(A.27b)}$$

$$P^r_{13}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle = |\vec{r}_3\vec{r}_2\vec{r}_1\rangle \ . \quad \text{(A.27c)}$$

One can remark that

$$\langle\vec{r}_1'\vec{r}_2'\vec{r}_3'|\hat{\delta}_{r_1r_3}\hat{\delta}_{r_2r_3}P^r_{xy}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle = \langle\vec{r}_1'\vec{r}_2'\vec{r}_3'|\hat{\delta}_{r_1r_3}\hat{\delta}_{r_2r_3}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle \ , \quad \text{(A.28a)}$$

where $xy\in\{12,23,13\}$, such that

$$\langle\vec{r}_1'\vec{r}_2'\vec{r}_3'|\hat{\vec{k}}_{xy}\hat{\delta}_{r_1r_3}\hat{\delta}_{r_2r_3}P^r_{xy}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle = -\langle\vec{r}_1'\vec{r}_2'\vec{r}_3'|\hat{\vec{k}}_{xy}\hat{\delta}_{r_1r_3}\hat{\delta}_{r_2r_3}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle \ , \quad \text{(A.29a)}$$

$$\langle\vec{r}_1'\vec{r}_2'\vec{r}_3'|\hat{\vec{k}}'_{xy}\hat{\delta}_{r_1r_3}\hat{\delta}_{r_2r_3}P^r_{xy}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle = +\langle\vec{r}_1'\vec{r}_2'\vec{r}_3'|\hat{\vec{k}}'_{xy}\hat{\delta}_{r_1r_3}\hat{\delta}_{r_2r_3}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle \ , \quad \text{(A.29b)}$$

$$\langle\vec{r}_1'\vec{r}_2'\vec{r}_3'|P^r_{xy}\hat{\vec{k}}_{xy}\hat{\delta}_{r_1r_3}\hat{\delta}_{r_2r_3}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle = +\langle\vec{r}_1'\vec{r}_2'\vec{r}_3'|\hat{\vec{k}}_{xy}\hat{\delta}_{r_1r_3}\hat{\delta}_{r_2r_3}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle \ , \quad \text{(A.29c)}$$

$$\langle\vec{r}_1'\vec{r}_2'\vec{r}_3'|P^r_{xy}\hat{\vec{k}}'_{xy}\hat{\delta}_{r_1r_3}\hat{\delta}_{r_2r_3}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle = -\langle\vec{r}_1'\vec{r}_2'\vec{r}_3'|\hat{\vec{k}}'_{xy}\hat{\delta}_{r_1r_3}\hat{\delta}_{r_2r_3}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle \ . \quad \text{(A.29d)}$$

One can also realize that

$$\langle \vec{r}_1' \vec{r}_2' \vec{r}_3' | \hat{\vec{k}}_{23} P_{12}^r | \vec{r}_1 \vec{r}_2 \vec{r}_3 \rangle = \vec{k}_{\vec{r}_1 \vec{r}_3} \delta_{r_1' r_2} \delta_{r_2' r_1} \delta_{r_3' r_3} \neq -\vec{k}_{\vec{r}_2 \vec{r}_3} \delta_{r_1' r_2} \delta_{r_2' r_1} \delta_{r_3' r_3} \ , \tag{A.30a}$$

$$\langle \vec{r}_1' \vec{r}_2' \vec{r}_3' | \hat{\vec{k}}_{23}' P_{12}^r | \vec{r}_1 \vec{r}_2 \vec{r}_3 \rangle = \vec{k}_{\vec{r}_1' \vec{r}_3'} \delta_{r_1' r_2} \delta_{r_2' r_1} \delta_{r_3' r_3} \neq -\vec{k}_{\vec{r}_2' \vec{r}_3'} \delta_{r_1' r_2} \delta_{r_2' r_1} \delta_{r_3' r_3} \ . \tag{A.30b}$$

Consequently, one must be careful using predefined rules regarding the application of coordinate exchange operators. All rules are given in Tab. {A.1}.

	$\hat{\vec{k}}_{12}$	$\hat{\vec{k}}_{12}'$	$\hat{\vec{k}}_{13}$	$\hat{\vec{k}}_{13}'$	$\hat{\vec{k}}_{23}$	$\hat{\vec{k}}_{23}'$
$\overrightarrow{P_{12}^r}$	-1	1	$\overrightarrow{P_{12}^r}$	$\overrightarrow{P_{12}^r}$	$\overrightarrow{P_{12}^r}$	$\overrightarrow{P_{12}^r}$
$\overrightarrow{P_{13}^r}$	$\overrightarrow{P_{13}^r}$	$\overrightarrow{P_{13}^r}$	-1	1	$\overrightarrow{P_{13}^r}$	$\overrightarrow{P_{13}^r}$
$\overrightarrow{P_{23}^r}$	$\overrightarrow{P_{23}^r}$	$\overrightarrow{P_{23}^r}$	$\overrightarrow{P_{23}^r}$	$\overrightarrow{P_{23}^r}$	-1	1
$\overleftarrow{P_{12}^r}$	1	-1	$\overleftarrow{P_{12}^r}$	$\overleftarrow{P_{12}^r}$	$\overleftarrow{P_{12}^r}$	$\overleftarrow{P_{12}^r}$
$\overleftarrow{P_{13}^r}$	$\overleftarrow{P_{13}^r}$	$\overleftarrow{P_{13}^r}$	1	-1	$\overleftarrow{P_{13}^r}$	$\overleftarrow{P_{13}^r}$
$\overleftarrow{P_{23}^r}$	$\overleftarrow{P_{23}^r}$	$\overleftarrow{P_{23}^r}$	$\overleftarrow{P_{23}^r}$	$\overleftarrow{P_{23}^r}$	1	-1

Table A.1: Possible simplification regarding the application of coordinate exchange operators on three-body states. A right (left) arrow denotes that the exchange operator acts on the ket (bra). The coordinate exchange operator is simply repeated whenever no shortcut is available such that it must be applied explicitly

A.4 Derivation of the EDF

In the present section Eqs. (3.3c,3.3e,3.5) are computed explicitly starting from Skyrme two- and three-body pseudo potentials.

A.4.1 Conventions

Kinetic, normal two- and three-body contributions to the energy can be expressed in coordinate⊗spin⊗isospi representation according to

$$E_{kin}^{\rho} = \int d(\vec{r}\sigma q) \Big\{ \langle \vec{r}' \sigma' q | \hat{t} | \vec{r} \sigma q \rangle \rho_q(\vec{r}\sigma, \vec{r}'\sigma') \Big\} \ , \tag{A.31a}$$

$$E_{Sk}^{\rho\rho} = \frac{1}{2} \int d(\vec{r}\sigma q) \Big\{ \langle \vec{r}_1' \sigma_1' q_1 \, \vec{r}_2' \sigma_2' q_2 | \hat{v}^{2Sk} \mathcal{A}_{12} | \vec{r}_1 \sigma_1 q_1 \, \vec{r}_2 \sigma_2 q_2 \rangle \rho_{q_1}(\vec{r}_1\sigma_1, \vec{r}_1'\sigma_1') \rho_{q_2}(\vec{r}_2\sigma_2, \vec{r}_2'\sigma_2') \Big\} \ , \tag{A.31b}$$

$$E_{Sk}^{\rho\rho\rho} = \frac{1}{2} \int d(\vec{r}\sigma q) \Big\{ \langle \vec{r}_1' \sigma_1' q_1 \, \vec{r}_2' \sigma_2' q_2 \, \vec{r}_3' \sigma_3' q_3 | \hat{v}_{\overline{123}}^{3Sk} \mathcal{A}_{123} | \vec{r}_1 \sigma_1 q_1 \, \vec{r}_2 \sigma_2 q_2 \, \vec{r}_3 \sigma_3 q_3 \rangle \rho_{q_1}(\vec{r}_1\sigma_1, \vec{r}_1'\sigma_1') \rho_{q_2}(\vec{r}_2\sigma_2, \vec{r}_2'\sigma_2') \rho_{q_3}(\vec{r}_3\sigma_3, \vec{r}_3'\sigma_3') \Big\} \ , \tag{A.31c}$$

where $\hat{v}^{3Sk}_{\overline{123}}$ has been defined in Sec. 3.4.1. Matter and spin non-local densities defined in Eqs. (3.13a,3.13b) are noted as

$$\rho^{q_1}_{\vec{r}_1\vec{r}_1'} \equiv \rho_{q_1}(\vec{r}_1,\vec{r}_1') = \sum_{\sigma_1\sigma_1'} \langle\sigma_1|\sigma_1'\rangle\, \rho_{q_1}(\vec{r}_1\sigma_1,\vec{r}_1'\sigma_1') \ , \tag{A.32a}$$

$$\vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'} \equiv \vec{s}_{q_1}(\vec{r}_1,\vec{r}_1') = \sum_{\sigma_1\sigma_1'} \langle\sigma_1|\vec{\sigma}|\sigma_1'\rangle\, \rho_{q_1}(\vec{r}_1\sigma_1,\vec{r}_1'\sigma_1') \ . \tag{A.32b}$$

A.4.1.1 Spin and isospin exchange operators

Spin exchange operator Expression 3.31 for the spin exchange operator is used, to make non-local spin densities appear, e.g.

$$\sum_{\sigma_1\sigma_1'}\sum_{\sigma_2\sigma_2'} \langle\sigma_1'\sigma_2'|P^s_{12}|\sigma_1\sigma_2\rangle \rho_{q_1}(\vec{r}_1\sigma_1,\vec{r}_1'\sigma_1')\rho_{q_2}(\vec{r}_2\sigma_2,\vec{r}_2'\sigma_2') = \frac{1}{2}\Big(\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_2\vec{r}_2'} + \vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'}\cdot\vec{s}^{q_2}_{\vec{r}_2\vec{r}_2'}\Big) \ . \tag{A.33}$$

The fact that isospin mixing is not considered, i.e. $\rho(\vec{r}_1\sigma_1 q_1,\vec{r}_1'\sigma_1' q_1') = 0$ for $q_1' \neq q_1$, allows us to replace isospin exchange operator by simple delta operator. Indeed

$$\langle q_1 ... q_i ... q_j ... q_N|P^t_{ij}|q_1 ... q_i ... q_j ... q_N\rangle = \langle q_1 ... q_i ... q_j ... q_N|q_1 ... q_j ... q_i ... q_N\rangle = \delta_{q_iq_j} \ , \tag{A.34}$$

so that isospin exchange operator P^t_{ij} is the operator whose matrix element gives $\delta_{q_iq_j}$. As a result, we will note

$$P^t_{12} = \hat{\delta}_{q_iq_j} \ . \tag{A.35}$$

A.4.1.2 Derivatives

For simplicity, the following shortcut notation is used for the application of gradient operators

$$\begin{aligned}
\vec{\nabla}_{r_1}\, \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\Big|_{\vec{r}_1=\vec{r}_1'} &= \frac{1}{2}\vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}} + i\vec{\mathcal{J}}^{q_1}_{\vec{r}} \equiv \vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}} \ , \\
\vec{\nabla}_{r_1'}\, \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\Big|_{\vec{r}_1=\vec{r}_1'} &= \frac{1}{2}\vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}} - i\vec{\mathcal{J}}^{q_1}_{\vec{r}} \equiv \vec{\nabla}'\mathcal{P}^{q_1}_{\vec{r}} \ , \\
\vec{\nabla}_{r_1}\cdot\vec{\nabla}_{r_1}\, \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\Big|_{\vec{r}_1=\vec{r}_1'} &= \frac{1}{2}\Delta\mathcal{P}^{q_1}_{\vec{r}} - \mathcal{T}^{q_1}_{\vec{r}} + i\vec{\nabla}\cdot\vec{\mathcal{J}}^{q_1}_{\vec{r}} \equiv \triangle\mathcal{P}^{q_1}_{\vec{r}} \ , \\
\vec{\nabla}_{r_1'}\cdot\vec{\nabla}_{r_1'}\, \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\Big|_{\vec{r}_1=\vec{r}_1'} &= \frac{1}{2}\Delta\mathcal{P}^{q_1}_{\vec{r}} - \mathcal{T}^{q_1}_{\vec{r}} - i\vec{\nabla}\cdot\vec{\mathcal{J}}^{q_1}_{\vec{r}} \equiv \triangle'\mathcal{P}^{q_1}_{\vec{r}} \ ,
\end{aligned} \tag{A.36}$$

where

$$\mathcal{P}^{q_1}_{\vec{r}} \ , \ \mathcal{T}^{q_1}_{\vec{r}} \ , \ \mathcal{J}^{q_1,\mu}_{\vec{r}} \equiv \begin{cases} \rho_{q_1}(\vec{r}) \ , \ \tau_{q_1}(\vec{r}) \ , \ j_{q_1,\mu}(\vec{r}) \text{ if } \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'} = \rho^{q_1}_{\vec{r}_1\vec{r}_1'} \\ s_{q_1,\nu}(\vec{r}) \ , \ T_{q_1,\nu}(\vec{r}) \ , \ J_{q_1,\mu\nu}(\vec{r}) \text{ if } \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'} = \vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'} \end{cases} \ . \tag{A.37}$$

As a result, one has

$$(\triangle + \triangle')\mathcal{P}^{q_1}_{\vec{r}} = \Delta\mathcal{P}^{q_1}_{\vec{r}} - 2\mathcal{T}^{q_1}_{\vec{r}} \ , \tag{A.38a}$$

$$(\triangle - \triangle')\mathcal{P}^{q_1}_{\vec{r}} = 2i\vec{\nabla}\cdot\vec{\mathcal{J}}^{q_1}_{\vec{r}} \ , \tag{A.38b}$$

$$\vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}\mathcal{P}^{q_2}_{\vec{r}} + \vec{\nabla}'\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}'\mathcal{P}^{q_2}_{\vec{r}} = \frac{1}{2}\vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}\mathcal{P}^{q_2}_{\vec{r}} - 2\vec{\mathcal{J}}^{q_1}_{\vec{r}}\vec{\mathcal{J}}^{q_2}_{\vec{r}} \ , \tag{A.38c}$$

$$\vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}\mathcal{P}^{q_2}_{\vec{r}} - \vec{\nabla}'\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}'\mathcal{P}^{q_2}_{\vec{r}} = i\vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}}\vec{\mathcal{J}}^{q_2}_{\vec{r}} + i\vec{\mathcal{J}}^{q_1}_{\vec{r}}\vec{\nabla}\mathcal{P}^{q_2}_{\vec{r}} \ , \tag{A.38d}$$

$$\vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}'\mathcal{P}^{q_2}_{\vec{r}} + \vec{\nabla}'\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}\mathcal{P}^{q_2}_{\vec{r}} = \frac{1}{2}\vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}\mathcal{P}^{q_2}_{\vec{r}} + 2\vec{\mathcal{J}}^{q_1}_{\vec{r}}\vec{\mathcal{J}}^{q_2}_{\vec{r}} \ , \tag{A.38e}$$

$$\vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}'\mathcal{P}^{q_2}_{\vec{r}} - \vec{\nabla}'\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}\mathcal{P}^{q_2}_{\vec{r}} = -i\vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}}\vec{\mathcal{J}}^{q_2}_{\vec{r}} + i\vec{\mathcal{J}}^{q_1}_{\vec{r}}\vec{\nabla}\mathcal{P}^{q_2}_{\vec{r}} \ , \tag{A.38f}$$

$$\sum_{\lambda\mu}\epsilon_{\lambda\mu\nu}\nabla'_\lambda\mathcal{P}^{q_1}_{\vec{r}}\nabla_\mu\mathcal{P}^{q_2}_{\vec{r}} + \nabla_\mu\mathcal{P}^{q_1}_{\vec{r}}\nabla'_\lambda\mathcal{P}^{q_2}_{\vec{r}} = i\nabla_\lambda\mathcal{P}^{q_1}_{\vec{r}}\mathcal{J}^{q_2}_{\vec{r},\mu} + i\mathcal{J}^{q_1}_{\vec{r},\mu}\nabla_\lambda\mathcal{P}^{q_2}_{\vec{r}} \ . \tag{A.38g}$$

Moreover the local and contact character of the Skyrme pseudo potential is such that the identity $\vec{r}_1' = ... = \vec{r}_N' = \vec{r}_1 = ... = \vec{r}_N = \vec{r}$ holds after having applied gradient operators. To take into account the latter property, a shortcut notation $\delta(\vec{r})$ is used such that

$$\int d\vec{r}_1'...d\vec{r}_N \; F(\vec{r}_1', ..., \vec{r}_N)\delta(\vec{r}) \equiv \int d\vec{r} \; F(\vec{r}_1', ..., \vec{r}_N)\Big|_{\vec{r}_1'=...=\vec{r}_N=\vec{r}} \tag{A.39}$$

A.4.2 Kinetic energy

The kinetic energy (Eq. A.31a) is

$$\begin{aligned} E^{\rho}_{kin} &= \int d(\vec{r}\sigma q) \, \langle \vec{r}'\sigma' q | \frac{\hat{\vec{p}}' \cdot \hat{\vec{p}}}{2m} | \vec{r}\sigma q \rangle \; \rho_q(\vec{r}\sigma, \vec{r}'\sigma') \\ &= \int d\vec{r}' d\vec{r} \sum_q \frac{\hbar^2}{2m} \, \delta(\vec{r} - \vec{r}') \, \vec{\nabla}_{\vec{r}'} \cdot \vec{\nabla}_{\vec{r}} \; \rho_q(\vec{r}, \vec{r}') \\ &= \frac{\hbar^2}{2m} \int d\vec{r} \sum_q \tau_q(\vec{r}) \; . \end{aligned} \tag{A.40}$$

A.4.3 Bilinear part of the EDF

The bilinear part of the EDF is calculated term by term starting from the two-body Skyrme pseudo potential (Eq. 3.52). Each term is computed in two steps. First one expresses the energy density in terms of non-local densities. Second, gradient operators are applied to provide the final expression of the quasi-local energy functional.

A.4.3.1 Interaction term Eq. 3.52a

The exchange operator part of the antisymmetrized interaction term can be reduced to

$$t_0(1 + x_0 P^s_{12})\mathcal{A}_{12} = t_0(1 - P^r_{12}P^s_{12}P^t_{12}) + t_0 x_0 (P^s_{12} - P^r_{12}P^t_{12}) \; . \tag{A.41}$$

Knowing that such a term acts only in S-wave, i.e. $L = 0$, such that $P^r_{12} = +1$, one has

$$\begin{aligned} E_{\rho\rho,t_0} &= \frac{1}{2} \int d(\vec{r}) \, v^{2Sk}_{t_0}(\vec{r}_1, \vec{r}_1', \vec{r}_2, \vec{r}_2') \, t_0 \Bigg\{ \sum_{q_1 q_2} \rho^{q_1}_{\vec{r}_1\vec{r}_1'} \rho^{q_2}_{\vec{r}_2\vec{r}_2'} - \frac{1}{2} \sum_{q_1} \left(\rho^{q_1}_{\vec{r}_1\vec{r}_1'} \rho^{q_1}_{\vec{r}_2\vec{r}_2'} + \vec{s}^{\,q_1}_{\vec{r}_1\vec{r}_1'} \vec{s}^{\,q_1}_{\vec{r}_2\vec{r}_2'} \right) \\ &\quad + x_0 \frac{1}{2} \sum_{q_1 q_2} \left(\rho^{q_1}_{\vec{r}_1\vec{r}_1'} \rho^{q_2}_{\vec{r}_2\vec{r}_2'} + \vec{s}^{\,q_1}_{\vec{r}_1\vec{r}_1'} \vec{s}^{\,q_2}_{\vec{r}_2\vec{r}_2'} \right) - x_0 \sum_{q_1} \rho^{q_1}_{\vec{r}_1\vec{r}_1'} \rho^{q_1}_{\vec{r}_2\vec{r}_2'} \Bigg\} \\ &= \int d(\vec{r}) \, v^{2Sk}_{t_0}(\vec{r}_1, \vec{r}_1', \vec{r}_2, \vec{r}_2') \Bigg\{ \sum_{q_1 \neq q_2} \left[\frac{t_0}{2}(1 + \frac{x_0}{2}) \rho^{q_1}_{\vec{r}_1\vec{r}_1'} \rho^{q_2}_{\vec{r}_2\vec{r}_2'} + \frac{t_0 x_0}{4} \vec{s}^{\,q_1}_{\vec{r}_1\vec{r}_1'} \vec{s}^{\,q_2}_{\vec{r}_2\vec{r}_2'} \right] \\ &\quad + \sum_{q_1} \left[\frac{t_0}{4}(1 - x_0) \rho^{q_1}_{\vec{r}_1\vec{r}_1'} \rho^{q_1}_{\vec{r}_2\vec{r}_2'} - \frac{t_0}{4}(1 - x_0) \vec{s}^{\,q_1}_{\vec{r}_1\vec{r}_1'} \vec{s}^{\,q_1}_{\vec{r}_2\vec{r}_2'} \right] \Bigg\} \; , \end{aligned} \tag{A.42}$$

where $v^{2Sk}_{t_i}(\vec{r}_1, \vec{r}_1', \vec{r}_2, \vec{r}_2')$ is the coordinate matrix element of the appropriate two-body Skyrme interaction term. In the case of interaction Eq. 3.52a, such a matrix element is simply made of delta operators. The quasi-local functional is thus obtained by setting $\vec{r}_1' = \vec{r}_2' = \vec{r}_1 = \vec{r}_2 = \vec{r}$, i.e.

$$\begin{aligned} E^{\rho\rho}_{Sk,t_0} = \int d\vec{r} \Bigg\{ & \sum_{q \neq q'} \left[\frac{1}{2} t_0 \left(1 + \frac{x_0}{2} \right) \rho_q \, \rho_{q'} \; + \; \frac{t_0 \, x_0}{4} \, \vec{s}_q \cdot \vec{s}_{q'} \right] \\ & + \sum_q \left[\frac{t_0}{4} \, (1 \, - \, x_0) \, \rho_q \, \rho_q \; - \; \frac{t_0}{4} \, (1 \, - \, x_0) \, \vec{s}_q \cdot \vec{s}_q \right] \Bigg\} \; . \end{aligned} \tag{A.43}$$

A.4.3.2 Interaction term Eq. 3.52b

The exchange operator part of the antisymmetrized interaction is the same as for Eq. 3.52a. Knowing that the present term also acts in S-wave only, i.e. $L = 0$, so that $P^r_{12} = 1$, one obtains the same non-local density matrix energy functional

$$E^{\rho\rho}_{Sk,t_1} = \int d(\vec{r})\, v^{2Sk}_{t_1}(\vec{r}_1,\vec{r}\,'_1,\vec{r}_2,\vec{r}\,'_2) \Bigg\{ \sum_{q_1\neq q_2} \Big[\frac{t_1}{4}(1+\frac{x_1}{2})\rho^{q_1}_{\vec{r}_1\vec{r}\,'_1}\rho^{q_2}_{\vec{r}_2\vec{r}\,'_2} + \frac{t_1 x_1}{8}\vec{s}^{\,q_1}_{\vec{r}_1\vec{r}\,'_1}\vec{s}^{\,q_2}_{\vec{r}_2\vec{r}\,'_2}\Big] + \sum_{q_1} \Big[\frac{t_1}{8}(1-x_1)\rho^{q_1}_{\vec{r}_1\vec{r}\,'_1}\rho^{q_1}_{\vec{r}_2\vec{r}\,'_2} - \frac{t_1}{8}(1-x_1)\vec{s}^{\,q_1}_{\vec{r}_1\vec{r}\,'_1}\vec{s}^{\,q_1}_{\vec{r}_2\vec{r}\,'_2}\Big] \Bigg\} \ , \tag{A.44}$$

as Eq. A.42, except that one must replace t_0 by $\dfrac{t_1}{2}$ and x_0 by x_1. The coordinate part of the interaction Eq. 3.52b is however different such that its matrix elements are given by

$$v^{2Sk}_{t_1}(\vec{r}_1,\vec{r}\,'_1,\vec{r}_2,\vec{r}\,'_2) = -\frac{1}{4}\Big(\vec{\nabla}^2_{\vec{r}\,'_1} + \vec{\nabla}^2_{\vec{r}\,'_2} + \vec{\nabla}^2_{\vec{r}_1} + \vec{\nabla}^2_{\vec{r}_2} - 2\vec{\nabla}_{\vec{r}\,'_1}\cdot\vec{\nabla}_{\vec{r}\,'_2} - 2\vec{\nabla}_{\vec{r}_1}\cdot\vec{\nabla}_{\vec{r}_2}\Big)\delta(\vec{r}) \ . \tag{A.45}$$

Corresponding gradient operators act on a given bilinear product of non-local density matrices according to

$$\begin{aligned} E^{\rho\rho}_{Sk,t_1} &\subset \int d(\vec{r})\, v^{2Sk}_{t_1}(\vec{r}_1,\vec{r}\,'_1,\vec{r}_2,\vec{r}\,'_2) \sum_{q_1\neq q_2} \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}\,'_1}\mathcal{P}^{q_2}_{\vec{r}_2\vec{r}\,'_2} \\ &= \frac{-1}{4}\int d\vec{r} \sum_{q_1\neq q_2} \Big\{ (\triangle+\triangle')\mathcal{P}^{q_1}_{\vec{r}}\mathcal{P}^{q_2}_{\vec{r}} + \mathcal{P}^{q_1}_{\vec{r}}(\triangle+\triangle')\mathcal{P}^{q_2}_{\vec{r}} - 2\vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}\mathcal{P}^{q_2}_{\vec{r}} - 2\vec{\nabla}'\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}'\mathcal{P}^{q_2}_{\vec{r}} \Big\} \\ &= \frac{-1}{4}\int d\vec{r} \sum_{q_1\neq q_2} \Big\{ (\Delta\mathcal{P}^{q_1}_{\vec{r}} - 2\mathcal{T}^{q_1}_{\vec{r}})\mathcal{P}^{q_2}_{\vec{r}} + \mathcal{P}^{q_1}_{\vec{r}}(\Delta\mathcal{P}^{q_2}_{\vec{r}} - 2\mathcal{T}^{q_2}_{\vec{r}}) - \vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}\mathcal{P}^{q_2}_{\vec{r}} + 4\vec{\mathcal{J}}^{q_1}_{\vec{r}}\vec{\mathcal{J}}^{q_2}_{\vec{r}} \Big\} \\ &= \frac{1}{4}\int d\vec{r} \sum_{q_1\neq q_2} \Big\{ 3\vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}\mathcal{P}^{q_2}_{\vec{r}} + 2\mathcal{T}^{q_1}_{\vec{r}}\mathcal{P}^{q_2}_{\vec{r}} + 2\mathcal{P}^{q_1}_{\vec{r}}\mathcal{T}^{q_2}_{\vec{r}} - 4\vec{\mathcal{J}}^{q_1}_{\vec{r}}\vec{\mathcal{J}}^{q_2}_{\vec{r}} \Big\} \ , \end{aligned} \tag{A.46}$$

where results from Sec. A.4.1.2 and an integration by part have been used. Eventually the contribution to the energy reads

$$\begin{aligned} E^{\rho\rho}_{Sk,t_1} = & \int d\vec{r} \sum_{q\neq q'} \Bigg\{ \frac{1}{16}t_1\Big(1+\frac{x_1}{2}\Big)\Big[3\,\vec{\nabla}\rho_q\cdot\vec{\nabla}\rho_{q'} + 4\,\tau_q\,\rho_{q'} - 4\,\vec{j}_q\cdot\vec{j}_{q'}\Big] \\ & + \frac{1}{32}t_1 x_1\Big[3\sum_{\mu\nu}\nabla_\mu s_{q,\nu}\nabla_\mu s_{q',\nu} + 4\,\vec{T}_q\cdot\vec{s}_{q'} - 4\sum_{\mu\nu}J_{q,\mu\nu}J_{q',\mu\nu}\Big]\Bigg\} \\ & + \int d\vec{r} \sum_{q} \Bigg\{ \frac{1}{32}t_1\,(1-x_1)\Big[3\,\vec{\nabla}\rho_q\cdot\vec{\nabla}\rho_q + 4\,\tau_q\,\rho_q - 4\,\vec{j}_q\cdot\vec{j}_q\Big] \\ & - \frac{1}{32}t_1(1-x_1)\Big[3\sum_{\mu\nu}\nabla_\mu s_{q,\nu}\nabla_\mu s_{q',\nu} + 4\,\vec{T}_q\cdot\vec{s}_q - 4\sum_{\mu\nu}J_{q,\mu\nu}J_{q,\mu\nu}\Big]\Bigg\} \ . \end{aligned} \tag{A.47}$$

A.4.3.3 Interaction term Eq. 3.52c

The exchange operator part of the antisymmetrized interaction term can be reduced according to

$$t_2(1+x_2P^s_{12})\mathcal{A}_{12} = t_2(1+P^s_{12}P^t_{12}) + t_2x_2(P^s_{12}+P^t_{12}) \ , \tag{A.48}$$

where P^r_{12} has been replaced by -1 given that Eq. 3.52c acts in P-wave only, i.e. $L=1$. Using Sec. A.4.1.1, one obtains

$$\begin{aligned} E^{\rho\rho}_{Sk,t_2} &= \frac{1}{2}\int d(\vec{r})\, v^{2Sk}_{t_2}(\vec{r}_1,\vec{r}_1',\vec{r}_2,\vec{r}_2')\, t_2 \Bigg\{ \sum_{q_1 q_2} \rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_2\vec{r}_2'} + \frac{1}{2}\sum_{q_1}\left(\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_1}_{\vec{r}_2\vec{r}_2'} + \vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'}\vec{s}^{q_1}_{\vec{r}_2\vec{r}_2'}\right) \\ &\quad + x_2\frac{1}{2}\sum_{q_1 q_2}\left(\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_2\vec{r}_2'} + \vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'}\vec{s}^{q_2}_{\vec{r}_2\vec{r}_2'}\right) + x_2\sum_{q_1}\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_1}_{\vec{r}_2\vec{r}_2'}\Bigg\} \\ &= \int d(\vec{r})\, v^{2Sk}_{t_2}(\vec{r}_1,\vec{r}_1',\vec{r}_2,\vec{r}_2')\Bigg\{ \sum_{q_1\neq q_2}\left[\frac{t_2}{2}(1+\frac{x_2}{2})\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_2\vec{r}_2'} + \frac{t_2x_2}{4}\vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'}\vec{s}^{q_2}_{\vec{r}_2\vec{r}_2'}\right] \\ &\quad + \sum_{q_1}\left[\frac{3t_2}{4}(1+x_2)\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_1}_{\vec{r}_2\vec{r}_2'} + \frac{t_2}{4}(1+x_2)\vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'}\vec{s}^{q_1}_{\vec{r}_2\vec{r}_2'}\right]\Bigg\}\ . \end{aligned} \tag{A.49}$$

Expressing the spatial part as

$$v^{2Sk}_{t_1}(\vec{r}_1,\vec{r}_1',\vec{r}_2,\vec{r}_2') = \frac{1}{4}\Big(\vec{\nabla}_{\vec{r}_1}\cdot\vec{\nabla}_{\vec{r}_1'} + \vec{\nabla}_{\vec{r}_2}\cdot\vec{\nabla}_{\vec{r}_2'} - \vec{\nabla}_{\vec{r}_1}\cdot\vec{\nabla}_{\vec{r}_2'} - \vec{\nabla}_{\vec{r}_2}\cdot\vec{\nabla}_{\vec{r}_1'}\Big)\delta(\vec{r})\ , \tag{A.50}$$

the gradient operators act on a given bilinear product of non-local density matrices according to

$$\begin{aligned} E^{\rho\rho}_{Sk,t_2} &\subset \int d(\vec{r})\, v^{2Sk}_{t_2}(\vec{r}_1,\vec{r}_1',\vec{r}_2,\vec{r}_2') \sum_{q_1\neq q_2}\mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\mathcal{P}^{q_2}_{\vec{r}_2\vec{r}_2'} \\ &= \frac{1}{4}\int d\vec{r}\sum_{q_1\neq q_2}\left\{\mathcal{T}^{q_1}_{\vec{r}}\mathcal{P}^{q_2}_{\vec{r}} + \mathcal{P}^{q_1}_{\vec{r}}\mathcal{T}^{q_2}_{\vec{r}} - \vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}'\mathcal{P}^{q_2}_{\vec{r}} - \vec{\nabla}'\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}\mathcal{P}^{q_2}_{\vec{r}}\right\} \\ &= \frac{1}{4}\int d\vec{r}\sum_{q_1\neq q_2}\left\{\mathcal{T}^{q_1}_{\vec{r}}\mathcal{P}^{q_2}_{\vec{r}} + \mathcal{P}^{q_1}_{\vec{r}}\mathcal{T}^{q_2}_{\vec{r}} - \frac{1}{2}\vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}\mathcal{P}^{q_2}_{\vec{r}} - 2\vec{\mathcal{J}}^{q_1}_{\vec{r}}\vec{\mathcal{J}}^{q_2}_{\vec{r}}\right\} \\ &= \frac{-1}{8}\int d\vec{r}\sum_{q_1\neq q_2}\left\{-2\mathcal{T}^{q_1}_{\vec{r}}\mathcal{P}^{q_2}_{\vec{r}} - 2\mathcal{P}^{q_1}_{\vec{r}}\mathcal{T}^{q_2}_{\vec{r}} + \vec{\nabla}\mathcal{P}^{q_1}_{\vec{r}}\vec{\nabla}\mathcal{P}^{q_2}_{\vec{r}} + 4\vec{\mathcal{J}}^{q_1}_{\vec{r}}\vec{\mathcal{J}}^{q_2}_{\vec{r}}\right\}\ , \end{aligned} \tag{A.51}$$

such that the contribution to the energy finally reads

$$\begin{aligned} E^{\rho\rho}_{Sk,t_2} = \int d\vec{r}\sum_{q\neq q'}\Bigg\{ &-\frac{1}{16}t_2\left(1+\frac{x_2}{2}\right)\left(\vec{\nabla}\rho_q\cdot\vec{\nabla}\rho_{q'} - 4\,\tau_q\,\rho_{q'} + 4\,\vec{j}_q\cdot\vec{j}_{q'}\right) \\ &-\frac{1}{32}t_2\,x_2\left(\sum_{\mu\nu}\nabla_\mu s_{q,\nu}\nabla_\mu s_{q',\nu} - 4\,\vec{T}_q\,\vec{s}_{q'} + 4\sum_{\mu\nu}J_{q,\mu\nu}J_{q',\mu\nu}\right)\Bigg\} \\ + \int d\vec{r}\sum_{q}\Bigg\{ &-\frac{3}{32}t_2\,(1+x_2)\left(\vec{\nabla}\rho_q\cdot\vec{\nabla}\rho_q - 4\,\tau_q\,\rho_q + 4\,\vec{j}_q\cdot\vec{j}_q\right) \\ &-\frac{1}{32}t_2(1+x_2)\left(\sum_{\mu\nu}\nabla_\mu s_{q,\nu}\nabla_\mu s_{q,\nu} - 4\,\vec{T}_q\,\vec{s}_q + 4\sum_{\mu\nu}J_{q,\mu\nu}J_{q,\mu\nu}\right)\Bigg\}\ . \end{aligned} \tag{A.52}$$

A.4.3.4 Interaction term Eq. 3.52d

The spin-orbit interaction term has a different structure compared to central terms. Indeed, the gradient operators are coupled to spin matrices. Moreover, no further spin or isospin exchange operator need to be included in the definition of the interaction term itself as they are known to be redundant in the present case. Finally, the interaction acts in P-wave and in the

spin-triplet state only such that $P^r_{12} = -1$ and $P^s_{12} = 1$. Eventually, the spin-isospin operator structure of the antisymmetrized spin-orbit term reads

$$iW_0(\hat{\sigma}_1 + \hat{\sigma}_2)\mathcal{A}_{12} = iW_0(\hat{\sigma}_1 + \hat{\sigma}_2)(1 + P^t_{12}) \ , \tag{A.53}$$

such that the density matrix functional is

$$\begin{aligned}
E^{\rho\rho}_{Sk,W_0} &= \frac{1}{2}\int d(\vec{r})\, \vec{v}^{2Sk}_{W_0}(\vec{r}_1,\vec{r}\,'_1,\vec{r}_2,\vec{r}\,'_2)\cdot iW_0\Bigg\{\sum_{q_1q_2}\left(\rho^{q_1}_{\vec{r}_1\vec{r}\,'_1}\vec{s}^{\,q_2}_{\vec{r}_2\vec{r}\,'_2} + \vec{s}^{\,q_1}_{\vec{r}_1\vec{r}\,'_1}\rho^{q_2}_{\vec{r}_2\vec{r}\,'_2}\right) \\
&\quad + \sum_{q_1}\left(\rho^{q_1}_{\vec{r}_1\vec{r}\,'_1}\vec{s}^{\,q_1}_{\vec{r}_2\vec{r}\,'_2} + \vec{s}^{\,q_1}_{\vec{r}_1\vec{r}\,'_1}\rho^{q_1}_{\vec{r}_2\vec{r}\,'_2}\right)\Bigg\} \\
&= \frac{1}{2}\int d(\vec{r})\, \vec{v}^{2Sk}_{W_0}(\vec{r}_1,\vec{r}\,'_1,\vec{r}_2,\vec{r}\,'_2)\cdot iW_0\Bigg\{\sum_{q_1\neq q_2}\left(\rho^{q_1}_{\vec{r}_1\vec{r}\,'_1}\vec{s}^{\,q_2}_{\vec{r}_2\vec{r}\,'_2} + \vec{s}^{\,q_1}_{\vec{r}_1\vec{r}\,'_1}\rho^{q_2}_{\vec{r}_2\vec{r}\,'_2}\right) \\
&\quad + 2\sum_{q_1}\left(\rho^{q_1}_{\vec{r}_1\vec{r}\,'_1}\vec{s}^{\,q_1}_{\vec{r}_2\vec{r}\,'_2} + \vec{s}^{\,q_1}_{\vec{r}_1\vec{r}\,'_1}\rho^{q_1}_{\vec{r}_2\vec{r}\,'_2}\right)\Bigg\} \\
&= \int d(\vec{r})\, \vec{v}^{2Sk}_{W_0}(\vec{r}_1,\vec{r}\,'_1,\vec{r}_2,\vec{r}\,'_2)\cdot iW_0\Bigg\{\sum_{q_1\neq q_2}\vec{s}^{\,q_1}_{\vec{r}_1\vec{r}\,'_1}\rho^{q_2}_{\vec{r}_2\vec{r}\,'_2} + 2\sum_{q_1}\vec{s}^{\,q_1}_{\vec{r}_1\vec{r}\,'_1}\rho^{q_1}_{\vec{r}_2\vec{r}\,'_2}\Bigg\} \ ,
\end{aligned} \tag{A.54}$$

where we have used that the spatial part of the interaction is symmetric with respect to the exchange of particle 1 and 2, i.e. $\vec{v}^{2Sk}_{W_0}(\vec{r}_1,\vec{r}\,'_1,\vec{r}_2,\vec{r}\,'_2) = \vec{v}^{2Sk}_{W_0}(\vec{r}_2,\vec{r}\,'_2,\vec{r}_1,\vec{r}\,'_1)$, in agreement with its definition

$$v^{2Sk}_{W_0,\nu}(\vec{r}_1,\vec{r}\,'_1,\vec{r}_2,\vec{r}\,'_2) = \frac{1}{4}\sum_{\lambda\mu}\epsilon_{\lambda\mu\nu}\Big(\nabla_{\vec{r}\,'_1,\lambda}\cdot\nabla_{\vec{r}_1,\mu} + \nabla_{\vec{r}\,'_2,\lambda}\cdot\nabla_{\vec{r}_2,\mu} - \nabla_{\vec{r}\,'_1,\lambda}\cdot\nabla_{\vec{r}_2,\mu} - \nabla_{\vec{r}\,'_2,\lambda}\cdot\nabla_{\vec{r}_1,\mu}\Big)\delta(\vec{r}) \ . \tag{A.55}$$

Using Sec. A.4.1.2, gradient operators act on a given bilinear product of non-local density matrices according to

$$\begin{aligned}
E^{\rho\rho}_{Sk,W_0} &\subset \int d(\vec{r})\, v^{2Sk}_{W_0,\nu}(\vec{r}_1,\vec{r}\,'_1,\vec{r}_2,\vec{r}\,'_2)\sum_{q_1\neq q_2}\mathcal{P}^{q_1}_{\vec{r}_1\vec{r}\,'_1}\mathcal{P}^{q_2}_{\vec{r}_2\vec{r}\,'_2} \\
&= \frac{1}{4}\int d\vec{r}\sum_{\lambda\mu\nu}\epsilon_{\lambda\mu\nu}\sum_{q_1\neq q_2}\left\{i\nabla_\lambda\mathcal{J}^{q_1}_{\vec{r},\mu}\mathcal{P}^{q_2}_{\vec{r}} + i\mathcal{P}^{q_1}_{\vec{r}}\nabla_\lambda\mathcal{J}^{q_2}_{\vec{r},\mu} - \nabla'_\lambda\mathcal{P}^{q_1}_{\vec{r}}\nabla_\mu\mathcal{P}^{q_2}_{\vec{r}} - \nabla_\mu\mathcal{P}^{q_1}_{\vec{r}}\nabla'_\lambda\mathcal{P}^{q_2}_{\vec{r}}\right\} \\
&= \frac{1}{4}\int d\vec{r}\sum_{\lambda\mu\nu}\epsilon_{\lambda\mu\nu}\sum_{q_1\neq q_2}\left\{i\nabla_\lambda\mathcal{J}^{q_1}_{\vec{r},\mu}\mathcal{P}^{q_2}_{\vec{r}} + i\mathcal{P}^{q_1}_{\vec{r}}\nabla_\lambda\mathcal{J}^{q_2}_{\vec{r},\mu} - i\nabla_\lambda\mathcal{P}^{q_1}_{\vec{r}}\mathcal{J}^{q_2}_{\vec{r},\mu} - i\mathcal{J}^{q_1}_{\vec{r},\mu}\nabla_\lambda\mathcal{P}^{q_2}_{\vec{r}}\right\} \\
&= \frac{1}{2}\int d\vec{r}\sum_{\lambda\mu\nu}\epsilon_{\lambda\mu\nu}\sum_{q_1\neq q_2}\left\{i\nabla_\lambda\mathcal{J}^{q_1}_{\vec{r},\mu}\mathcal{P}^{q_2}_{\vec{r}} + i\mathcal{P}^{q_1}_{\vec{r}}\nabla_\lambda\mathcal{J}^{q_2}_{\vec{r},\mu}\right\} \\
&= \frac{1}{2}\int d\vec{r}\sum_{\lambda\mu\nu}\epsilon_{\lambda\mu\nu}\sum_{q_1\neq q_2}\left\{i\nabla_\lambda\mathcal{J}^{q_1}_{\vec{r},\mu}\mathcal{P}^{q_2}_{\vec{r}} + i\nabla_\mu\mathcal{P}^{q_1}_{\vec{r}}\mathcal{J}^{q_2}_{\vec{r},\lambda}\right\} \ .
\end{aligned} \tag{A.56}$$

One of the two generic non-local densities $\mathcal{P}^q_{\vec{r}\,\vec{r}\,'}$ has to be a spin density matrix with vector index ν. The contribution to the energy eventually reads

$$\begin{aligned}
E^{\rho\rho}_{Sk,W_0} &= -\int d\vec{r}\sum_{q\neq q'}\frac{W_0}{2}\left[(\vec{\nabla}\cdot\vec{J}_q)\,\rho_{q'} + (\vec{\nabla}\times\vec{s}_q)\cdot\vec{j}_{q'}\right] \\
&\quad - \int d\vec{r}\sum_q W_0\left[(\vec{\nabla}\cdot\vec{J}_q)\,\rho_q + (\vec{\nabla}\times\vec{s}_q)\cdot\vec{j}_q\right] \ .
\end{aligned} \tag{A.57}$$

A.4.3.5 Complete two-body EDF

The complete bilinear part of the EDF expressed in neutron-proton representation takes the form

$$\begin{aligned}\mathcal{E}_{Sk}^{\rho\rho} &= \sum_q \Big\{ A^{\rho\rho}\,\rho_q\rho_q + A^{\rho\Delta\rho}\,\rho_q\Delta\rho_q + A^{\rho\tau}\left(\rho_q\tau_q - \vec{j}_q\cdot\vec{j}_q\right) + A^{ss}\,\vec{s}_q\cdot\vec{s}_q + A^{s\Delta s}\,\vec{s}_q\cdot\Delta\vec{s}_q \\ &\qquad + A^{\rho\nabla J}\left(\rho_q\vec{\nabla}\cdot\vec{J}_q + \vec{j}_q\cdot\vec{\nabla}\times\vec{s}_q\right) + A^{JJ}\Big(\sum_{\mu\nu} J_{q,\mu\nu}J_{q,\mu\nu} - \vec{s}_q\cdot\vec{T}_q\Big)\Big\} \\ &+ \sum_{q\neq q'}\Big\{ B^{\rho\rho}\,\rho_q\rho_{q'} + B^{\rho\Delta\rho}\,\rho_q\Delta\rho_{q'} + B^{\rho\tau}\left(\rho_q\tau_{q'} - \vec{j}_q\cdot\vec{j}_{q'}\right) + B^{ss}\,\vec{s}_q\cdot\vec{s}_{q'} + B^{s\Delta s}\,\vec{s}_q\cdot\Delta\vec{s}_{q'} \\ &\qquad + B^{\rho\nabla J}\left(\rho_q\vec{\nabla}\cdot\vec{J}_{q'} + \vec{j}_q\cdot\vec{\nabla}\times\vec{s}_{q'}\right) + B^{JJ}\Big(\sum_{\mu\nu} J_{q,\mu\nu}J_{q',\mu\nu} - \vec{s}_q\cdot\vec{T}_{q'}\Big)\Big\}\ , \end{aligned} \tag{A.58}$$

where functional coefficients are related to interaction ones through

$$A^{\rho\rho} = \frac{1}{4}t_0(1-x_0) \quad , \quad B^{\rho\rho} = \frac{1}{2}t_0\Big(1+\frac{x_0}{2}\Big) \tag{A.59a}$$

$$A^{ss} = -\frac{1}{4}t_0(1-x_0) \quad , \quad B^{ss} = \frac{1}{4}t_0x_0 \tag{A.59b}$$

$$A^{\rho\tau} = \frac{1}{8}[t_1(1-x_1)+3t_2(1+x_2)] \quad , \quad B^{\rho\tau} = \frac{1}{4}\Big[t_1\Big(1+\frac{x_1}{2}\Big)+t_2\Big(1+\frac{x_2}{2}\Big)\Big] \tag{A.59c}$$

$$A^{\rho\Delta\rho} = \frac{3}{32}[-t_1(1-x_1)+t_2(1+x_2)], \quad B^{\rho\Delta\rho} = -\frac{1}{16}\Big[3t_1\Big(1+\frac{x_1}{2}\Big)-t_2\Big(1+\frac{x_2}{2}\Big)\Big] \tag{A.59d}$$

$$A^{\rho\nabla J} = -W_0 \quad , \quad B^{\rho\nabla J} = -\frac{1}{2}W_0 \tag{A.59e}$$

$$A^{JJ} = \frac{1}{8}\Big[t_1(1-x_1)-t_2(1+x_2)\Big] \quad , \quad B^{JJ} = -\frac{1}{8}(t_1x_1+t_2x_2) \tag{A.59f}$$

$$A^{s\Delta s} = \frac{1}{32}\Big[3t_1(1-x_1)+t_2(1+x_2)\Big], \quad B^{s\Delta s} = -\frac{1}{32}(3t_1x_1-t_2x_2)\ . \tag{A.59g}$$

To obtain the form of the EDF given by Eqs. (3.53,3.54), one has to go from neutron-proton representation to isoscalar-isovector representation using Eq. 3.15, such that

$$A_0^{\rho} = \frac{1}{2}(A^{\rho\rho}+B^{\rho\rho}) \quad , \quad A_1^{\rho} = \frac{1}{2}(A^{\rho\rho}-B^{\rho\rho}) \tag{A.60a}$$

$$A_0^{s} = \frac{1}{2}(A^{ss}+B^{ss}) \quad , \quad A_1^{s} = \frac{1}{2}(A^{ss}-B^{ss}) \tag{A.60b}$$

$$A_0^{\tau} = \frac{1}{2}(A^{\rho\tau}+B^{\rho\tau}) \quad , \quad A_1^{\tau} = \frac{1}{2}(A^{\rho\tau}-B^{\rho\tau}) \tag{A.60c}$$

$$A_0^{J} = \frac{1}{2}(A^{JJ}+B^{JJ}) \quad , \quad A_1^{J} = \frac{1}{2}(A^{JJ}-B^{JJ}) \tag{A.60d}$$

$$A_0^{\nabla\rho} = \frac{-1}{2}(A^{\rho\Delta\rho}+B^{\rho\Delta\rho}) \quad , \quad A_1^{\nabla\rho} = \frac{-1}{2}(A^{\rho\Delta\rho}-B^{\rho\Delta\rho}) \tag{A.60e}$$

$$A_0^{\nabla s} = \frac{-1}{2}(A^{s\Delta s}+B^{s\Delta s}) \quad , \quad A_1^{\nabla s} = \frac{-1}{2}(A^{s\Delta s}-B^{s\Delta s}) \tag{A.60f}$$

$$A_0^{\nabla J} = \frac{1}{2}(A^{\rho\nabla J}+B^{\rho\nabla J}) \quad , \quad A_1^{\nabla J} = \frac{1}{2}(A^{\rho\nabla J}-B^{\rho\nabla J})\,, \tag{A.60g}$$

where $\vec{\nabla}\rho\cdot\vec{\nabla}\rho$ and $\vec{\nabla}s\cdot\vec{\nabla}s$ are obtained from $\rho\Delta\rho$ and $s\Delta s$ thanks to an integration by part.

A.4.4 Trilinear part of the EDF

As the potential energy deriving from the three-body pseudo potential is significantly more lengthy to compute, only the contribution originating from interaction term (Eq. 3.87b) is explicitly derived. Such a derivation provides a good illustration of the steps performed by the code (Sec. 3.4.4.1) that starts from the non-reduced interaction, see Eqs. (3.64,3.75,3.70).

A.4.4.1 Exchange operators and antisymmetrizer

The exchange operator structure of the antisymmetrized interaction term is obtained through

$$\begin{aligned}\frac{u_1}{2}(1+y_1P_{12}^s)\mathcal{A}_{123} &= +\frac{u_1}{2}\left[+1-P_{12}^rP_{12}^sP_{12}^t-2P_{23}^rP_{23}^sP_{23}^t+2P_{12}^rP_{23}^rP_{12}^sP_{23}^sP_{12}^tP_{23}^t\right] \\ &\quad +\frac{u_1y_1}{2}\left[+P_{12}^s-P_{12}^rP_{12}^t-2P_{23}^rP_{12}^sP_{23}^sP_{23}^t+2P_{12}^rP_{23}^rP_{23}^sP_{12}^tP_{23}^t\right] \ ,\end{aligned} \tag{A.61}$$

where Eq. 3.22b and the symmetry under the exchange of particle 1 and 2, so that $P_{23}^x = P_{13}^x$ have been used.

A.4.4.2 Function of non-local densities

The functional of non-local densities is obtained similarly to the bilinear case, except for a few differences.
First, double exchange operators appear in the calculation. For isospin exchange operators the conclusion drawn before does not change such that $P_{xy}^tP_{yz}^t = \hat{\delta}_{q_xq_y}\hat{\delta}_{q_yq_z}$. For spin exchange operators one has

$$\begin{aligned}P_{12}^sP_{23}^s &= \frac{1}{4}(1+\sigma_1\cdot\sigma_2+\sigma_2\cdot\sigma_3+\sigma_1\cdot\sigma_2\sigma_2\cdot\sigma_3) \\ &= \frac{1}{4}(1+\sigma_1\cdot\sigma_2+\sigma_2\cdot\sigma_3+\sigma_1\cdot\sigma_3-\sum_{ijk}i\epsilon_{ijk}\sigma_{1,i}\sigma_{2,j}\sigma_{3,k}) \ ,\end{aligned} \tag{A.62}$$

where one has used the following property of Pauli matrices

$$\sigma_i\sigma_j = i\epsilon_{ijk}\sigma_k+\delta_{ij}\mathbb{I} \ . \tag{A.63}$$

A second difference is that coordinate exchange operators do not simplify *a priori*, such that they must be applied consistently when computing the functional of non-local densities and when applying gradient operators. The convention used in the present chapter is to exchange coordinates at the level of the non-local densities, e.g.

$$\begin{aligned}\int d(\vec{r})\langle\vec{r}_1'\vec{r}_2'\vec{r}_3'|\hat{v}_{123}^{3Sk}P_{13}^r|\vec{r}_1\vec{r}_2\vec{r}_3\rangle\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_2\vec{r}_2'}\rho^{q_3}_{\vec{r}_3\vec{r}_3'} &= \int d(\vec{r})\langle\vec{r}_1'\vec{r}_2'\vec{r}_3'|\hat{v}_{123}^{3Sk}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle\rho^{q_1}_{\vec{r}_3\vec{r}_1'}\rho^{q_2}_{\vec{r}_2\vec{r}_2'}\rho^{q_3}_{\vec{r}_1\vec{r}_3'} \ , \\ \int d(\vec{r})\langle\vec{r}_1'\vec{r}_2'\vec{r}_3'|\hat{v}_{123}^{3Sk}P_{12}^rP_{23}^r|\vec{r}_1\vec{r}_2\vec{r}_3\rangle\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_2\vec{r}_2'}\rho^{q_3}_{\vec{r}_3\vec{r}_3'} &= \int d(\vec{r})\langle\vec{r}_1'\vec{r}_2'\vec{r}_3'|\hat{v}_{123}^{3Sk}|\vec{r}_3\vec{r}_1\vec{r}_2\rangle\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_2\vec{r}_2'}\rho^{q_3}_{\vec{r}_3\vec{r}_3'} \\ &= \int d(\vec{r})\langle\vec{r}_1'\vec{r}_2'\vec{r}_3'|\hat{v}_{123}^{3Sk}|\vec{r}_1\vec{r}_2\vec{r}_3\rangle\rho^{q_1}_{\vec{r}_2\vec{r}_1'}\rho^{q_2}_{\vec{r}_3\vec{r}_2'}\rho^{q_3}_{\vec{r}_1\vec{r}_3'} \ .\end{aligned} \tag{A.64}$$

In summary, exchange operators are applied according to

$$\begin{aligned}\int d(\vec{r}\sigma q)\Big\{\langle\vec{r}_1'\sigma_1'q_1\,\vec{r}_2'\sigma_2'q_2\,\vec{r}_3'\sigma_3'q_3|\hat{v}_{123}^{3Sk}P_{123}^{rst}|\vec{r}_1\sigma_1q_1\,\vec{r}_2\sigma_2q_2\,\vec{r}_3\sigma_3q_3\rangle\rho_{q_1}(\vec{r}_1\sigma_1,\vec{r}_1'\sigma_1')\rho_{q_2}(\vec{r}_2\sigma_2,\vec{r}_2'\sigma_2') \\ \rho_{q_3}(\vec{r}_3\sigma_3,\vec{r}_3'\sigma_3')\Big\} = \int d(\vec{r}q)\langle\vec{r}_1'q_1\,\vec{r}_2'q_2\,\vec{r}_3'q_3|\hat{v}_{123}^{3Sk}|\vec{r}_1q_1\,\vec{r}_2q_2\,\vec{r}_3q_3\rangle\mathcal{P}^{q_x}_{\vec{r}_a\vec{r}_b'}\mathcal{P}^{q_y}_{\vec{r}_c\vec{r}_d'}\mathcal{P}^{q_z}_{\vec{r}_e\vec{r}_f'} \ ,\end{aligned} \tag{A.65}$$

P^{rst}_{123}	1	P^{x}_{12}	P^{x}_{13}	P^{x}_{23}	$P^{x}_{12}P^{x}_{23}$	$P^{x}_{13}P^{x}_{23}$
$\overrightarrow{x=r}$	$a=1,\ b=1$ $c=2,\ d=2$ $e=3,\ f=3$	$a=2,\ b=1$ $c=1,\ d=2$ $e=3,\ f=3$	$a=3,\ b=1$ $c=2,\ d=2$ $e=1,\ f=3$	$a=1,\ b=1$ $c=3,\ d=2$ $e=2,\ f=3$	$a=2,\ b=1$ $c=3,\ d=2$ $e=1,\ f=3$	$a=3,\ b=1$ $c=1,\ d=2$ $e=2,\ f=3$
$\overleftarrow{x=r}$	$a=1,\ b=1$ $c=2,\ d=2$ $e=3,\ f=3$	$a=1,\ b=2$ $c=2,\ d=1$ $e=3,\ f=3$	$a=1,\ b=3$ $c=2,\ d=2$ $e=3,\ f=1$	$a=1,\ b=1$ $c=2,\ d=3$ $e=3,\ f=2$	$a=1,\ b=3$ $c=2,\ d=1$ $e=3,\ f=2$	$a=1,\ b=2$ $c=2,\ d=3$ $e=3,\ f=1$
$x=t$ $x=t$ $x=t$	$x=1$ $y=2$ $z=3$	$x=1$ $y=1$ $z=3$	$x=1$ $y=2$ $z=1$	$x=1$ $y=2$ $z=2$	$x=1$ $y=1$ $z=1$	$x=1$ $y=1$ $z=1$
$x=s$	$\mathcal{PPP}=$ $\rho\rho\rho$	$\mathcal{PPP}=$ $\frac{1}{2}\rho\rho\rho$ $+\frac{1}{2}ss\rho$	$\mathcal{PPP}=$ $\frac{1}{2}\rho\rho\rho$ $+\frac{1}{2}s\rho s$	$\mathcal{PPP}=$ $\frac{1}{2}\rho\rho\rho$ $+\frac{1}{2}\rho ss$	$\mathcal{PPP}=$ $\frac{1}{4}\rho\rho\rho$ $+\frac{1}{4}ss\rho$ $+\frac{1}{4}s\rho s$ $+\frac{1}{4}\rho ss$ $-\frac{i}{4}sss$	$\mathcal{PPP}=$ $\frac{1}{4}\rho\rho\rho$ $+\frac{1}{4}ss\rho$ $+\frac{1}{4}s\rho s$ $+\frac{1}{4}\rho ss$ $+\frac{i}{4}sss$

Table A.2: Rules to apply exchange operators in view of obtaining functional of non-local densities. The right (left) arrow on $x=r$ denotes that the coordinate exchange operators act on the ket (bra). Spin exchange operators determine the matter or spin nature of the densities, whereas isospin and coordinate exchange operators determine their isospin and coordinate content.

where the product of three non-local densities depend on the content of P^{rst}_{123} in terms of two-body exchange operators. For corresponding rules see Tab. {A.2}.

The functional of non-local densities originating from the first line of Eq. A.61 reads

$$E^{\rho\rho\rho}_{Sk}(u_1)=\frac{1}{2}\int d(\vec{r})v^{3Sk}_{\overline{123}}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_1\,',\vec{r}_2\,',\vec{r}_3\,')\frac{u_1}{2}\Bigg\{ \tag{A.66}$$

$$\sum_{q_1q_2q_3}\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_2\vec{r}_2'}\rho^{q_3}_{\vec{r}_3\vec{r}_3'}-\sum_{q_1q_3}\frac{1}{2}\Big(\rho^{q_1}_{\vec{r}_2\vec{r}_1'}\rho^{q_1}_{\vec{r}_1\vec{r}_2'}+\vec{s}^{\,q_1}_{\vec{r}_2\vec{r}_1'}\vec{s}^{\,q_1}_{\vec{r}_1\vec{r}_2'}\Big)\rho^{q_3}_{\vec{r}_3\vec{r}_3'}-2\sum_{q_1q_2}\frac{1}{2}\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\Big(\rho^{q_2}_{\vec{r}_3\vec{r}_2'}\rho^{q_2}_{\vec{r}_2\vec{r}_3'}+\vec{s}^{\,q_2}_{\vec{r}_3\vec{r}_2'}\vec{s}^{\,q_2}_{\vec{r}_2\vec{r}_3'}\Big)$$

$$+2\sum_{q_1}\frac{1}{4}\Big(\rho^{q_1}_{\vec{r}_2\vec{r}_1'}\rho^{q_1}_{\vec{r}_3\vec{r}_2'}\rho^{q_1}_{\vec{r}_1\vec{r}_3'}+\vec{s}^{\,q_1}_{\vec{r}_2\vec{r}_1'}\vec{s}^{\,q_1}_{\vec{r}_3\vec{r}_2'}\rho^{q_1}_{\vec{r}_1\vec{r}_3'}+\vec{s}^{\,q_1}_{\vec{r}_2\vec{r}_1'}\rho^{q_1}_{\vec{r}_3\vec{r}_2'}\vec{s}^{\,q_1}_{\vec{r}_1\vec{r}_3'}+\rho^{q_1}_{\vec{r}_2\vec{r}_1'}\vec{s}^{\,q_1}_{\vec{r}_3\vec{r}_2'}\vec{s}^{\,q_1}_{\vec{r}_1\vec{r}_3'}-i\vec{s}^{\,q_1}_{\vec{r}_2\vec{r}_1'}\times\vec{s}^{\,q_1}_{\vec{r}_3\vec{r}_2'}\cdot\vec{s}^{\,q_1}_{\vec{r}_1\vec{r}_3'}\Big)\Bigg\}\ ,$$

whereas for the second term one has

$$E^{\rho\rho\rho}_{Sk}(u_1y_1)=\frac{1}{2}\int d(\vec{r})v^{3Sk}_{\overline{123}}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_1\,',\vec{r}_2\,',\vec{r}_3\,')\frac{u_1y_1}{2}\Bigg\{ \tag{A.67}$$

$$\sum_{q_1q_2q_3}\frac{1}{2}\Big(\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_2\vec{r}_2'}+\vec{s}^{\,q_1}_{\vec{r}_1\vec{r}_1'}\vec{s}^{\,q_2}_{\vec{r}_2\vec{r}_2'}\Big)\rho^{q_3}_{\vec{r}_3\vec{r}_3'}-\sum_{q_1q_3}\rho^{q_1}_{\vec{r}_2\vec{r}_1'}\rho^{q_1}_{\vec{r}_1\vec{r}_2'}\rho^{q_3}_{\vec{r}_3\vec{r}_3'}$$

$$-2\sum_{q_1q_2}\frac{1}{4}\Big(\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_3\vec{r}_2'}\rho^{q_2}_{\vec{r}_2\vec{r}_3'}+\vec{s}^{\,q_1}_{\vec{r}_1\vec{r}_1'}\vec{s}^{\,q_2}_{\vec{r}_3\vec{r}_2'}\rho^{q_2}_{\vec{r}_2\vec{r}_3'}+\vec{s}^{\,q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_3\vec{r}_2'}\vec{s}^{\,q_2}_{\vec{r}_2\vec{r}_3'}+\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\vec{s}^{\,q_2}_{\vec{r}_3\vec{r}_2'}\vec{s}^{\,q_2}_{\vec{r}_2\vec{r}_3'}-i\vec{s}^{\,q_1}_{\vec{r}_1\vec{r}_1'}\times\vec{s}^{\,q_2}_{\vec{r}_3\vec{r}_2'}\cdot\vec{s}^{\,q_2}_{\vec{r}_2\vec{r}_3'}\Big)$$

$$+ 2\sum_{q_1} \frac{1}{2}\rho^{q_1}_{\vec{r}_2\vec{r}_1'}\Big(\rho^{q_1}_{\vec{r}_3\vec{r}_2'}\rho^{q_1}_{\vec{r}_1\vec{r}_3'} + \vec{s}^{q_1}_{\vec{r}_3\vec{r}_2'}\vec{s}^{q_1}_{\vec{r}_1\vec{r}_3'}\Big)\Bigg\} \ .$$

Knowing that

$$\sum_{q_1q_2q_3} \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\mathcal{P}^{q_2}_{\vec{r}_2\vec{r}_2'}\mathcal{P}^{q_3}_{\vec{r}_3\vec{r}_3'} = \sum_{q_1\neq q_3} \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\mathcal{P}^{q_1}_{\vec{r}_2\vec{r}_2'}\mathcal{P}^{q_3}_{\vec{r}_3\vec{r}_3'} + \sum_{q_1\neq q_2} \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\mathcal{P}^{q_2}_{\vec{r}_2\vec{r}_2'}\mathcal{P}^{q_2}_{\vec{r}_3\vec{r}_3'}$$
$$+ \sum_{q_1\neq q_2} \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\mathcal{P}^{q_2}_{\vec{r}_2\vec{r}_2'}\mathcal{P}^{q_1}_{\vec{r}_3\vec{r}_3'} + \sum_{q_1} \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\mathcal{P}^{q_1}_{\vec{r}_2\vec{r}_2'}\mathcal{P}^{q_1}_{\vec{r}_3\vec{r}_3'} \tag{A.68a}$$

$$\sum_{q_1q_3} \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\mathcal{P}^{q_1}_{\vec{r}_2\vec{r}_2'}\mathcal{P}^{q_3}_{\vec{r}_3\vec{r}_3'} = \sum_{q_1\neq q_3} \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\mathcal{P}^{q_1}_{\vec{r}_2\vec{r}_2'}\mathcal{P}^{q_3}_{\vec{r}_3\vec{r}_3'} + \sum_{q_1} \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\mathcal{P}^{q_1}_{\vec{r}_2\vec{r}_2'}\mathcal{P}^{q_1}_{\vec{r}_3\vec{r}_3'} \tag{A.68b}$$

$$\sum_{q_1q_2} \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\mathcal{P}^{q_2}_{\vec{r}_2\vec{r}_2'}\mathcal{P}^{q_2}_{\vec{r}_3\vec{r}_3'} = \sum_{q_1\neq q_2} \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\mathcal{P}^{q_2}_{\vec{r}_2\vec{r}_2'}\mathcal{P}^{q_2}_{\vec{r}_3\vec{r}_3'} + \sum_{q_1} \mathcal{P}^{q_1}_{\vec{r}_1\vec{r}_1'}\mathcal{P}^{q_1}_{\vec{r}_2\vec{r}_2'}\mathcal{P}^{q_1}_{\vec{r}_3\vec{r}_3'} \ , \tag{A.68c}$$

one has for the contribution depending on parameter u_1

$$E^{\rho\rho\rho}_{Sk}(u_1) = \frac{u_1}{4}\int d(\vec{r})v^{3Sk}_{\overline{123}}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_1\,',\vec{r}_2\,',\vec{r}_3\,')$$
$$\Bigg\{ \sum_{q_1\neq q_3}\Big[\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_1}_{\vec{r}_2\vec{r}_2'}\rho^{q_3}_{\vec{r}_3\vec{r}_3'} - \frac{1}{2}\Big(\rho^{q_1}_{\vec{r}_2\vec{r}_1'}\rho^{q_1}_{\vec{r}_1\vec{r}_2'} + \vec{s}^{q_1}_{\vec{r}_2\vec{r}_1'}\vec{s}^{q_1}_{\vec{r}_1\vec{r}_2'}\Big)\rho^{q_3}_{\vec{r}_3\vec{r}_3'}\Big] \tag{A.69a}$$
$$+ \sum_{q_1\neq q_2}\Big[\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_2\vec{r}_2'}\rho^{q_2}_{\vec{r}_3\vec{r}_3'} - 2\frac{1}{2}\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\Big(\rho^{q_2}_{\vec{r}_3\vec{r}_2'}\rho^{q_2}_{\vec{r}_2\vec{r}_3'} + \vec{s}^{q_2}_{\vec{r}_3\vec{r}_2'}\vec{s}^{q_2}_{\vec{r}_2\vec{r}_3'}\Big)\Big] \tag{A.69b}$$
$$+ \sum_{q_1\neq q_2}\Big[\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_2\vec{r}_2'}\rho^{q_1}_{\vec{r}_3\vec{r}_3'}\Big] \tag{A.69c}$$
$$+ \sum_{q_1}\Big[\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_1}_{\vec{r}_2\vec{r}_2'}\rho^{q_1}_{\vec{r}_3\vec{r}_3'} - \frac{1}{2}\Big(\rho^{q_1}_{\vec{r}_2\vec{r}_1'}\rho^{q_1}_{\vec{r}_1\vec{r}_2'} + \vec{s}^{q_1}_{\vec{r}_2\vec{r}_1'}\vec{s}^{q_1}_{\vec{r}_1\vec{r}_2'}\Big)\rho^{q_1}_{\vec{r}_3\vec{r}_3'} - 2\frac{1}{2}\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\Big(\rho^{q_1}_{\vec{r}_3\vec{r}_2'}\rho^{q_1}_{\vec{r}_2\vec{r}_3'} + \vec{s}^{q_1}_{\vec{r}_3\vec{r}_2'}\vec{s}^{q_1}_{\vec{r}_2\vec{r}_3'}\Big)$$
$$+ 2\frac{1}{4}\Big(\rho^{q_1}_{\vec{r}_2\vec{r}_1'}\rho^{q_1}_{\vec{r}_3\vec{r}_2'}\rho^{q_1}_{\vec{r}_1\vec{r}_3'} + \vec{s}^{q_1}_{\vec{r}_2\vec{r}_1'}\vec{s}^{q_1}_{\vec{r}_3\vec{r}_2'}\rho^{q_1}_{\vec{r}_1\vec{r}_3'} + \vec{s}^{q_1}_{\vec{r}_2\vec{r}_1'}\rho^{q_1}_{\vec{r}_3\vec{r}_2'}\vec{s}^{q_1}_{\vec{r}_1\vec{r}_3'} + \rho^{q_1}_{\vec{r}_2\vec{r}_1'}\vec{s}^{q_1}_{\vec{r}_3\vec{r}_2'}\vec{s}^{q_1}_{\vec{r}_1\vec{r}_3'} - i\vec{s}^{q_1}_{\vec{r}_2\vec{r}_1'}\times\vec{s}^{q_1}_{\vec{r}_3\vec{r}_2'}\cdot\vec{s}^{q_1}_{\vec{r}_1\vec{r}_3'}\Big)\Big]\Bigg\} \ , \tag{A.69d}$$

and for the one depending on parameters u_1y_1

$$E^{\rho\rho\rho}_{Sk}(u_1y_1) = \frac{u_1y_1}{4}\int d(\vec{r})v^{3Sk}_{\overline{123}}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_1\,',\vec{r}_2\,',\vec{r}_3\,')$$
$$\Bigg\{ \sum_{q_1\neq q_3}\Big[\frac{1}{2}\Big(\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_1}_{\vec{r}_2\vec{r}_2'} + \vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'}\vec{s}^{q_1}_{\vec{r}_2\vec{r}_2'}\Big)\rho^{q_3}_{\vec{r}_3\vec{r}_3'} - \rho^{q_1}_{\vec{r}_2\vec{r}_1'}\rho^{q_1}_{\vec{r}_1\vec{r}_2'}\rho^{q_3}_{\vec{r}_3\vec{r}_3'}\Big] \tag{A.70a}$$
$$+ \sum_{q_1\neq q_2}\Big[\frac{1}{2}\Big(\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_2\vec{r}_2'} + \vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'}\vec{s}^{q_2}_{\vec{r}_2\vec{r}_2'}\Big)\rho^{q_1}_{\vec{r}_3\vec{r}_3'}\Big] \tag{A.70b}$$
$$+ \sum_{q_1\neq q_2}\Big[\frac{1}{2}\Big(\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_2\vec{r}_2'} + \vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'}\vec{s}^{q_2}_{\vec{r}_2\vec{r}_2'}\Big)\rho^{q_2}_{\vec{r}_3\vec{r}_3'} \tag{A.70c}$$
$$- 2\frac{1}{4}\Big(\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_3\vec{r}_2'}\rho^{q_2}_{\vec{r}_2\vec{r}_3'} + \vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'}\vec{s}^{q_2}_{\vec{r}_3\vec{r}_2'}\rho^{q_2}_{\vec{r}_2\vec{r}_3'} + \vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_2}_{\vec{r}_3\vec{r}_2'}\vec{s}^{q_2}_{\vec{r}_2\vec{r}_3'} + \rho^{q_1}_{\vec{r}_1\vec{r}_1'}\vec{s}^{q_2}_{\vec{r}_3\vec{r}_2'}\vec{s}^{q_2}_{\vec{r}_2\vec{r}_3'} - i\vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'}\times\vec{s}^{q_2}_{\vec{r}_3\vec{r}_2'}\cdot\vec{s}^{q_2}_{\vec{r}_2\vec{r}_3'}\Big)\Big]$$
$$+ \sum_{q_1}\Big[\frac{1}{2}\Big(\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_1}_{\vec{r}_2\vec{r}_2'} + \vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'}\vec{s}^{q_1}_{\vec{r}_2\vec{r}_2'}\Big)\rho^{q_1}_{\vec{r}_3\vec{r}_3'} - \rho^{q_1}_{\vec{r}_2\vec{r}_1'}\rho^{q_1}_{\vec{r}_1\vec{r}_2'}\rho^{q_1}_{\vec{r}_3\vec{r}_3'} \tag{A.70d}$$

$$- 2\frac{1}{4}\Big(\rho^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_1}_{\vec{r}_3\vec{r}_2'}\rho^{q_1}_{\vec{r}_2\vec{r}_3'} + \vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'}\vec{s}^{q_1}_{\vec{r}_3\vec{r}_2'}\rho^{q_1}_{\vec{r}_2\vec{r}_3'} + \vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'}\rho^{q_1}_{\vec{r}_3\vec{r}_2'}\vec{s}^{q_1}_{\vec{r}_2\vec{r}_3'} + \rho^{q_1}_{\vec{r}_1\vec{r}_1'}\vec{s}^{q_1}_{\vec{r}_3\vec{r}_2'}\vec{s}^{q_1}_{\vec{r}_2\vec{r}_3'} - i\vec{s}^{q_1}_{\vec{r}_1\vec{r}_1'} \times \vec{s}^{q_1}_{\vec{r}_3\vec{r}_2'} \cdot \vec{s}^{q_1}_{\vec{r}_2\vec{r}_3'}\Big)$$
$$+ 2\frac{1}{2}\rho^{q_1}_{\vec{r}_2\vec{r}_1'}\Big(\rho^{q_1}_{\vec{r}_3\vec{r}_2'}\rho^{q_1}_{\vec{r}_1\vec{r}_3'} + \vec{s}^{q_1}_{\vec{r}_3\vec{r}_2'}\vec{s}^{q_1}_{\vec{r}_1\vec{r}_3'}\Big)\Big]\Big\} \ .$$

As the expression of the functional of non-local densities is complicated, the application of gradient operators is fastidious. Consequently, the application of gradients is subdivided in several parts following conventions introduced in Sec. A.4.1.2. The interaction matrix element of the interaction term of interest is

$$v^{3Sk}_{\overline{123}}(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_1',\vec{r}_2',\vec{r}_3') = -\frac{1}{4}\Big(\vec{\nabla}^2_{\vec{r}_1'} + \vec{\nabla}^2_{\vec{r}_2'} + \vec{\nabla}^2_{\vec{r}_1} + \vec{\nabla}^2_{\vec{r}_2} - 2\vec{\nabla}_{\vec{r}_1'}\cdot\vec{\nabla}_{\vec{r}_2'} - 2\vec{\nabla}_{\vec{r}_1}\cdot\vec{\nabla}_{\vec{r}_2}\Big)\delta(\vec{r}) \ . \quad \text{(A.71)}$$

A.4.4.3 Application of gradients on Eq. A.69

Part Eq. A.69a

$$E^{\rho_{q_1}\rho_{q_1}\rho_{q_3}}_{Sk}(u_1) = -\frac{u_1}{16}\int d\vec{r}\sum_{q_1\neq q_3}\Bigg\{\Big[\ \triangle'\,\rho_{q_1}\rho_{q_1}\rho_{q_3} + \triangle\rho_{q_1}\rho_{q_1}\rho_{q_3} + \rho_{q_1}\,\triangle'\,\rho_{q_1}\rho_{q_3} + \rho_{q_1}\,\triangle\,\rho_{q_1}\rho_{q_3}$$
$$- 2\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_1}\rho_{q_3} - 2\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1}\rho_{q_3}\Big] - \frac{1}{2}\Big[\ \triangle'\,\rho_{q_1}\rho_{q_1}\rho_{q_3} + \rho_{q_1}\,\triangle\,\rho_{q_1}\rho_{q_3} + \rho_{q_1}\,\triangle'\,\rho_{q_1}\rho_{q_3}$$
$$+ \triangle\rho_{q_1}\rho_{q_1}\rho_{q_3} - 2\nabla'\rho_{q_1}\nabla'_\mu\rho_{q_1}\rho_{q_3} - 2\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1}\rho_{q_3}\Big] - \frac{1}{2}\Big[\ \triangle'\,s_{q_1,\nu}s_{q_1,\nu}\rho_{q_3} + s_{q_1,\nu}\,\triangle\,s_{q_1,\nu}\rho_{q_3}$$
$$+ s_{q_1,\nu}\,\triangle'\,s_{q_1,\nu}\rho_{q_3} + \triangle's_{q_1,\nu}s_{q_1,\nu}\rho_{q_3} - 2\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_1,\nu}\rho_{q_3} - 2\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_1,\nu}\rho_{q_3}\Big]\Bigg\}$$
$$= -\frac{u_1}{16}\int d\vec{r}\sum_{q_1\neq q_3}\Bigg\{+\frac{1}{2}\Big[2(\triangle'+\triangle)\rho_{q_1}\rho_{q_1}\rho_{q_3} - 2(\nabla'\rho_{q_1}\nabla'_\mu\rho_{q_1} + \nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1})\rho_{q_3}\Big]$$
$$- \frac{1}{2}\Big[2(\triangle'+\triangle)s_{q_1,\nu}s_{q_1,\nu}\rho_{q_3} - 2(\nabla's_{q_1,\nu}\nabla'_\mu s_{q_1,\nu} + \nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_1,\nu})\rho_{q_3}\Big]\Bigg\} \ . \quad \text{(A.72)}$$

Part Eq. A.69b

$$E^{\rho_{q_1}\rho_{q_2}\rho_{q_2}}_{Sk}(u_1) = -\frac{u_1}{16}\int d\vec{r}\sum_{q_1\neq q_2}\Bigg\{\Big[\ \triangle'\,\rho_{q_1}\rho_{q_2}\rho_{q_2} + \triangle\rho_{q_1}\rho_{q_2}\rho_{q_2} + \rho_{q_1}\,\triangle'\,\rho_{q_2}\rho_{q_2} + \rho_{q_1}\,\triangle\,\rho_{q_2}\rho_{q_2}$$
$$- 2\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_2}\rho_{q_2} - 2\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_2}\rho_{q_2}\Big] - \Big[\ \triangle'\,\rho_{q_1}\rho_{q_2}\rho_{q_2} + \triangle\rho_{q_1}\rho_{q_2}\rho_{q_2} + \rho_{q_1}\,\triangle'\,\rho_{q_2}\rho_{q_2}$$
$$+ \rho_{q_1}\rho_{q_2}\,\triangle\,\rho_{q_2} - 2\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_2}\rho_{q_2} - 2\nabla_\mu\rho_{q_1}\rho_{q_2}\nabla_\mu\rho_{q_2}\Big] - \Big[\ \triangle'\,\rho_{q_1}s_{q_2,\nu}s_{q_2,\nu} + \triangle\rho_{q_1}s_{q_2,\nu}s_{q_2,\nu}$$

$$+\rho_{q_1}\triangle' s_{q_2,\nu}s_{q_2,\nu}+\rho_{q_1}s_{q_2,\nu}\triangle s_{q_2,\nu}-2\nabla'_\mu\rho_{q_1}\nabla'_\mu s_{q_2,\nu}s_{q_2,\nu}-2\nabla_\mu\rho_{q_1}s_{q_2,\nu}\nabla_\mu s_{q_2,\nu}\Big]\Big\}$$
$$=-\frac{u_1}{16}\int d\vec{r}\sum_{q_1\neq q_2}\Big\{-\Big[(\triangle'+\triangle)\rho_{q_1}s_{q_2,\nu}s_{q_2,\nu}+\rho_{q_1}(\triangle'+\triangle)s_{q_2,\nu}s_{q_2,\nu}$$
$$-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu s_{q_2,\nu}+\nabla_\mu\rho_{q_1}\nabla_\mu s_{q_2,\nu})s_{q_2,\nu}\Big]\Big\}\ . \tag{A.73}$$

Part Eq. A.69c

$$E_{Sk}^{\rho_{q_1}\rho_{q_2}\rho_{q_1}}(u_1)=-\frac{u_1}{16}\int d\vec{r}\sum_{q_1\neq q_2}\Big\{\Big[(\triangle'+\triangle)\rho_{q_1}\rho_{q_2}\rho_{q_1}+\rho_{q_1}(\triangle'+\triangle)\rho_{q_2}\rho_{q_1}$$
$$-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_2}+\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_2})\rho_{q_1}\Big]\Big\}\ . \tag{A.74}$$

Part Eq. A.69d

$$E_{Sk}^{\rho_{q_1}\rho_{q_1}\rho_{q_1}}(u_1)=-\frac{u_1}{16}\int d\vec{r}\sum_{q_1}\Big\{-\frac{1}{2}\Big[2(\triangle'+\triangle)\rho_{q_1}\rho_{q_1}\rho_{q_1}-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_1}+\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1})\rho_{q_1}\Big]$$
$$-\Big[2(\triangle'+\triangle)s_{q_1,\nu}s_{q_1,\nu}\rho_{q_1}+(\triangle'+\triangle)\rho_{q_1}s_{q_1,\nu}s_{q_1,\nu}-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu s_{q_1,\nu}+\nabla_\mu\rho_{q_1}\nabla_\mu s_{q_1,\nu})s_{q_1,\nu}$$
$$-(\nabla' s_{q_1,\nu}\nabla'_\mu s_{q_1,\nu}+\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_1,\nu})\rho_{q_1}\Big]+\Big[(\triangle'+\triangle)\rho_{q_1}\rho_{q_1}\rho_{q_1}-(\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_1}+\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1})\rho_{q_1}\Big]$$
$$+\Big[2(\triangle'+\triangle)s_{q_1,\nu}s_{q_1,\nu}\rho_{q_1}+(\triangle'+\triangle)\rho_{q_1}s_{q_1,\nu}s_{q_1,\nu}-(\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_1,\nu}+\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_1,\nu})\rho_{q_1}$$
$$-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu s_{q_1,\nu}+\nabla_\mu\rho_{q_1}\nabla_\mu s_{q_1,\nu})s_{q_1,\nu}\Big]-\frac{i}{2}\epsilon_{\nu\lambda k}\Big[(\triangle'+\triangle)s_{q_1,\nu}s_{q_1,\lambda}s_{q_1,k}+(\triangle'-\triangle)s_{q_1,\nu}s_{q_1,\lambda}s_{q_1,k}$$
$$-2(\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_1,\lambda}-\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_1,\lambda})s_{q_1,k}\Big]\Big\}=0\ , \tag{A.75}$$

where we have used that

$$\epsilon_{\nu\lambda k}s_{q_1,\lambda}s_{q_1,k}=\epsilon_{\nu\lambda k}\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_1,\lambda}=\epsilon_{\nu\lambda k}\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_1,\lambda}=0\ . \tag{A.76}$$

Adding Eqs. (A.72,A.73,A.74,A.75)

$$
\begin{aligned}
E_{Sk}^{\rho\rho\rho}(u_1) = &-\frac{u_1}{16}\int d\vec{r}\sum_{q_1\neq q_2}\Bigg\{+\frac{1}{2}\Big[\Big(2\Delta\rho_{q_1}-4\tau_{q_1}\Big)\rho_{q_1}\rho_{q_2}-\Big(\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1}-4j_{q_1,\mu}j_{q_1,\mu}\Big)\rho_{q_2}\Big]\\
&-\frac{1}{2}\Big[\Big(2\Delta s_{q_1,\nu}-4T_{q_1,\nu}\Big)s_{q_1,\nu}\rho_{q_2}-\Big(\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_1,\nu}-4J_{q_1,\mu\nu}J_{q_1,\mu\nu}\Big)\rho_{q_2}\Big]\\
&-\Big[\Big(\Delta\rho_{q_2}-2\tau_{q_2}\Big)s_{q_1,\nu}s_{q_1,\nu}+\rho_{q_2}\Big(\Delta s_{q_1,\nu}-2T_{q_1,\nu}\Big)s_{q_1,\nu}-\Big(\nabla_\mu\rho_{q_2}\nabla_\mu s_{q_1,\nu}-4j_{q_2,\mu}J_{q_1,\mu\nu}\Big)s_{q_1,\nu}\Big]\\
&+\Big[\Big(\Delta\rho_{q_1}-2\tau_{q_1}\Big)\rho_{q_2}\rho_{q_1}+\rho_{q_1}\Big(\Delta\rho_{q_2}-2\tau_{q_2}\Big)\rho_{q_1}-\Big(\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_2}-4j_{q_1,\mu}j_{q_2,\mu}\Big)\rho_{q_1}\Big]\Bigg\}\\
= &-\frac{u_1}{16}\int d\vec{r}\sum_{q_1\neq q_2}\Bigg\{\Big[\Big(2\Delta\rho_{q_1}-4\tau_{q_1}\Big)\rho_{q_1}\rho_{q_2}+\Big(\Delta\rho_{q_2}-2\tau_{q_2}\Big)\rho_{q_1}\rho_{q_1}\\
&-\Big(\frac{1}{2}\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1}-2j_{q_1,\mu}j_{q_1,\mu}\Big)\rho_{q_2}-\Big(\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_2}-4j_{q_1,\mu}j_{q_2,\mu}\Big)\rho_{q_1}\Big]\\
&-\Big[\Big(2\Delta s_{q_1,\nu}-4T_{q_1,\nu}\Big)s_{q_1,\nu}\rho_{q_2}+\Big(\Delta\rho_{q_2}-2\tau_{q_2}\Big)s_{q_1,\nu}s_{q_1,\nu}-\Big(\frac{1}{2}\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_1,\nu}-2J_{q_1,\mu\nu}J_{q_1,\mu\nu}\Big)\rho_{q_2}\\
&-\Big(\nabla_\mu\rho_{q_2}\nabla_\mu s_{q_1,\nu}-4j_{q_2,\mu}J_{q_1,\mu\nu}\Big)s_{q_1,\nu}\Big]\Bigg\}\ . \qquad \text{(A.77)}
\end{aligned}
$$

A.4.4.4 Application of gradients on Eq. A.70

Part Eq. A.70a

$$
\begin{aligned}
E_{Sk}^{\rho_{q_1}\rho_{q_1}\rho_{q_3}}(u_1y_1) = &-\frac{u_1y_1}{16}\int d\vec{r}\sum_{q_1\neq q_3}\Bigg\{\frac{1}{2}\Big[2(\triangle'+\triangle)\rho_{q_1}\rho_{q_1}\rho_{q_3}-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_1}+\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1})\rho_{q_3}\\
&2(\triangle'+\triangle)s_{q_1,\nu}s_{q_1,\nu}\rho_{q_3}-2(\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_1,\nu}+\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_1,\nu})\rho_{q_3}\Big]\\
&-\Big[2(\triangle'+\triangle)\rho_{q_1}\rho_{q_1}\rho_{q_3}-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_1}+\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1})\rho_{q_3}\Big]\Bigg\}\ . \qquad \text{(A.78)}
\end{aligned}
$$

Part Eq. A.70b

$$
\begin{aligned}
E_{Sk}^{\rho_{q_1}\rho_{q_2}\rho_{q_1}}(u_1y_1) = &-\frac{u_1y_1}{16}\int d\vec{r}\sum_{q_1\neq q_2}\frac{1}{2}\Bigg\{(\triangle'+\triangle)\rho_{q_1}\rho_{q_2}\rho_{q_1}+(\triangle'+\triangle)\rho_{q_2}\rho_{q_1}\rho_{q_1}\\
&-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_2}+\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_2})\rho_{q_1}+(\triangle'+\triangle)s_{q_1,\nu}s_{q_2,\nu}\rho_{q_1}+(\triangle'+\triangle)s_{q_2,\nu}s_{q_1,\nu}\rho_{q_1}\\
&-2(\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_2,\nu}+\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_2,\nu})\rho_{q_1}\Bigg\}\ . \qquad \text{(A.79)}
\end{aligned}
$$

Part Eq. A.70c

$$
\begin{aligned}
E_{Sk}^{\rho_{q_1}\rho_{q_2}\rho_{q_2}}(u_1y_1) = &-\frac{u_1y_1}{16}\int d\vec{r}\sum_{q_1\neq q_2}\Bigg\{\frac{1}{2}\Big[(\triangle'+\triangle)\rho_{q_1}\rho_{q_2}\rho_{q_2}+(\triangle'+\triangle)\rho_{q_2}\rho_{q_1}\rho_{q_2}\\
&-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_2}+\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_2})\rho_{q_2}+(\triangle'+\triangle)s_{q_1,\nu}s_{q_2,\nu}\rho_{q_2}\\
&+(\triangle'+\triangle)s_{q_2,\nu}s_{q_1,\nu}\rho_{q_2}-2(\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_2,\nu}+\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_2,\nu})\rho_{q_2}\Big]\\
&-\frac{1}{2}\Big[(\triangle'+\triangle)\rho_{q_1}\rho_{q_2}\rho_{q_2}+(\triangle'+\triangle)\rho_{q_2}\rho_{q_1}\rho_{q_2}-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_2}+\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_2})\rho_{q_2}\Big]\\
&-\frac{1}{2}\Big[(\triangle'+\triangle)s_{q_1,\nu}s_{q_2,\nu}\rho_{q_2}+\triangle's_{q_2,\nu}s_{q_1,\nu}\rho_{q_2}+\triangle\rho_{q_2}s_{q_1,\nu}s_{q_2,\nu}-2\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_2,\nu}\rho_{q_2}\\
&-2\nabla_\mu s_{q_1,\nu}\nabla_\mu\rho_{q_2}s_{q_2,\nu}\Big]-\frac{1}{2}\Big[(\triangle'+\triangle)\rho_{q_1}s_{q_2,\nu}s_{q_2,\nu}+(\triangle'+\triangle)s_{q_2,\nu}\rho_{q_1}s_{q_2,\nu}\\
&-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu s_{q_2,\nu}+\nabla_\mu\rho_{q_1}\nabla_\mu s_{q_2,\nu})s_{q_2,\nu}\Big]-\frac{1}{2}\Big[(\triangle'+\triangle)s_{q_1,\nu}\rho_{q_2}s_{q_2,\nu}\\
&+\triangle'\rho_{q_2}s_{q_1,\nu}s_{q_2,\nu}+\triangle s_{q_2,\nu}s_{q_1,\nu}\rho_{q_2}-2\nabla'_\mu s_{q_1,\nu}\nabla'_\mu\rho_{q_2}s_{q_2,\nu}-2\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_2,\nu}\rho_{q_2}\Big]\\
&+\frac{i}{2}\epsilon_{\nu\lambda k}\Big[(\triangle'+\triangle)s_{q_1,\nu}s_{q_2,\lambda}s_{q_2,k}+(\triangle'-\triangle)s_{q_2,\lambda}s_{q_1,\nu}s_{q_2,k}\\
&-2(\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_2,\lambda}-\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_2,\lambda})s_{q_2,k}\Big]\Bigg\}\\
= &-\frac{u_1y_1}{16}\int d\vec{r}\sum_{q_1\neq q_2}\Bigg\{-\frac{1}{2}\Big[(\triangle'+\triangle)\rho_{q_1}s_{q_2,\nu}s_{q_2,\nu}+(\triangle'+\triangle)s_{q_2,\nu}\rho_{q_1}s_{q_2,\nu}\\
&-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu s_{q_2,\nu}+\nabla_\mu\rho_{q_1}\nabla_\mu s_{q_2,\nu})s_{q_2,\nu}\Big]-\frac{1}{2}\Big[(\triangle'+\triangle)s_{q_1,\nu}\rho_{q_2}s_{q_2,\nu}\\
&+(\triangle'+\triangle)\rho_{q_2}s_{q_1,\nu}s_{q_2,\nu}-2(\nabla'_\mu s_{q_1,\nu}\nabla'_\mu\rho_{q_2}+\nabla_\mu s_{q_1,\nu}\nabla_\mu\rho_{q_2})s_{q_2,\nu}\Big]\\
&+\frac{i}{2}\epsilon_{\nu\lambda k}\Big[(\triangle'-\triangle)s_{q_2,\lambda}s_{q_1,\nu}s_{q_2,k}-2(\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_2,\lambda}-\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_2,\lambda})s_{q_2,k}\Big]\Bigg\}\ . \qquad \text{(A.80)}
\end{aligned}
$$

Part Eq. A.70d

$$
\begin{aligned}
E_{Sk}^{\rho_{q_1}\rho_{q_1}\rho_{q_1}} = &-\frac{u_1y_1}{16}\int d\vec{r}\sum_{q_1}\Bigg\{-\Big[2(\triangle'+\triangle)\rho_{q_1}\rho_{q_1}\rho_{q_1}-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_1}+\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1})\rho_{q_1}\Big]\\
&-\Big[(\triangle'+\triangle)\rho_{q_1}s_{q_1,\nu}s_{q_1,\nu}+(\triangle'+\triangle)s_{q_1,\nu}\rho_{q_1}s_{q_1,\nu}-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu s_{q_1,\nu}+\nabla_\mu\rho_{q_1}\nabla_\mu s_{q_1,\nu})s_{q_1,\nu}\Big]
\end{aligned}
$$

$$
\begin{aligned}
&+\left[2(\triangle'+\triangle)\rho_{q_1}\rho_{q_1}\rho_{q_1}-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_1}+\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1})\rho_{q_1}\right]\\
&+\left[(\triangle'+\triangle)\rho_{q_1}s_{q_1,\nu}s_{q_1,\nu}+(\triangle'+\triangle)s_{q_1,\nu}\rho_{q_1}s_{q_1,\nu}-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu s_{q_1,\nu}+\nabla_\mu\rho_{q_1}\nabla_\mu s_{q_1,\nu})s_{q_1,\nu}\right]\\
&+\frac{i}{2}\epsilon_{\nu\lambda k}\left[(\triangle'-\triangle)s_{q_1,\lambda}s_{q_1,\nu}s_{q_1,k}-2(\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_1,\lambda}-\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_1,\lambda})s_{q_1,k}\right]\Bigg\}\\
&=0\ . \qquad \text{(A.81)}
\end{aligned}
$$

Adding Eqs. (A.78,A.80,A.79,A.81)

$$
\begin{aligned}
&E_{Sk}^{\rho\rho\rho}(u_1y_1)=-\frac{u_1y_1}{16}\int d\vec{r}\sum_{q_1\neq q_2}\Bigg\{\frac{1}{2}\Bigg[2(\triangle'+\triangle)\rho_{q_1}\rho_{q_1}\rho_{q_2}-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_1}+\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1})\rho_{q_2}\\
&+2(\triangle'+\triangle)s_{q_1,\nu}s_{q_1,\nu}\rho_{q_2}-2(\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_1,\nu}+\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_1,\nu})\rho_{q_2}\Bigg]\\
&-\left[2(\triangle'+\triangle)\rho_{q_1}\rho_{q_1}\rho_{q_2}-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_1}+\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1})\rho_{q_2}\right]\\
&+\frac{1}{2}\Bigg[(\triangle'+\triangle)\rho_{q_1}\rho_{q_2}\rho_{q_1}+(\triangle'+\triangle)\rho_{q_2}\rho_{q_1}\rho_{q_1}-2(\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_2}+\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_2})\rho_{q_1}\\
&+(\triangle'+\triangle)s_{q_1,\nu}s_{q_2,\nu}\rho_{q_1}+(\triangle'+\triangle)s_{q_2,\nu}s_{q_1,\nu}\rho_{q_1}-2(\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_2,\nu}+\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_2,\nu})\rho_{q_1}\Bigg]\\
&-\frac{1}{2}\Bigg[(\triangle'+\triangle)\rho_{q_2}s_{q_1,\nu}s_{q_1,\nu}+(\triangle'+\triangle)s_{q_1,\nu}\rho_{q_2}s_{q_1,\nu}-2(\nabla'_\mu\rho_{q_2}\nabla'_\mu s_{q_1,\nu}+\nabla_\mu\rho_{q_2}\nabla_\mu s_{q_1,\nu})s_{q_1,\nu}\Bigg]\\
&-\frac{1}{2}\Bigg[(\triangle'+\triangle)s_{q_2,\nu}\rho_{q_1}s_{q_1,\nu}+(\triangle'+\triangle)\rho_{q_1}s_{q_2,\nu}s_{q_1,\nu}-2(\nabla'_\mu s_{q_2,\nu}\nabla'_\mu\rho_{q_1}+\nabla_\mu s_{q_2,\nu}\nabla_\mu\rho_{q_1})s_{q_1,\nu}\Bigg]\\
&+\frac{i}{2}\epsilon_{\nu\lambda k}\left[(\triangle'-\triangle)s_{q_2,\lambda}s_{q_1,\nu}s_{q_2,k}-2(\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_2,\lambda}-\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_2,\lambda})s_{q_2,k}\right]\Bigg\}\\
&=-\frac{u_1y_1}{16}\int d\vec{r}\sum_{q_1\neq q_2}\Bigg\{\Bigg[-\frac{1}{2}(\triangle'+\triangle)\rho_{q_1}\rho_{q_1}\rho_{q_2}+\frac{1}{2}(\triangle'+\triangle)\rho_{q_2}\rho_{q_1}\rho_{q_1}\\
&+(\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_1}+\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1})\rho_{q_2}-(\nabla'_\mu\rho_{q_1}\nabla'_\mu\rho_{q_2}+\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_2})\rho_{q_1}\Bigg]\\
&+\Bigg[\frac{1}{2}(\triangle'+\triangle)s_{q_1,\nu}s_{q_1,\nu}\rho_{q_2}-\frac{1}{2}(\triangle'+\triangle)\rho_{q_2}s_{q_1,\nu}s_{q_1,\nu}\\
&-(\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_1,\nu}+\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_1,\nu})\rho_{q_2}+(\nabla'_\mu\rho_{q_2}\nabla'_\mu s_{q_1,\nu}+\nabla_\mu\rho_{q_2}\nabla_\mu s_{q_1,\nu})s_{q_1,\nu}\Bigg]\\
&+\Bigg[\frac{1}{2}(\triangle'+\triangle)s_{q_1,\nu}s_{q_2,\nu}\rho_{q_1}-\frac{1}{2}(\triangle'+\triangle)\rho_{q_1}s_{q_2,\nu}s_{q_1,\nu}\\
&-(\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_2,\nu}+\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_2,\nu})\rho_{q_1}+(\nabla'_\mu s_{q_2,\nu}\nabla'_\mu\rho_{q_1}+\nabla_\mu s_{q_2,\nu}\nabla_\mu\rho_{q_1})s_{q_1,\nu}\Bigg]\\
&+\frac{i}{2}\epsilon_{\nu\lambda k}\left[(\triangle'-\triangle)s_{q_2,\lambda}s_{q_1,\nu}s_{q_2,k}-2(\nabla'_\mu s_{q_1,\nu}\nabla'_\mu s_{q_2,\lambda}-\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_2,\lambda})s_{q_2,k}\right]\Bigg\}\\
&=-\frac{u_1y_1}{16}\int d\vec{r}\sum_{q_1\neq q_2}\Bigg\{\Bigg[-(\frac{1}{2}\Delta\rho_{q_1}-\tau_{q_1})\rho_{q_1}\rho_{q_2}+(\frac{1}{2}\Delta\rho_{q_2}-\tau_{q_2})\rho_{q_1}\rho_{q_1}\\
&+(\frac{1}{2}\vec{\nabla}\rho_{q_1}\vec{\nabla}\rho_{q_1}-2j_{q_1,\mu}j_{q_1,\mu})\rho_{q_2}-(\frac{1}{2}\vec{\nabla}\rho_{q_1}\vec{\nabla}\rho_{q_2}-2j_{q_1,\mu}j_{q_2,\mu})\rho_{q_1}\Bigg]
\end{aligned}
$$

$$
\begin{aligned}
&+\Big[(\frac{1}{2}\Delta s_{q_1,\nu}-T_{q_1,\nu})s_{q_1,\nu}\rho_{q_2}-(\frac{1}{2}\Delta\rho_{q_2}-\tau_{q_2})s_{q_1,\nu}s_{q_1,\nu}\\
&-(\frac{1}{2}\vec{\nabla}s_{q_1,\nu}\vec{\nabla}s_{q_1,\nu}-2J_{q_1,\mu\nu}J_{q_1,\mu\nu})\rho_{q_2}+(\frac{1}{2}\vec{\nabla}\rho_{q_2}\vec{\nabla}s_{q_1,\nu}-2j_{q_2,\mu}J_{q_1,\mu\nu})s_{q_1,\nu}\Big]\\
&+\Big[(\frac{1}{2}\Delta s_{q_1,\nu}-T_{q_1,\nu})s_{q_2,\nu}\rho_{q_1}-(\frac{1}{2}\Delta\rho_{q_1}-\tau_{q_1})s_{q_2,\nu}s_{q_1,\nu}\\
&-(\frac{1}{2}\vec{\nabla}s_{q_1,\nu}\vec{\nabla}s_{q_2,\nu}-2J_{q_1,\mu\nu}J_{q_2,\mu\nu})\rho_{q_1}+(\frac{1}{2}\vec{\nabla}s_{q_2,\nu}\vec{\nabla}\rho_{q_1}-2J_{q_2,\mu\nu}j_{q_1,\mu})s_{q_1,\nu}\Big]\\
&+\epsilon_{\nu\lambda k}\Big[-2\nabla_\mu s_{q_1,\nu}J_{q_2,\mu\lambda}s_{q_2,k}+\nabla_\mu s_{q_2,\nu}J_{q_2,\mu\lambda}s_{q_1,k}+\nabla_\mu s_{q_2,\nu}J_{q_1,\mu\lambda}s_{q_2,k}\Big]\Big\}\ .
\end{aligned}
\tag{A.82}
$$

A.4.4.5 Resulting trilinear EDF

The trilinear energy density functional originating from interaction term Eq. 3.87b is obtained adding Eqs. (A.77,A.82) and reads

$$
\begin{aligned}
\mathcal{E}^{\rho\rho\rho}_{Sk}=\sum_{q_1\neq q_2}\Big[\ & B^{\Delta\rho_1\rho_1\rho_2}\Delta\rho_{q_1}\rho_{q_1}\rho_{q_2}+B^{\Delta\rho_1\rho_2\rho_2}\Delta\rho_{q_1}\rho_{q_2}\rho_{q_2}+B^{\tau_1\rho_1\rho_2}\tau_{q_1}\rho_{q_1}\rho_{q_2}\\
&+B^{\tau_1\rho_2\rho_2}\tau_{q_1}\rho_{q_2}\rho_{q_2}+B^{\nabla\rho_1\nabla\rho_1\rho_2}\nabla_u\rho_{q_1}\nabla_u\rho_{q_1}\rho_{q_2}+B^{\nabla\rho_1\nabla\rho_2\rho_1}\nabla_u\rho_{q_1}\nabla_u\rho_{q_2}\rho_{q_1}\\
&+B^{j_1j_1\rho_2}j_{q_1,\mu}j_{q_1,\mu}\rho_{q_2}+B^{j_1j_2\rho_1}j_{q_1,\mu}j_{q_2,\mu}\rho_{q_1}+B^{\Delta s_1s_1\rho_2}\Delta s_{q_1,\nu}s_{q_1,\nu}\rho_{q_2}\\
&+B^{\Delta s_1s_2\rho_1}\Delta s_{q_1,\nu}s_{q_2,\nu}\rho_{q_1}+B^{T_1s_1\rho_2}T_{q_1,\nu}s_{q_1,\nu}\rho_{q_2}+B^{T_1s_2\rho_1}T_{q_1,\nu}s_{q_2,\nu}\rho_{q_1}\\
&+B^{\nabla s_1\nabla s_1\rho_2}\nabla_u s_{q_1,\nu}\nabla_u s_{q_1,\nu}\rho_{q_2}+B^{\nabla s_1\nabla s_2\rho_1}\nabla_u s_{q_1,\nu}\nabla_u s_{q_2,\nu}\rho_{q_1}\\
&+B^{J_1J_1\rho_2}J_{q_1,\mu\nu}J_{q_1,\mu\nu}\rho_{q_2}+B^{J_1J_2\rho_1}J_{q_1,\mu\nu}J_{q_2,\mu\nu}\rho_{q_1}\\
&+B^{\Delta\rho_1s_1s_2}\Delta\rho_{q_1}s_{q_1,\nu}s_{q_2,\nu}+B^{\Delta\rho_1s_2s_2}\Delta\rho_{q_1}s_{q_2,\nu}s_{q_2,\nu}\\
&+B^{\tau_1s_1s_2}\tau_{q_1}s_{q_1,\nu}s_{q_2,\nu}+B^{\tau_1s_2s_2}\tau_{q_1}s_{q_2,\nu}s_{q_2,\nu}+B^{\nabla\rho_1\nabla s_2s_1}\nabla_u\rho_{q_1}\nabla_u s_{q_2,\nu}s_{q_1,\nu}\\
&+B^{\nabla\rho_1\nabla s_2s_2}\nabla_u\rho_{q_1}\nabla_u s_{q_2,\nu}s_{q_2,\nu}+B^{j_1J_2s_1}j_{q_1,\mu}J_{q_2,\mu\nu}s_{q_1,\nu}+B^{j_1J_2s_2}j_{q_1,\mu}J_{q_2,\mu\nu}s_{q_2,\nu}\\
&+B^{J_1\nabla s_1s_2}\epsilon_{\nu\lambda k}\nabla_\mu s_{q_1,\nu}J_{q_1,\mu\lambda}s_{q_2,k}+B^{J_1\nabla s_2s_2}\epsilon_{\nu\lambda k}\nabla_\mu s_{q_2,\nu}J_{q_1,\mu\lambda}s_{q_2,k}\\
&+B^{J_1\nabla s_2s_1}\epsilon_{\nu\lambda k}\nabla_\mu s_{q_2,\nu}J_{q_1,\mu\lambda}s_{q_1,k}\Big]\ .
\end{aligned}
\tag{A.83}
$$

The functional parameters are related to those of the pseudo potential through

$$
\begin{aligned}
B^{\Delta\rho_1\rho_1\rho_2}&=-u_1/8+u_1y_1/32 &,\quad B^{\Delta\rho_1\rho_2\rho_2}&=-u_1/16-u_1y_1/32 &\text{(A.84a)}\\
B^{\Delta s_1s_1\rho_2}&=+u_1/8-u_1y_1/32 &,\quad B^{\Delta s_1s_2\rho_1}&=-u_1y_1/32 &\text{(A.84b)}\\
B^{\Delta\rho_1s_1s_2}&=+u_1y_1/32 &,\quad B^{\Delta\rho_1s_2s_2}&=+u_1/16+u_1y_1/32 &\text{(A.84c)}\\
B^{\tau_1\rho_1\rho_2}&=+u_1/4-u_1y_1/16 &,\quad B^{\tau_1\rho_2\rho_2}&=+u_1/8+u_1y_1/16 &\text{(A.84d)}\\
B^{T_1s_1\rho_2}&=-u_1/4+u_1y_1/16 &,\quad B^{T_1s_2\rho_1}&=+u_1y_1/16 &\text{(A.84e)}\\
B^{\tau_1s_1s_2}&=-u_1y_1/16 &,\quad B^{\tau_1s_2s_2}&=-u_1/8-u_1y_1/16 &\text{(A.84f)}\\
B^{\nabla\rho_1\nabla\rho_1\rho_2}&=+u_1/32-u_1y_1/32 &,\quad B^{\nabla\rho_1\nabla\rho_2\rho_1}&=+u_1/16+u_1y_1/32 &\text{(A.84g)}\\
B^{\nabla s_1\nabla s_1\rho_2}&=-u_1/32+u_1y_1/32 &,\quad B^{\nabla s_1\nabla s_2\rho_1}&=+u_1y_1/32 &\text{(A.84h)}\\
B^{\nabla\rho_1\nabla s_2s_1}&=-u_1y_1/32 &,\quad B^{\nabla\rho_1\nabla s_2s_2}&=-u_1/16-u_1y_1/32 &\text{(A.84i)}\\
B^{j_1j_1\rho_2}&=-u_1/8+u_1y_1/8 &,\quad B^{j_1j_2\rho_1}&=-u_1/4-u_1y_1/8 &\text{(A.84j)}\\
B^{J_1J_1\rho_2}&=+u_1/8-u_1y_1/8 &,\quad B^{J_1J_2\rho_1}&=-u_1y_1/8 &\text{(A.84k)}\\
B^{j_1J_2s_1}&=+u_1y_1/8 &,\quad B^{j_1J_2s_2}&=+u_1/4+u_1y_1/8 &\text{(A.84l)}
\end{aligned}
$$

$$B^{J_1\nabla s_1 s_2} = -u_1 y_1/16 \quad , \quad B^{J_1\nabla s_2 s_2} = -u_1 y_1/16 \tag{A.84m}$$
$$B^{J_1\nabla s_2 s_1} = +u_1 y_1/8 \quad . \tag{A.84n}$$

A.4.4.6 Complete trilinear EDF

The complete trilinear EDF derived from interaction Eqs. (3.87,3.88) is decomposed in its time-even part

$$\begin{aligned}\mathcal{E}^{\rho\rho\rho}_{Sk} = \sum_{q_1}\Big[& B^{\tau_1\rho_1\rho_1}\tau_{q_1}\rho_{q_1}\rho_{q_1} + B^{\nabla\rho_1\nabla\rho_1\rho_1}\nabla_u\rho_{q_1}\nabla_u\rho_{q_1}\rho_{q_1} + B^{J_1J_1\rho_1}J_{q_1,\mu\nu}J_{q_1,\mu\nu}\rho_{q_1}\Big] \\ + \sum_{q_1\neq q_2}\Big[& B^{\rho_1\rho_1\rho_2}\rho_{q_1}\rho_{q_1}\rho_{q_2} + B^{\tau_1\rho_1\rho_2}\tau_{q_1}\rho_{q_1}\rho_{q_2} + B^{\tau_1\rho_2\rho_2}\tau_{q_1}\rho_{q_2}\rho_{q_2} \\ & + B^{\nabla\rho_1\nabla\rho_1\rho_2}\nabla_u\rho_{q_1}\nabla_u\rho_{q_1}\rho_{q_2} + B^{\nabla\rho_1\nabla\rho_2\rho_1}\nabla_u\rho_{q_1}\nabla_u\rho_{q_2}\rho_{q_1} \\ & + B^{J_1J_1\rho_2}J_{q_1,\mu\nu}J_{q_1,\mu\nu}\rho_{q_2} + B^{J_1J_2\rho_1}J_{q_1,\mu\nu}J_{q_2,\mu\nu}\rho_{q_1}\Big] \ ,\end{aligned} \tag{A.85}$$

and its time-odd

$$\begin{aligned}\mathcal{E}^{\rho\rho\rho}_{Sk} = \sum_{q_1}\Big[& B^{\tau_1 s_1 s_1}\tau_{q_1}s_{q_1,\nu}s_{q_1,\nu} + B^{j_1j_1\rho_1}j_{q_1,\mu}j_{q_1,\mu}\rho_{q_1} + B^{j_1J_1s_1}j_{q_1,\mu}J_{q_1,\mu\nu}s_{q_1,\nu} \\ & + B^{\nabla s_1\nabla s_1\rho_1}\nabla_u s_{q_1,\nu}\nabla_u s_{q_1,\nu}\rho_{q_1} + B^{\nabla\rho_1\nabla s_1 s_1}\nabla_u\rho_{q_1}\nabla_u s_{q_1,\nu}s_{q_1,\nu} \\ & + B^{\nabla s_1 J_1 s_1}\epsilon_{abc}\nabla_u s_{q_1,a}J_{q_1,\mu b}s_{q_1,c}\Big] \\ + \sum_{q_1\neq q_2}\Big[& B^{j_1j_1\rho_2}j_{q_1,\mu}j_{q_1,\mu}\rho_{q_2} + B^{j_1j_2\rho_1}j_{q_1,\mu}j_{q_2,\mu}\rho_{q_1} + B^{s_1s_1\rho_2}s_{q_1,\nu}s_{q_1,\nu}\rho_{q_2} \\ & + B^{T_1s_1\rho_2}T_{q_1,\nu}s_{q_1,\nu}\rho_{q_2} + B^{T_1s_2\rho_1}T_{q_1,\nu}s_{q_2,\nu}\rho_{q_1} + B^{\tau_1s_1s_2}\tau_{q_1}s_{q_1,\nu}s_{q_2,\nu} \\ & + B^{\tau_1s_2s_2}\tau_{q_1}s_{q_2,\nu}s_{q_2,\nu} + B^{\nabla s_1\nabla s_1\rho_2}\nabla_u s_{q_1,\nu}\nabla_u s_{q_1,\nu}\rho_{q_2} \\ & + B^{\nabla s_1\nabla s_2\rho_1}\nabla_u s_{q_1,\nu}\nabla_u s_{q_2,\nu}\rho_{q_1} + B^{\nabla\rho_1\nabla s_1s_2}\nabla_u\rho_{q_1}\nabla_u s_{q_1,\nu}s_{q_2,\nu} \\ & + B^{\nabla\rho_1\nabla s_2s_1}\nabla_u\rho_{q_1}\nabla_u s_{q_2,\nu}s_{q_1,\nu} + B^{\nabla\rho_1\nabla s_2s_2}\nabla_u\rho_{q_1}\nabla_u s_{q_2,\nu}s_{q_2,\nu} \\ & + B^{j_1J_1s_2}j_{q_1,\mu}J_{q_1,\mu\nu}s_{q_2,\nu} + B^{j_1J_2s_1}j_{q_1,\mu}J_{q_2,\mu\nu}s_{q_1,\nu} + B^{j_1J_2s_2}j_{q_1,\mu}J_{q_2,\mu\nu}s_{q_2,\nu} \\ & + B^{\nabla s_1J_1s_2}\epsilon_{abc}\nabla_u s_{q_1,a}J_{q_1,\mu b}s_{q_2,c} + B^{\nabla s_1J_2s_1}\epsilon_{abc}\nabla_u s_{q_1,a}J_{q_2,\mu b}s_{q_1,c} \\ & + B^{\nabla s_1J_2s_2}\epsilon_{abc}\nabla_u s_{q_1,a}J_{q_2,\mu b}s_{q_2,c}\Big] \ .\end{aligned} \tag{A.86}$$

The relation between time-even and time-odd three-body functional coefficients and those of the three-body interaction are given in Tab. {A.3} and Tab. {A.4}. To obtain the functional in terms of isoscalar-isovector densities Eqs. (3.91,3.92), one uses Eq. 3.15, such that

$$\mathcal{P}^{q_1}\mathcal{P}^{q_1}\mathcal{P}^{q_1} = \frac{1}{4}\Big(\mathcal{P}^0\mathcal{P}^0\mathcal{P}^0 + \mathcal{P}^0\mathcal{P}^1\mathcal{P}^1 + \mathcal{P}^1\mathcal{P}^0\mathcal{P}^1 + \mathcal{P}^1\mathcal{P}^1\mathcal{P}^0\Big) \tag{A.87a}$$
$$\mathcal{P}^{q_1}\mathcal{P}^{q_1}\mathcal{P}^{q_2} = \frac{1}{4}\Big(\mathcal{P}^0\mathcal{P}^0\mathcal{P}^0 - \mathcal{P}^0\mathcal{P}^1\mathcal{P}^1 - \mathcal{P}^1\mathcal{P}^0\mathcal{P}^1 + \mathcal{P}^1\mathcal{P}^1\mathcal{P}^0\Big) \tag{A.87b}$$
$$\mathcal{P}^{q_1}\mathcal{P}^{q_2}\mathcal{P}^{q_2} = \frac{1}{4}\Big(\mathcal{P}^0\mathcal{P}^0\mathcal{P}^0 + \mathcal{P}^0\mathcal{P}^1\mathcal{P}^1 - \mathcal{P}^1\mathcal{P}^0\mathcal{P}^1 - \mathcal{P}^1\mathcal{P}^1\mathcal{P}^0\Big) \tag{A.87c}$$
$$\mathcal{P}^{q_1}\mathcal{P}^{q_2}\mathcal{P}^{q_1} = \frac{1}{4}\Big(\mathcal{P}^0\mathcal{P}^0\mathcal{P}^0 - \mathcal{P}^0\mathcal{P}^1\mathcal{P}^1 + \mathcal{P}^1\mathcal{P}^0\mathcal{P}^1 - \mathcal{P}^1\mathcal{P}^1\mathcal{P}^0\Big) \ , \tag{A.87d}$$

$Func\backslash Int$	u_0	u_1	u_1y_1	u_2	u_2y_{21}	u_2y_{22}
$B^{\rho_1\rho_1\rho_2} =$	$+\frac{3}{4}$	$+0$	$+0$	$+0$	$+0$	$+0$
$B^{\tau_1\rho_1\rho_1} =$	$+0$	$+0$	$+0$	$+\frac{3}{16}$	$+\frac{3}{16}$	$-\frac{3}{16}$
$B^{\tau_1\rho_1\rho_2} =$	$+0$	$+\frac{1}{4}$	$-\frac{1}{16}$	$+\frac{5}{8}$	$+\frac{1}{2}$	$+\frac{5}{8}$
$B^{\tau_1\rho_2\rho_2} =$	$+0$	$+\frac{1}{8}$	$+\frac{1}{16}$	$+\frac{1}{8}$	$+\frac{1}{16}$	$-\frac{1}{16}$
$B^{\nabla\rho_1\nabla\rho_1\rho_1} =$	$+0$	$+0$	$+0$	$-\frac{3}{64}$	$-\frac{3}{64}$	$+\frac{3}{64}$
$B^{\nabla\rho_1\nabla\rho_1\rho_2} =$	$+0$	$+\frac{5}{32}$	$-\frac{1}{16}$	$-\frac{1}{8}$	$-\frac{7}{64}$	$-\frac{11}{64}$
$B^{\nabla\rho_1\nabla\rho_2\rho_1} =$	$+0$	$+\frac{5}{16}$	$+\frac{1}{16}$	$-\frac{1}{16}$	$-\frac{1}{32}$	$+\frac{1}{32}$
$B^{J_1J_1\rho_1} =$	$+0$	$+0$	$+0$	$-\frac{3}{16}$	$-\frac{3}{16}$	$+\frac{3}{16}$
$B^{J_1J_1\rho_2} =$	$+0$	$+\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{1}{4}$	$-\frac{3}{16}$	$-\frac{3}{16}$
$B^{J_1J_2\rho_1} =$	$+0$	$+0$	$-\frac{1}{8}$	$+0$	$-\frac{1}{8}$	$+\frac{1}{8}$

Table A.3: Time-even functional A.85 coefficients are expressed in terms of pseudo potential parameters.

where $\mathcal{P} \in \{\rho, \Delta\rho, \vec{\nabla}\rho, \tau, \vec{j}, \vec{s}, \Delta\vec{s}, \nabla_\mu s_\nu, \vec{T}, J_{\mu\nu}\}$. Thus

$$B^{\mathcal{P}^0\mathcal{P}^0\mathcal{P}^0} = \frac{1}{4}\Big(B^{\mathcal{P}^{q_1}\mathcal{P}^{q_1}\mathcal{P}^{q_1}} + B^{\mathcal{P}^{q_1}\mathcal{P}^{q_1}\mathcal{P}^{q_2}} + B^{\mathcal{P}^{q_1}\mathcal{P}^{q_2}\mathcal{P}^{q_2}} + B^{\mathcal{P}^{q_1}\mathcal{P}^{q_2}\mathcal{P}^{q_1}}\Big) \tag{A.88a}$$

$$B^{\mathcal{P}^0\mathcal{P}^1\mathcal{P}^1} = \frac{1}{4}\Big(B^{\mathcal{P}^{q_1}\mathcal{P}^{q_1}\mathcal{P}^{q_1}} - B^{\mathcal{P}^{q_1}\mathcal{P}^{q_1}\mathcal{P}^{q_2}} + B^{\mathcal{P}^{q_1}\mathcal{P}^{q_2}\mathcal{P}^{q_2}} - B^{\mathcal{P}^{q_1}\mathcal{P}^{q_2}\mathcal{P}^{q_1}}\Big) \tag{A.88b}$$

$$B^{\mathcal{P}^1\mathcal{P}^0\mathcal{P}^1} = \frac{1}{4}\Big(B^{\mathcal{P}^{q_1}\mathcal{P}^{q_1}\mathcal{P}^{q_1}} - B^{\mathcal{P}^{q_1}\mathcal{P}^{q_1}\mathcal{P}^{q_2}} - B^{\mathcal{P}^{q_1}\mathcal{P}^{q_2}\mathcal{P}^{q_2}} + B^{\mathcal{P}^{q_1}\mathcal{P}^{q_2}\mathcal{P}^{q_1}}\Big) \tag{A.88c}$$

$$B^{\mathcal{P}^1\mathcal{P}^1\mathcal{P}^0} = \frac{1}{4}\Big(B^{\mathcal{P}^{q_1}\mathcal{P}^{q_1}\mathcal{P}^{q_1}} + B^{\mathcal{P}^{q_1}\mathcal{P}^{q_1}\mathcal{P}^{q_2}} - B^{\mathcal{P}^{q_1}\mathcal{P}^{q_2}\mathcal{P}^{q_2}} - B^{\mathcal{P}^{q_1}\mathcal{P}^{q_2}\mathcal{P}^{q_1}}\Big)\ , \tag{A.88d}$$

where $B^{\mathcal{P}^{0/1}\mathcal{P}^{0/1}\mathcal{P}^{0/1}}$ represents the coefficient in front of the functional term of the form $\mathcal{P}^{0/1}\mathcal{P}^{0/1}\mathcal{P}^{0/1}$. Last but not least the functional term $\Delta\rho\rho\rho$ and $\Delta ss\rho$ are changed into $\vec{\nabla}\rho\vec{\nabla}\rho\rho$ and $\vec{\nabla}s\vec{\nabla}s\rho$ through an integration by part. Moreover, we define couplings that reabsorb one power of a density in order to recover Tabs. {3.2-3.3}.

A.5 Gauge invariant correlations

Correlation between couplings of the trilinear EDF (Eq. 3.97), due to gauge invariant conditions (Eq. 3.96) is expanded in the present section.
Using Eq. 3.20, condition Eq. 3.96a is equivalent to

$$2\Big(B_0^\tau + B_0^j\Big)\,\nabla_\mu\phi(\vec{r})\,j_{0,\mu}\rho_0\rho_0 + \Big(B_0^\tau + B_0^j\Big)\,\nabla_\mu\phi(\vec{r})\nabla_\mu\phi(\vec{r})\,\rho_0\rho_0\rho_0 = 0\ , \tag{A.89}$$

where repeated indices are summed and where B_0^τ and B_0^j refer to EDF couplings Tabs. {3.2-3.3} without the density dependence. Condition Eq. A.89 leads to Eq. 3.97a.
Condition Eq. 3.96b is equivalent to

$$\begin{aligned}&\Big(2B_0^{\tau s} + B_0^{Js}\Big)\,\nabla_\mu\phi(\vec{r})\,j_{0,\mu}s_{0,\nu}s_{0,\nu} + \Big(2B_0^T + 2B_0^J + B_0^{Js}\Big)\,\nabla_\mu\phi(\vec{r})\,J_{0,\mu\nu}s_{0,\nu}\rho_0\\ &+ \Big(B_0^T + B_0^{\tau s} + B_0^J + B_0^{Js}\Big)\,\nabla_\mu\phi(\vec{r})\nabla_\mu\phi(\vec{r})\,\rho_0 s_{0,\nu}s_{0,\nu} = 0\ ,\end{aligned} \tag{A.90}$$

$Func\backslash Int$	u_0	u_1	u_1y_1	u_2	u_2y_{21}	u_2y_{22}
$B^{s_1s_1\rho_2} =$	$-\frac{3}{4}$	$+0$	$+0$	$+0$	$+0$	$+0$
$B^{T_1s_1\rho_2} =$	$+0$	$-\frac{1}{4}$	$+\frac{1}{16}$	$+\frac{1}{8}$	$+\frac{1}{8}$	$+\frac{1}{4}$
$B^{T_1s_2\rho_1} =$	$+0$	$+0$	$+\frac{1}{16}$	$+0$	$+\frac{1}{8}$	$+\frac{1}{4}$
$B^{\tau_1s_1s_1} =$	$+0$	$+0$	$+0$	$-\frac{3}{16}$	$-\frac{3}{16}$	$+\frac{3}{16}$
$B^{\tau_1s_1s_2} =$	$+0$	$+0$	$-\frac{1}{16}$	$+0$	$+0$	$+\frac{3}{8}$
$B^{\tau_1s_2s_2} =$	$+0$	$-\frac{1}{8}$	$-\frac{1}{16}$	$-\frac{1}{8}$	$-\frac{1}{16}$	$+\frac{1}{16}$
$B^{\nabla s_1\nabla s_1\rho_1} =$	$+0$	$+0$	$+0$	$-\frac{3}{64}$	$-\frac{3}{64}$	$+\frac{3}{64}$
$B^{\nabla s_1\nabla s_1\rho_2} =$	$+0$	$-\frac{5}{32}$	$+\frac{1}{16}$	$-\frac{1}{16}$	$-\frac{3}{64}$	$-\frac{3}{64}$
$B^{\nabla s_1\nabla s_2\rho_1} =$	$+0$	$+0$	$+\frac{1}{16}$	$+0$	$-\frac{1}{32}$	$+\frac{1}{32}$
$B^{\nabla\rho_1\nabla s_1s_1} =$	$+0$	$+0$	$+0$	$+\frac{3}{32}$	$+\frac{3}{32}$	$-\frac{3}{32}$
$B^{\nabla\rho_1\nabla s_1s_2} =$	$+0$	$+0$	$+0$	$+0$	$-\frac{1}{32}$	$-\frac{5}{32}$
$B^{\nabla\rho_1\nabla s_2s_1} =$	$+0$	$+0$	$-\frac{1}{16}$	$+0$	$+\frac{1}{32}$	$-\frac{1}{32}$
$B^{\nabla\rho_1\nabla s_2s_2} =$	$+0$	$-\frac{5}{16}$	$-\frac{1}{16}$	$+\frac{1}{16}$	$+\frac{1}{32}$	$-\frac{1}{32}$
$B^{j_1J_1s_1} =$	$+0$	$+0$	$+0$	$+\frac{3}{8}$	$+\frac{3}{8}$	$-\frac{3}{8}$
$B^{j_1J_1s_2} =$	$+0$	$+0$	$+0$	$+0$	$-\frac{1}{8}$	$-\frac{5}{8}$
$B^{j_1J_2s_1} =$	$+0$	$+0$	$+\frac{1}{8}$	$+0$	$+\frac{1}{8}$	$-\frac{1}{8}$
$B^{j_1J_2s_2} =$	$+0$	$+\frac{1}{4}$	$+\frac{1}{8}$	$+\frac{1}{4}$	$+\frac{1}{8}$	$-\frac{1}{8}$
$B^{\nabla s_1J_1s_1} =$	$+0$	$+0$	$+0$	$-\frac{3}{16}$	$-\frac{3}{16}$	$+\frac{3}{16}$
$B^{\nabla s_1J_1s_2} =$	$+0$	$+0$	$-\frac{1}{16}$	$+0$	$-\frac{1}{16}$	$+\frac{1}{16}$
$B^{\nabla s_1J_2s_1} =$	$+0$	$+0$	$-\frac{1}{16}$	$+0$	$-\frac{1}{16}$	$+\frac{1}{16}$
$B^{\nabla s_1J_2s_2} =$	$+0$	$+0$	$+\frac{1}{8}$	$+0$	$-\frac{1}{16}$	$+\frac{1}{16}$
$B^{j_1j_1\rho_1} =$	$+0$	$+0$	$+0$	$-\frac{3}{16}$	$-\frac{3}{16}$	$+\frac{3}{16}$
$B^{j_1j_1\rho_2} =$	$+0$	$-\frac{1}{8}$	$+\frac{1}{8}$	$-\frac{1}{2}$	$-\frac{7}{16}$	$-\frac{11}{16}$
$B^{j_1j_2\rho_1} =$	$+0$	$-\frac{1}{4}$	$-\frac{1}{8}$	$-\frac{1}{4}$	$-\frac{1}{8}$	$+\frac{1}{8}$

Table A.4: Time-odd functional A.86 coefficients are expressed in terms of pseudo potential parameters.

leading to condition Eq. 3.97b.
Condition Eq. 3.96c is equivalent to

$$\left(2B_{10}^{\tau}+B_{10}^{j}\right)\nabla_{\mu}\phi(\vec{r})\,j_{0,\mu}\rho_1\rho_1+\left(2B_{1}^{\tau}+2B_{1}^{j}+B_{10}^{j}\right)\nabla_{\mu}\phi(\vec{r})\,j_{1,\mu}\rho_1\rho_0$$
$$+\left(B_{1}^{\tau}+B_{10}^{\tau}+B_{1}^{j}+B_{10}^{j}\right)\nabla_{\mu}\phi(\vec{r})\nabla_{\mu}\phi(\vec{r})\,\rho_1\rho_1\rho_0=0\ , \tag{A.91}$$

leading to condition Eq. 3.97c.
Condition Eq. 3.96d is equivalent to

$$\left(2B_{10}^{\tau}+B_{10}^{j}\right)\nabla_{\mu}\phi(\vec{r})\,j_{0,\mu}s_{1,\nu}s_{1,\nu}+\left(2B_{1}^{\tau}+2B_{1}^{j}+B_{10}^{j}\right)\nabla_{\mu}\phi(\vec{r})\,J_{1,\mu\nu}s_{1,\nu}\rho_0$$
$$+\left(B_{1}^{\tau}+B_{10}^{\tau}+B_{1}^{j}+B_{10}^{j}\right)\nabla_{\mu}\phi(\vec{r})\nabla_{\mu}\phi(\vec{r})\,s_{1,\nu}s_{1,\nu}\rho_0=0\ , \tag{A.92}$$

leading to condition Eq. 3.97d.
Condition Eq. 3.96e is equivalent to

$$\begin{aligned}&\left(2B_1^{\tau s}+B_1^{Js}+B_{10}^{Js}\right)\nabla_\mu\phi(\vec{r})\,j_{1,\mu}s_{1,\nu}s_{0,\nu}+\left(2B_{10}^{T}+B_{10}^{J}+B_{10}^{Js}\right)\nabla_\mu\phi(\vec{r})\,J_{0,\mu\nu}s_{1,\nu}\rho_1\\&+\left(2B_{01}^{T}+B_{10}^{J}+B_{1}^{Js}\right)\nabla_\mu\phi(\vec{r})\,J_{1,\mu\nu}s_{0,\nu}\rho_1\\&+\left(B_{10}^{T}+B_{01}^{T}+B_1^{\tau s}+B_{10}^{J}+B_1^{Js}+B_{10}^{Js}\right)\nabla_\mu\phi(\vec{r})\nabla_\mu\phi(\vec{r})\,s_{0,\nu}s_{1,\nu}\rho_1=0\ ,\end{aligned}\tag{A.93}$$

leading to condition Eq. 3.97e.
Condition Eq. 3.96f is equivalent to

$$B_0^{\nabla sJ}\,\epsilon_{\nu\lambda k}\,\nabla_\mu\phi(\vec{r})\,s_{0,k}\nabla_\mu s_{0,\nu}s_{0,\lambda}=0\ ,\tag{A.94}$$

which is true for any $B_0^{\nabla sJ}$. Condition Eq. 3.96g is equivalent to

$$\begin{aligned}&B_1^{\nabla sJ}\,\epsilon_{\nu\lambda k}\,\nabla_\mu\phi(\vec{r})\,s_{0,k}\nabla_\mu s_{1,\nu}s_{1,\lambda}+B_{10}^{\nabla sJ}\,\epsilon_{\nu\lambda k}\,\nabla_\mu\phi(\vec{r})\,s_{1,k}\nabla_\mu s_{1,\nu}s_{0,\lambda}\\&+B_{01}^{\nabla sJ}\,\epsilon_{\nu\lambda k}\,\nabla_\mu\phi(\vec{r})\,s_{1,k}\nabla_\mu s_{0,\nu}s_{1,\lambda}=0\ ,\end{aligned}\tag{A.95}$$

which can be rewritten using the Levi-Civita operator properties

$$(B_1^{\nabla sJ}-B_{10}^{\nabla sJ})\,\epsilon_{\nu\lambda k}\,\nabla_\mu\phi(\vec{r})\,s_{0,k}\nabla_\mu s_{1,\nu}s_{1,\lambda}=0\ ,\tag{A.96}$$

leading to condition Eq. 3.97f.

Appendix B

Formal computation code output for the two-body pseudo potential

Abstract: In this section the Latex output file of the formal computation code treating the derivation of the bilinear functional is reported. The code has been used with two-body pseudo-potential Eq. 3.52. Functional derivatives and infinite nuclear matter properties that have not been given explicitly in the chapters devoted to the two-body Skyrme pseudo-potential, are reproduced here.

Contents

The present document is the formal computation code output in which the calculated quantities are reported. The .tex and .pdf files are copied in the output directory chosen at the execution, where one also finds all results in separated output files and in a non-LaTeX version. First, let us remark that as the LaTeX file is generated by the code, equations might appear misshapen in certain cases, e.g. too long lines or equations alignement problems may appear. However, the .tex file can be changed manually to reshape equations. For complementary explanations on derived properties and the method used to derive them one should refer to Chap. 3 and Chap. 4.

B.1 Formal code input : two-body Skyrme pseudo potential

This section deals with the inputs used by the code. In case it does not correspond to what one had expected, one should run the code again with appropriate inputs.

B.1.1 Gradient structure

The inputs file asks for specific gradient and exchange operator structures, the latter being named $P^{\{x\}}$. The code multiplies each bilinear gradient operator structure entered by $P^{\{x\}}$ and calculates the hermitian counterpart so that the resulting EDF must be real by construction. In the present case, the code uses The pseudo potential the code just has used is

$$\begin{aligned} V^{Sk} = &+ P^{\{x^0\}}\delta(\vec{r}_1-\vec{r}_2) \\ &+ \frac{1}{2}\left[P^{\{x^1\}}\left(k'_{12,u}k'_{12,u}\right) + \left(k_{12,u}k_{12,u}\right)P^{\{x^1\}}\right]\delta(\vec{r}_1-\vec{r}_2) \\ &+ \frac{1}{2}\left[P^{\{x^2\}}\left(k_{12,u}k'_{12,u}\right) + \left(k'_{12,u}k_{12,u}\right)P^{\{x^2\}}\right]\delta(\vec{r}_1-\vec{r}_2) \ . \end{aligned}$$

B.1.2 Exchange operators $P^{\{x\}}$

The corresponding exchange operators are

$$\begin{aligned} P^{\{x^0\}} &= + t_0 + t_0x_0P^{\sigma}_{12} \ , \\ P^{\{x^1\}} &= + t_1 + t_1x_1P^{\sigma}_{12} \ , \\ P^{\{x^2\}} &= + t_2 + t_2x_2P^{\sigma}_{12} \ . \end{aligned}$$

B.1.3 Parameters correlations

The pseudo potential used might have correlated parameters. This would appear after the functional has been calculated. In order to save space, only the functional from which correlated parameters have been suppressed is presented. Unfortunately, all correlations cannot be found using this particular code that can only identify parameters that are correlated in pairs. Parameters located on the right-hand side of the following equations are correlated to those located on the left hand side.

$$\begin{aligned} t_0 &\Leftarrow \\ t_0x_0 &\Leftarrow \\ t_1 &\Leftarrow \\ t_1x_1 &\Leftarrow \\ t_2 &\Leftarrow \\ t_2x_2 &\Leftarrow \end{aligned}$$

To find linear combinations of more than two parameters one needs to construct the matrix of coefficients Tab. {B.2} and use the singular value decomposition , see Sec. 3.4.3. One computes the square matrix X by multiplying the matrix of coefficients M with its transpose

$$X = M^T M \ .$$

Diagonalizing X, one accesses linear combinations of correlated parameters, i.e. they are given by the eigenvectors with null eigenvalues. To do so one can use either the matrix of coefficients given in the output directories with any given routine or use the script in the Others/ directory to get the devoted mathematica commands.

B.1.4 Less-correlated exchange operators $P^{\{x\}}$

The pseudo potential from which detected correlations have been suppressed corresponds to the following reduced exchange operators

$$\begin{aligned} P^{\{x^0\}} &= +\,t_0 + t_0 x_0 P^\sigma_{12} \ , \\ P^{\{x^1\}} &= +\,t_1 + t_1 x_1 P^\sigma_{12} \ , \\ P^{\{x^2\}} &= +\,t_2 + t_2 x_2 P^\sigma_{12} \ . \end{aligned}$$

B.2 Energy Density Functional

B.2.1 Skyrme bilinear functional in neutron-proton representation

The bilinear Skyrme functional computed in neutron-proton representation reads

$$\begin{aligned} E^{\rho\rho} = \int d\vec{r} \Bigg\{ & \sum_{q_1} \Big[+ A^\rho_1 \, \rho_{q_1}\rho_{q_1} + A^s_1 \, s_{q_1,\nu}s_{q_1,\nu} + A^\tau_1 \, \tau_{q_1}\rho_{q_1} + A^T_1 \, T_{q_1,\nu}s_{q_1,\nu} \\ & + A^{\nabla\rho}_1 \, \nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1} + A^{\nabla s}_1 \, \nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_1,\nu} + A^j_1 \, j_{q_1,\mu}j_{q_1,\mu} + A^J_1 \, J_{q_1,\mu\nu}J_{q_1,\mu\nu} \Big] \\ & + \sum_{q_1\neq q_2} \Big[+ A^{\rho_1\rho_2}\rho_{q_1}\rho_{q_2} + A^{s_1s_2}s_{q_1,\nu}s_{q_2,\nu} + A^{\tau_1\rho_2}\tau_{q_1}\rho_{q_2} + A^{T_1s_2}T_{q_1,\nu}s_{q_2,\nu} \\ & + A^{\nabla\rho_1\nabla\rho_2}\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_2} + A^{\nabla s_1\nabla s_2}\nabla_\mu s_{q_1,\nu}\nabla_\mu s_{q_2,\nu} + A^{j_1j_2}j_{q_1,\mu}j_{q_2,\mu} + A^{J_1J_2}J_{q_1,\mu\nu}J_{q_2,\mu\nu} \Big] \Bigg\} \ . \end{aligned}$$

where the functional coefficients are related to those of the pseudo-potential given in input according to TAB. {B.1}. The expression of those coefficients can be found in a different format in the output directory or commented in the .tex file. For practical reason one might want to use the time-even part of the functional only, given by

$$\begin{aligned} E^{\rho\rho} = \int d\vec{r} \Bigg\{ & \sum_{q_1} \Big[+ A^\rho_1 \, \rho_{q_1}\rho_{q_1} + A^\tau_1 \, \tau_{q_1}\rho_{q_1} + A^{\nabla\rho}_1 \, \nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_1} + A^J_1 \, J_{q_1,\mu\nu}J_{q_1,\mu\nu} \Big] \\ & + \sum_{q_1\neq q_2} \Big[+ A^{\rho_1\rho_2}\rho_{q_1}\rho_{q_2} + A^{\tau_1\rho_2}\tau_{q_1}\rho_{q_2} + A^{\nabla\rho_1\nabla\rho_2}\nabla_\mu\rho_{q_1}\nabla_\mu\rho_{q_2} + A^{J_1J_2}J_{q_1,\mu\nu}J_{q_2,\mu\nu} \Big] \Bigg\} \ . \end{aligned}$$

B.2.2 Skyrme bilinear functional in isoscalar-isovector representation

The Skyrme functional is then calculated in isoscalar-isovector representation and reads

$$\begin{aligned} E^{\rho\rho} = \int d\vec{r} \Bigg\{ & + A^\rho_0 \, \rho_0\rho_0 + A^\rho_1 \, \rho_1\rho_1 + A^s_0 \, s_{0,\nu}s_{0,\nu} + A^s_1 \, s_{1,\nu}s_{1,\nu} \\ & + A^\tau_0 \, \tau_0\rho_0 + A^\tau_1 \, \tau_1\rho_1 + A^T_0 \, T_{0,\nu}s_{0,\nu} + A^T_1 \, T_{1,\nu}s_{1,\nu} \\ & + A^{\nabla\rho}_0 \, \nabla_\mu\rho_0\nabla_\mu\rho_0 + A^{\nabla\rho}_1 \, \nabla_\mu\rho_1\nabla_\mu\rho_1 + A^{\nabla s}_0 \, \nabla_\mu s_{0,\nu}\nabla_\mu s_{0,\nu} + A^{\nabla s}_1 \, \nabla_\mu s_{1,\nu}\nabla_\mu s_{1,\nu} \\ & + A^j_0 \, j_{0,\mu}j_{0,\mu} + A^j_1 \, j_{1,\mu}j_{1,\mu} + A^J_0 \, J_{0,\mu\nu}J_{0,\mu\nu} + A^J_1 \, J_{1,\mu\nu}J_{1,\mu\nu} \Bigg\} \ . \end{aligned}$$

$Func\backslash Int$	t_0	t_0x_0	t_1	t_1x_1	t_2	t_2x_2
$A_1^{\rho} =$	$+\frac{1}{4}$	$-\frac{1}{4}$	$+0$	$+0$	$+0$	$+0$
$A^{\rho_1\rho_2} =$	$+\frac{1}{2}$	$+\frac{1}{4}$	$+0$	$+0$	$+0$	$+0$
$A_1^{s} =$	$-\frac{1}{4}$	$+\frac{1}{4}$	$+0$	$+0$	$+0$	$+0$
$A^{s_1s_2} =$	$+0$	$+\frac{1}{4}$	$+0$	$+0$	$+0$	$+0$
$A_1^{\tau} =$	$+0$	$+0$	$+\frac{1}{8}$	$-\frac{1}{8}$	$+\frac{3}{8}$	$+\frac{3}{8}$
$A^{\tau_1\rho_2} =$	$+0$	$+0$	$+\frac{1}{4}$	$+\frac{1}{8}$	$+\frac{1}{4}$	$+\frac{1}{8}$
$A_1^{T} =$	$+0$	$+0$	$-\frac{1}{8}$	$+\frac{1}{8}$	$+\frac{1}{8}$	$+\frac{1}{8}$
$A^{T_1s_2} =$	$+0$	$+0$	$+0$	$+\frac{1}{8}$	$+0$	$+\frac{1}{8}$
$A_1^{\nabla\rho} =$	$+0$	$+0$	$+\frac{3}{32}$	$-\frac{3}{32}$	$-\frac{3}{32}$	$-\frac{3}{32}$
$A^{\nabla\rho_1\nabla\rho_2} =$	$+0$	$+0$	$+\frac{3}{16}$	$+\frac{3}{32}$	$-\frac{1}{16}$	$-\frac{1}{32}$
$A_1^{\nabla s} =$	$+0$	$+0$	$-\frac{3}{32}$	$+\frac{3}{32}$	$-\frac{1}{32}$	$-\frac{1}{32}$
$A^{\nabla s_1\nabla s_2} =$	$+0$	$+0$	$+0$	$+\frac{3}{32}$	$+0$	$-\frac{1}{32}$
$A_1^{j} =$	$+0$	$+0$	$-\frac{1}{8}$	$+\frac{1}{8}$	$-\frac{3}{8}$	$-\frac{3}{8}$
$A^{j_1j_2} =$	$+0$	$+0$	$-\frac{1}{4}$	$-\frac{1}{8}$	$-\frac{1}{4}$	$-\frac{1}{8}$
$A_1^{J} =$	$+0$	$+0$	$+\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{1}{8}$
$A^{J_1J_2} =$	$+0$	$+0$	$+0$	$-\frac{1}{8}$	$+0$	$-\frac{1}{8}$

Table B.1: Functional coefficients in neutron-proton representation expressed in terms of pseudo-potential parameters.

where the functional coefficients are related to those of the pseudo-potential given in input according to Tab. {B.2}. For practical reason one might want to use the time-even part of the functional only given by

$$E^{\rho\rho} = \int d\vec{r} \Big\{ + A_0^{\rho}\,\rho_0\rho_0 + A_1^{\rho}\,\rho_1\rho_1 + A_0^{\tau}\,\tau_0\rho_0 + A_1^{\tau}\,\tau_1\rho_1 + A_0^{\nabla\rho}\,\nabla_\mu\rho_0\nabla_\mu\rho_0 + A_1^{\nabla\rho}\,\nabla_\mu\rho_1\nabla_\mu\rho_1 + A_0^{J}\,J_{0,\mu\nu}J_{0,\mu\nu} + A_1^{J}\,J_{1,\mu\nu}J_{1,\mu\nu} \Big\} .$$

B.3 Functional derivatives

The one-body fields obtained through functional derivatives read

$$U_q \equiv \frac{\delta\mathcal{E}}{\delta\rho_q} = +2A_1^{\rho}\,\rho_q + 2A^{\rho_1\rho_2}\rho_{\bar{q}} + A_1^{\tau}\,\tau_q + A^{\tau_1\rho_2}\tau_{\bar{q}} - 2A_1^{\nabla\rho}\,\Delta\rho_q - 2A^{\nabla\rho_1\nabla\rho_2}\Delta\rho_{\bar{q}} \ ,$$

$$S_{q,\nu} \equiv \frac{\delta\mathcal{E}}{\delta s_{q,\mu}} = +2A_1^{s}\,s_{q,\nu} + 2A^{s_1s_2}s_{\bar{q},\nu} + A_1^{T}\,T_{q,\nu} + A^{T_1s_2}T_{\bar{q},\nu} - 2A_1^{\nabla s}\,\Delta s_{q,\nu} - 2A^{\nabla s_1\nabla s_2}\Delta s_{\bar{q},\nu} \ ,$$

$Func\backslash Int$	t_0	t_0x_0	t_1	t_1x_1	t_2	t_2x_2
A_0^ρ =	$+\frac{3}{8}$	$+0$	$+0$	$+0$	$+0$	$+0$
A_1^ρ =	$-\frac{1}{8}$	$-\frac{1}{4}$	$+0$	$+0$	$+0$	$+0$
A_0^s =	$-\frac{1}{8}$	$+\frac{1}{4}$	$+0$	$+0$	$+0$	$+0$
A_1^s =	$-\frac{1}{8}$	$+0$	$+0$	$+0$	$+0$	$+0$
A_0^τ =	$+0$	$+0$	$+\frac{3}{16}$	$+0$	$+\frac{5}{16}$	$+\frac{1}{4}$
A_1^τ =	$+0$	$+0$	$-\frac{1}{16}$	$-\frac{1}{8}$	$+\frac{1}{16}$	$+\frac{1}{8}$
A_0^T =	$+0$	$+0$	$-\frac{1}{16}$	$+\frac{1}{8}$	$+\frac{1}{16}$	$+\frac{1}{8}$
A_1^T =	$+0$	$+0$	$-\frac{1}{16}$	$+0$	$+\frac{1}{16}$	$+0$
$A_0^{\nabla\rho}$ =	$+0$	$+0$	$+\frac{9}{64}$	$+0$	$-\frac{5}{64}$	$-\frac{1}{16}$
$A_1^{\nabla\rho}$ =	$+0$	$+0$	$-\frac{3}{64}$	$-\frac{3}{32}$	$-\frac{1}{64}$	$-\frac{1}{32}$
$A_0^{\nabla s}$ =	$+0$	$+0$	$-\frac{3}{64}$	$+\frac{3}{32}$	$-\frac{1}{64}$	$-\frac{1}{32}$
$A_1^{\nabla s}$ =	$+0$	$+0$	$-\frac{3}{64}$	$+0$	$-\frac{1}{64}$	$+0$
A_0^j =	$+0$	$+0$	$-\frac{3}{16}$	$+0$	$-\frac{5}{16}$	$-\frac{1}{4}$
A_1^j =	$+0$	$+0$	$+\frac{1}{16}$	$+\frac{1}{8}$	$-\frac{1}{16}$	$-\frac{1}{8}$
A_0^J =	$+0$	$+0$	$+\frac{1}{16}$	$-\frac{1}{8}$	$-\frac{1}{16}$	$-\frac{1}{8}$
A_1^J =	$+0$	$+0$	$+\frac{1}{16}$	$+0$	$-\frac{1}{16}$	$+0$

Table B.2: Functional coefficients in isoscalar-isovector representation expressed in terms of pseudo-potential parameters.

$$
\begin{aligned}
B_q \equiv \frac{\delta\mathcal{E}}{\delta\tau_q} &= +\,A_1^\tau\ \rho_q + A^{\tau_1\rho_2}\rho_{\bar{q}}\ , \\
C_{q,\nu} \equiv \frac{\delta\mathcal{E}}{\delta T_{q,\nu}} &= +\,A_1^T\ s_{q,\nu} + A^{T_1 s_2} s_{\bar{q},\nu}\ , \\
A_{q,\nu} \equiv \frac{\delta\mathcal{E}}{\delta j_{q,\mu}} &= +\,2A_1^j\ j_{q,\mu} + 2A^{j_1 j_2} j_{\bar{q},\mu}\ , \\
W_{q,\mu\nu} \equiv \frac{\delta\mathcal{E}}{\delta J_{q,\mu\nu}} &= +\,2A_1^J\ J_{q,\mu\nu} + 2A^{J_1 J_2} J_{\bar{q},\mu\nu}\ ,
\end{aligned}
$$

where $\bar{q} \equiv -q$.

B.4 Infinite Nuclear Matter

The code also computes a set of infinite nuclear matter properties. The four basic degrees of freedom of homogeneous INM are the isoscalar scalar density ρ_0, the isovector scalar density ρ_1, the isoscalar vector density s_0, and the isovector vector density s_1. Each of them can be written as a function of the scalar isoscalar density following

$$
\begin{aligned}
\rho_1 &\equiv \rho_0 I_\tau\ , \\
s_0 &\equiv \rho_0 I_\sigma\ , \\
s_1 &\equiv \rho_0 I_{\sigma\tau}\ ,
\end{aligned}
$$

where I_τ is the relative isospin excess, I_σ is the relative spin excess, and $I_{\sigma\tau}$ is the relative spin-isospin excess, with $-1 \leq I_i \leq 1$. Moreover, Fermi momentum is related to isoscalar density

through

$$\rho_0 = \frac{2}{3\pi^2} k_F^3 \ . \tag{B.1}$$

Matter and spin kinetic densities are then given by

$$\begin{aligned}
\tau_0 &= \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \rho_0^{\frac{5}{3}} F_{5/3}^{(0)}(I_\tau, I_\sigma, I_{\sigma\tau}) \ , \\
\tau_1 &= \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \rho_0^{\frac{5}{3}} F_{5/3}^{(\tau)}(I_\tau, I_\sigma, I_{\sigma\tau}) \ , \\
T_0 &= \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \rho_0^{\frac{5}{3}} F_{5/3}^{(\sigma)}(I_\tau, I_\sigma, I_{\sigma\tau}) \ , \\
T_1 &= \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \rho_0^{\frac{5}{3}} F_{5/3}^{(\sigma\tau)}(I_\tau, I_\sigma, I_{\sigma\tau}) \ ,
\end{aligned}$$

where $F^{(0)}, F^{(\tau)}, F^{(\sigma)}$ and $F^{(\sigma\tau)}$ are defined as

$$\begin{aligned}
F_m^{(0)}(I_\tau, I_\sigma, I_{\sigma\tau}) \equiv & \frac{1}{4}\Big[(1+I_\tau+I_\sigma+I_{\sigma\tau})^m + (1+I_\tau-I_\sigma-I_{\sigma\tau})^m \\
& + (1-I_\tau+I_\sigma-I_{\sigma\tau})^m + (1-I_\tau-I_\sigma+I_{\sigma\tau})^m\Big] \ , \\
F_m^{(\tau)}(I_\tau, I_\sigma, I_{\sigma\tau}) \equiv & \frac{1}{4}\Big[(1+I_\tau+I_\sigma+I_{\sigma\tau})^m + (1+I_\tau-I_\sigma-I_{\sigma\tau})^m \\
& - (1-I_\tau+I_\sigma-I_{\sigma\tau})^m - (1-I_\tau-I_\sigma+I_{\sigma\tau})^m\Big] \ , \\
F_m^{(\sigma)}(I_\tau, I_\sigma, I_{\sigma\tau}) \equiv & \frac{1}{4}\Big[(1+I_\tau+I_\sigma+I_{\sigma\tau})^m - (1+I_\tau-I_\sigma-I_{\sigma\tau})^m \\
& + (1-I_\tau+I_\sigma-I_{\sigma\tau})^m - (1-I_\tau-I_\sigma+I_{\sigma\tau})^m\Big] \ , \\
F_m^{(\sigma\tau)}(I_\tau, I_\sigma, I_{\sigma\tau}) \equiv & \frac{1}{4}\Big[(1+I_\tau+I_\sigma+I_{\sigma\tau})^m - (1+I_\tau-I_\sigma-I_{\sigma\tau})^m \\
& - (1-I_\tau+I_\sigma-I_{\sigma\tau})^m + (1-I_\tau-I_\sigma+I_{\sigma\tau})^m\Big] \ .
\end{aligned}$$

All others one-body local densities are null in homogenous nuclear matter. Note that the properties given below is just the contribution coming from the two-body potential given in input, it then have to be added to the properties coming from the others potential one wants to used.

B.4.1 Spin and isospin Symmetric Nuclear Matter

Spin and isospin symmetric nuclear matter is defined by $\rho_1 = I_\tau = 0$ and $I_\sigma = I_{\sigma\tau} = 0$. The equation of state is given in this case by

$$\frac{E}{A} = +\frac{1}{2}A_1^\rho \, \rho_0 + \frac{3}{10}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau \, \rho_0^{\frac{5}{3}} \ ,$$

while the pressure, from which the saturation density is obtained, is expressed as

$$P = +\frac{1}{2}A_1^\rho \, \rho_0^2 + \frac{1}{2}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau \, \rho_0^{\frac{8}{3}} \ .$$

The incompressibility writes as

$$K = +9A_1^\rho \, \rho_0 + 9\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau \, \rho_0^{\frac{5}{3}} + 3\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau \, \rho_0^{\frac{5}{3}} \ ,$$

such that at the saturation point one finds that

$$K_\infty = +\,3\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{5}{3}}\ .$$

B.4.2 Isospin Asymmetric Nuclear Matter

Isospin asymmetric nuclear matter is characterized by $I_\tau \neq 0$. The equation of state is given by

$$\frac{E}{A} = +\,\frac{1}{2}A_1^\rho\,\rho_0\Big[1+I_\tau^2\Big] + \frac{3}{10}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{5}{3}} F_{5/3}^{(0)}(I_\tau,0,0) + \frac{3}{10}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{5}{3}} F_{5/3}^{(\tau)}(I_\tau,0,0)\ .$$

The pressure, is expressed as

$$P = +\,\frac{1}{2}A_1^\rho\,\rho_0^2\Big[1+I_\tau^2\Big] + \frac{1}{2}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{8}{3}} F_{5/3}^{(0)}(I_\tau,0,0) + \frac{1}{2}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{8}{3}} F_{5/3}^{(\tau)}(I_\tau,0,0)\ .$$

The critical value of the isospin for which the saturation point disappears is obtained thanks to

$$\frac{\partial P}{\partial \rho} = +\,A_1^\rho\,\rho_0\Big[1+I_\tau^2\Big] + \frac{4}{3}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{5}{3}} F_{5/3}^{(0)}(I_\tau,0,0) + \frac{4}{3}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{5}{3}} F_{5/3}^{(\tau)}(I_\tau,0,0)\ ,$$

$$\frac{\partial^2 P}{\partial \rho^2} = +\,A_1^\rho\,\Big[1+I_\tau^2\Big] + \frac{20}{9}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{2}{3}} F_{5/3}^{(0)}(I_\tau,0,0) + \frac{20}{9}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{2}{3}} F_{5/3}^{(\tau)}(I_\tau,0,0)\ .$$

The symmetry energy is

$$\begin{aligned} S = &+\,\frac{1}{2}A_1^\rho\,\rho_0 + \frac{1}{6}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{5}{3}} F_{-1/3}^{(0)}(I_\tau,0,0) \\ &+\,\frac{1}{6}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{5}{3}} F_{-1/3}^{(\tau)}(I_\tau,0,0)\ , \end{aligned}$$

such that the symmetry coefficient reads

$$a_I = +\,\frac{1}{2}A_1^\rho\,\rho_0 + \frac{1}{6}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{5}{3}}\ .$$

The coefficient L is

$$L = +\,\frac{3}{2}A_1^\rho\,\rho_0 + \frac{5}{6}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{5}{3}}\ .$$

The symmetry incompressibility is obtained through

$$K_{sym} = +\,\frac{5}{3}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{5}{3}}\ .$$

B.4.3 Pure Neutron Matter

For $I_\tau = 1$ the infinite nuclear matter is composed uniquely of neutrons. The equation of state is given by

$$\frac{E}{A} = +\,A_1^\rho\,\rho_0 + \frac{3}{10}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} 2^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{5}{3}} + \frac{3}{10}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} 2^{\frac{2}{3}} A_1^\tau\,\rho_0^{\frac{5}{3}}\ .$$

B.4.4 Spin-isospin polarized nuclear matter

The most general equation of state is

$$\begin{aligned}\frac{E}{A} =& + \frac{1}{2}A_1^\rho\ \rho_0\Big[1+I_\tau^2\Big] + \frac{1}{2}A_1^s\ \rho_0\Big[I_\sigma^2+I_{\sigma\tau}^2\Big] \\ &+ \frac{3}{10}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\ \rho_0^{\frac{5}{3}} F_{5/3}^{(0)}(I_\tau,I_\sigma,I_{\sigma\tau}) + \frac{3}{10}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^\tau\ \rho_0^{\frac{5}{3}} F_{5/3}^{(\tau)}(I_\tau,I_\sigma,I_{\sigma\tau}) \\ &+ \frac{3}{10}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^T\ \rho_0^{\frac{5}{3}} F_{5/3}^{(\sigma)}(I_\tau,I_\sigma,I_{\sigma\tau})I_\sigma + \frac{3}{10}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} A_1^T\ \rho_0^{\frac{5}{3}} F_{5/3}^{(\sigma\tau)}(I_\tau,I_\sigma,I_{\sigma\tau})I_{\sigma\tau}\ .\end{aligned}$$

B.4.5 Landau parameters

The Landau parameters are calculated from the residual interaction, i.e. using the following second derivatives of the energy functional

$$\begin{aligned}V_0^{\rho\rho} &\equiv \frac{\partial^2\mathcal{E}}{\partial\rho_0\partial\rho_0} = +2A_0^\rho\ , \\ V_1^{\rho\rho} &\equiv \frac{\partial^2\mathcal{E}}{\partial\rho_1\partial\rho_1} = +2A_1^\rho\ , \\ V_0^{ss} &\equiv \frac{\partial^2\mathcal{E}}{\partial s_0\partial s_0} = +2A_0^s\ , \\ V_1^{ss} &\equiv \frac{\partial^2\mathcal{E}}{\partial s_1\partial s_1} = +2A_1^s\ , \\ V_0^{\tau\rho} &\equiv \frac{\partial^2\mathcal{E}}{\partial\tau_0\partial\rho_0} = +A_0^\tau\ , \\ V_1^{\tau\rho} &\equiv \frac{\partial^2\mathcal{E}}{\partial\tau_1\partial\rho_1} = +A_1^\tau\ , \\ V_0^{Ts} &\equiv \frac{\partial^2\mathcal{E}}{\partial T_0\partial s_0} = +A_0^T\ , \\ V_1^{Ts} &\equiv \frac{\partial^2\mathcal{E}}{\partial T_1\partial s_1} = +A_1^T\ , \\ V_0^{jj} &\equiv \frac{\partial^2\mathcal{E}}{\partial j_0\partial j_0} = +2A_0^j\ , \\ V_1^{jj} &\equiv \frac{\partial^2\mathcal{E}}{\partial j_1\partial j_1} = +2A_1^j\ , \\ V_0^{JJ} &\equiv \frac{\partial^2\mathcal{E}}{\partial J_0\partial J_0} = +2A_0^J\ , \\ V_1^{JJ} &\equiv \frac{\partial^2\mathcal{E}}{\partial J_1\partial J_1} = +2A_1^J\ , \\ V_0^{\nabla\rho\nabla\rho} &\equiv \frac{\partial^2\mathcal{E}}{\partial\nabla\rho_0\partial\nabla\rho_0} = +2A_0^{\nabla\rho}\ , \\ V_1^{\nabla\rho\nabla\rho} &\equiv \frac{\partial^2\mathcal{E}}{\partial\nabla\rho_1\partial\nabla\rho_1} = +2A_1^{\nabla\rho}\ , \\ V_0^{\nabla s\nabla s} &\equiv \frac{\partial^2\mathcal{E}}{\partial\nabla s_0\partial\nabla s_0} = +2A_0^{\nabla s}\ , \\ V_1^{\nabla s\nabla s} &\equiv \frac{\partial^2\mathcal{E}}{\partial\nabla s_1\partial\nabla s_1} = +2A_1^{\nabla s}\ .\end{aligned}$$

The Landau parameters are then given by

$$\begin{aligned} F_l &= N_0 f_l \ , \\ F'_l &= N_0 f'_l \ , \\ G_l &= N_0 g_l \ , \\ G'_l &= N_0 g'_l \ , \end{aligned} \tag{B.2}$$

where $N_0 = \dfrac{2m_0^*}{\pi^2\hbar^2} k_F$, with m_0^* the isocalar effective mass, and

$$\begin{aligned} f_0 =& V_0^{\rho\rho} + 2k_F^2 V_0^{\rho\tau} = +2A_0^{\rho} + 2A_0^{\tau}\ k_F^2 \ , \\ f'_0 =& V_1^{\rho\rho} + 2k_F^2 V_1^{\rho\tau} = +2A_1^{\rho} + 2A_1^{\tau}\ k_F^2 \ , \\ g_0 =& V_0^{ss} + 2k_F^2 V_0^{sT} = +2A_0^{s} + 2A_0^{T}\ k_F^2 \ , \\ g'_0 =& V_1^{ss} + 2k_F^2 V_1^{sT} = +2A_1^{s} + 2A_1^{T}\ k_F^2 \ , \\ f_1 =& k_F^2 V_0^{jj} = +2A_0^{j}\ k_F^2 \ , \\ f'_1 =& k_F^2 V_1^{jj} = +2A_1^{j}\ k_F^2 \ , \\ g_1 =& k_F^2 V_0^{JJ} = +2A_0^{J}\ k_F^2 \ , \\ g'_1 =& k_F^2 V_1^{JJ} = +2A_1^{J}\ k_F^2 \ . \end{aligned}$$

Appendix C

Formal computation code output for the three-body pseudo potential

Abstract: In this section the Latex output file of the formal computation code treating the derivation of the trilinear functional is reported. The code has been used with three-body pseudo-potential Eqs. (3.87,3.88). Functional derivatives and infinite nuclear matter properties that have not been given explicitly in the chapters devoted to the three-body Skyrme pseudo-potential, are reproduced here.

Contents

The present document is the formal computation code output in which the calculated quantities are reported. The .tex and .pdf files are copied in the output directory chosen at the execution, where one also finds all results in separated output files and in a non-LaTeX version. First, let us remark that as the LaTeX file is generated by the code, equations might appear misshapen in certain cases, e.g. too long lines or equations alignement problems may appear. However, the .tex file can be changed manually to reshape equations. For complementary explanations on derived properties and the method used to derive them one should refer to Chap. 3 and Chap. 4.

C.1 Formal code input : three-body Skyrme pseudo potential

This section deals with the inputs used by the code. In case it does not correspond to what one had expected, one should run the code again with appropriate inputs.

C.1.1 Gradient structure

The inputs file asks for specific gradient and exchange operator structures, the latter being named $P^{\{x\}}$. The code multiplies each bilinear gradient operator structure entered by $P^{\{x\}}$ and calculates the hermitian counterpart so that the resulting EDF must be real by construction. In the present case, the code uses The pseudo potential the code just has used is

$$\begin{aligned} V^{Sk} = &+ 3P^{\{x^0\}}\delta(\vec{r}_1-\vec{r}_2)\delta(\vec{r}_1-\vec{r}_3) \\ &+ \frac{3}{2}\left[P^{\{x^1\}}\Big(k'_{12,u}k'_{12,u}\Big) + \Big(k_{12,u}k_{12,u}\Big)P^{\{x^1\}}\right]\delta(\vec{r}_1-\vec{r}_2)\delta(\vec{r}_1-\vec{r}_3) \\ &+ \frac{3}{2}\left[P^{\{x^2\}}\Big(k_{12,u}k'_{12,u}\Big) + \Big(k'_{12,u}k_{12,u}\Big)P^{\{x^2\}}\right]\delta(\vec{r}_1-\vec{r}_2)\delta(\vec{r}_1-\vec{r}_3) \ . \end{aligned}$$

C.1.2 Exchange operators $P^{\{x\}}$

The corresponding exchange operators are

$$\begin{aligned} P^{\{x^0\}} &= + u_0 \ , \\ P^{\{x^1\}} &= + u_1 + u_1 y_1 P^{\sigma}_{12} \ , \\ P^{\{x^2\}} &= + u_2 + u_2 y_{21} P^{\sigma}_{12} + u_2 y_{22} P^{\sigma}_{13} + u_2 y_{22} P^{\sigma}_{23} \ . \end{aligned}$$

C.1.3 Parameters correlations

The pseudo potential used might have correlated parameters. This would appear after the functional has been calculated. In order to save space, only the functional from which correlated parameters have been suppressed is presented. Unfortunately, all correlations cannot be found using this particular code that can only identify parameters that are correlated in pairs. Parameters located on the right-hand side of the following equations are correlated to those located on the left hand side.

$$\begin{aligned} u_0 &\Leftarrow \\ u_1 &\Leftarrow \\ u_1 y_1 &\Leftarrow \\ u_2 &\Leftarrow \\ u_2 y_{21} &\Leftarrow \\ u_2 y_{22} &\Leftarrow \end{aligned}$$

To find linear combinations of more than two parameters one needs to construct the matrix of coefficients Tabs. {C.3-C.4} and use the singular value decomposition , see Sec. 3.4.3. One computes the square matrix X by multiplying the matrix of coefficients M with its transpose

$$X = M^T M \ .$$

Diagonalizing X, one accesses linear combinations of correlated parameters, i.e. they are given by the eigenvectors with null eigenvalues. To do so one can use either the matrix of coefficients given in the output directories with any given routine or use the script in the Others/ directory to get the devoted mathematica commands.

C.1.4 Less-correlated exchange operators $P^{\{x\}}$

The pseudo potential from which detected correlations have been suppressed corresponds to the following reduced exchange operators

$$
\begin{aligned}
P^{\{x^0\}} &= +\, u_0 \ , \\
P^{\{x^1\}} &= +\, u_1 + u_1 y_1 P^{\sigma}_{12} \ , \\
P^{\{x^2\}} &= +\, u_2 + u_2 y_{21} P^{\sigma}_{12} + u_2 y_{22} P^{\sigma}_{13} + u_2 y_{22} P^{\sigma}_{23} \ .
\end{aligned}
$$

C.2 Energy Density Functional

C.2.1 Skyrme trilinear functional in neutron-proton representation

The trilinear Skyrme functional computed in neutron-proton representation reads

$$
\begin{aligned}
E^{\rho\rho\rho} = \int d\vec{r} \Bigg\{ \sum_{q_1} \Bigg[& + B^{\tau_1\rho_1\rho_1} \tau_{q_1}\rho_{q_1}\rho_{q_1} + B^{\tau_1 s_1 s_1} \tau_{q_1} s_{q_1,\nu} s_{q_1,\nu} + B^{\nabla\rho_1\nabla\rho_1\rho_1} \nabla_\mu\rho_{q_1} \nabla_\mu\rho_{q_1}\rho_{q_1} \\
& + B^{\nabla s_1\nabla s_1\rho_1} \nabla_\mu s_{q_1,\nu} \nabla_\mu s_{q_1,\nu}\rho_{q_1} + B^{\nabla\rho_1\nabla s_1 s_1} \nabla_\mu\rho_{q_1} \nabla_\mu s_{q_1,\nu} s_{q_1,\nu} + B^{j_1 j_1\rho_1} j_{q_1,\mu} j_{q_1,\mu}\rho_{q_1} \\
& + B^{J_1 J_1\rho_1} J_{q_1,\mu\nu} J_{q_1,\mu\nu}\rho_{q_1} + B^{j_1 J_1 s_1} j_{q_1,\mu} J_{q_1,\mu\nu} s_{q_1,\nu} + B^{\nabla s_1 J_1 s_1} \epsilon_{abc} \nabla_\mu s_{q_1,a} J_{q_1,\mu b} s_{q_1,c} \Bigg] \\
& + \sum_{q_1\neq q_2} \Bigg[+ B^{\rho_1\rho_1\rho_2} \rho_{q_1}\rho_{q_1}\rho_{q_2} + B^{s_1 s_1\rho_2} s_{q_1,\nu} s_{q_1,\nu}\rho_{q_2} + B^{\tau_1\rho_1\rho_2} \tau_{q_1}\rho_{q_1}\rho_{q_2} \\
& + B^{\tau_1\rho_2\rho_2} \tau_{q_1}\rho_{q_2}\rho_{q_2} + B^{T_1 s_1\rho_2} T_{q_1,\nu} s_{q_1,\nu}\rho_{q_2} + B^{T_1 s_2\rho_1} T_{q_1,\nu} s_{q_2,\nu}\rho_{q_1} \\
& + B^{\tau_1 s_1 s_2} \tau_{q_1} s_{q_1,\nu} s_{q_2,\nu} + B^{\tau_1 s_2 s_2} \tau_{q_1} s_{q_2,\nu} s_{q_2,\nu} + B^{\nabla\rho_1\nabla\rho_1\rho_2} \nabla_\mu\rho_{q_1} \nabla_\mu\rho_{q_1}\rho_{q_2} \\
& + B^{\nabla\rho_1\nabla\rho_2\rho_1} \nabla_\mu\rho_{q_1} \nabla_\mu\rho_{q_2}\rho_{q_1} + B^{\nabla s_1\nabla s_1\rho_2} \nabla_\mu s_{q_1,\nu} \nabla_\mu s_{q_1,\nu}\rho_{q_2} + B^{\nabla s_1\nabla s_2\rho_1} \nabla_\mu s_{q_1,\nu} \nabla_\mu s_{q_2,\nu}\rho_{q_1} \\
& + B^{\nabla\rho_1\nabla s_1 s_2} \nabla_\mu\rho_{q_1} \nabla_\mu s_{q_1,\nu} s_{q_2,\nu} + B^{\nabla\rho_1\nabla s_2 s_1} \nabla_\mu\rho_{q_1} \nabla_\mu s_{q_2,\nu} s_{q_1,\nu} + B^{\nabla\rho_1\nabla s_2 s_2} \nabla_\mu\rho_{q_1} \nabla_\mu s_{q_2,\nu} s_{q_2,\nu} \\
& + B^{j_1 j_1\rho_2} j_{q_1,\mu} j_{q_1,\mu}\rho_{q_2} + B^{j_1 j_2\rho_1} j_{q_1,\mu} j_{q_2,\mu}\rho_{q_1} + B^{J_1 J_1\rho_2} J_{q_1,\mu\nu} J_{q_1,\mu\nu}\rho_{q_2} \\
& + B^{J_1 J_2\rho_1} J_{q_1,\mu\nu} J_{q_2,\mu\nu}\rho_{q_1} + B^{j_1 J_1 s_2} j_{q_1,\mu} J_{q_1,\mu\nu} s_{q_2,\nu} + B^{j_1 J_2 s_1} j_{q_1,\mu} J_{q_2,\mu\nu} s_{q_1,\nu} \\
& + B^{j_1 J_2 s_2} j_{q_1,\mu} J_{q_2,\mu\nu} s_{q_2,\nu} + B^{\nabla s_1 J_1 s_2} \epsilon_{abc} \nabla_\mu s_{q_1,a} J_{q_1,\mu b} s_{q_2,c} + B^{\nabla s_1 J_2 s_1} \epsilon_{abc} \nabla_\mu s_{q_1,a} J_{q_2,\mu b} s_{q_1,c} \\
& + B^{\nabla s_1 J_2 s_2} \epsilon_{abc} \nabla_\mu s_{q_1,a} J_{q_2,\mu b} s_{q_2,c} \Bigg] \Bigg\} \ .
\end{aligned}
$$

where the functional coefficients are related to those of the pseudo-potential given in input according to Tabs. {C.1-C.2}. The expression of those coefficients can be found in a different format in the output directory or commented in the .tex file. For practical reason one might want to use the time-even part of the functional only, given by

$$
\begin{aligned}
E^{\rho\rho\rho} = \int d\vec{r} \Bigg\{ \sum_{q_1} \Bigg[& + B^{\tau_1\rho_1\rho_1} \tau_{q_1}\rho_{q_1}\rho_{q_1} + B^{\nabla\rho_1\nabla\rho_1\rho_1} \nabla_\mu\rho_{q_1} \nabla_\mu\rho_{q_1}\rho_{q_1} + B^{J_1 J_1\rho_1} J_{q_1,\mu\nu} J_{q_1,\mu\nu}\rho_{q_1} \Bigg] \\
& + \sum_{q_1\neq q_2} \Bigg[+ B^{\rho_1\rho_1\rho_2} \rho_{q_1}\rho_{q_1}\rho_{q_2} + B^{\tau_1\rho_1\rho_2} \tau_{q_1}\rho_{q_1}\rho_{q_2} + B^{\tau_1\rho_2\rho_2} \tau_{q_1}\rho_{q_2}\rho_{q_2} + B^{\nabla\rho_1\nabla\rho_1\rho_2} \nabla_\mu\rho_{q_1} \nabla_\mu\rho_{q_1}\rho_{q_2} \\
& + B^{\nabla\rho_1\nabla\rho_2\rho_1} \nabla_\mu\rho_{q_1} \nabla_\mu\rho_{q_2}\rho_{q_1} + B^{J_1 J_1\rho_2} J_{q_1,\mu\nu} J_{q_1,\mu\nu}\rho_{q_2} + B^{J_1 J_2\rho_1} J_{q_1,\mu\nu} J_{q_2,\mu\nu}\rho_{q_1} \Bigg] \Bigg\} \ .
\end{aligned}
$$

$Func\backslash Int$	u_0	u_1	u_1y_1	u_2	u_2y_{21}	u_2y_{22}
$B^{\rho_1\rho_1\rho_2} =$	$+\frac{3}{4}$	$+0$	$+0$	$+0$	$+0$	$+0$
$B^{\tau_1\rho_1\rho_1} =$	$+0$	$+0$	$+0$	$+\frac{3}{16}$	$+\frac{3}{16}$	$-\frac{3}{16}$
$B^{\tau_1\rho_1\rho_2} =$	$+0$	$+\frac{1}{4}$	$-\frac{1}{16}$	$+\frac{5}{8}$	$+\frac{1}{2}$	$+\frac{5}{8}$
$B^{\tau_1\rho_2\rho_2} =$	$+0$	$+\frac{1}{8}$	$+\frac{1}{16}$	$+\frac{1}{8}$	$+\frac{1}{16}$	$-\frac{1}{16}$
$B^{\nabla\rho_1\nabla\rho_1\rho_1} =$	$+0$	$+0$	$+0$	$-\frac{3}{64}$	$-\frac{3}{64}$	$+\frac{3}{64}$
$B^{\nabla\rho_1\nabla\rho_1\rho_2} =$	$+0$	$+\frac{5}{32}$	$-\frac{1}{16}$	$-\frac{1}{8}$	$-\frac{7}{64}$	$-\frac{11}{64}$
$B^{\nabla\rho_1\nabla\rho_2\rho_1} =$	$+0$	$+\frac{5}{16}$	$+\frac{1}{16}$	$-\frac{1}{16}$	$-\frac{1}{32}$	$+\frac{1}{32}$
$B^{J_1J_1\rho_1} =$	$+0$	$+0$	$+0$	$-\frac{3}{16}$	$-\frac{3}{16}$	$+\frac{3}{16}$
$B^{J_1J_1\rho_2} =$	$+0$	$+\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{1}{4}$	$-\frac{3}{16}$	$-\frac{3}{16}$
$B^{J_1J_2\rho_1} =$	$+0$	$+0$	$-\frac{1}{8}$	$+0$	$-\frac{1}{8}$	$+\frac{1}{8}$

Table C.1: Time-even functional coefficients in neutron-proton representation expressed in terms of pseudo-potential parameters.

C.2.2 Skyrme trilinear functional in isoscalar-isovector representation

The Skyrme functional is then calculated in isoscalar-isovector representation and reads

$$
\begin{aligned}
E^{\rho\rho\rho} = \int d\vec{r} \Big\{ & + B_0^{\rho}\ \rho_0\rho_0\rho_0 + B_1^{\rho}\ \rho_0\rho_1\rho_1 + B_0^{s}\ s_{0,\nu}s_{0,\nu}\rho_0 \\
& + B_{10}^{s}\ s_{0,\nu}s_{1,\nu}\rho_1 + B_1^{s}\ s_{1,\nu}s_{1,\nu}\rho_0 + B_0^{\tau}\ \tau_0\rho_0\rho_0 \\
& + B_{10}^{\tau}\ \tau_0\rho_1\rho_1 + B_1^{\tau}\ \tau_1\rho_0\rho_1 + B_0^{T}\ T_{0,\nu}s_{0,\nu}\rho_0 \\
& + B_{10}^{T}\ T_{0,\nu}s_{1,\nu}\rho_1 + B_{01}^{T}\ T_{1,\nu}s_{0,\nu}\rho_1 + B_1^{T}\ T_{1,\nu}s_{1,\nu}\rho_0 \\
& + B_0^{\tau s}\ \tau_0 s_{0,\nu}s_{0,\nu} + B_{10}^{\tau s}\ \tau_0 s_{1,\nu}s_{1,\nu} + B_1^{\tau s}\ \tau_1 s_{0,\nu}s_{1,\nu} \\
& + B_0^{\nabla\rho}\ \nabla_\mu\rho_0\nabla_\mu\rho_0\rho_0 + B_{10}^{\nabla\rho}\ \nabla_\mu\rho_0\nabla_\mu\rho_1\rho_1 + B_1^{\nabla\rho}\ \nabla_\mu\rho_1\nabla_\mu\rho_1\rho_0 \\
& + B_0^{\nabla s}\ \nabla_\mu s_{0,\nu}\nabla_\mu s_{0,\nu}\rho_0 + B_{10}^{\nabla s}\ \nabla_\mu s_{0,\nu}\nabla_\mu s_{1,\nu}\rho_1 + B_1^{\nabla s}\ \nabla_\mu s_{1,\nu}\nabla_\mu s_{1,\nu}\rho_0 \\
& + B_0^{\nabla\rho s}\ \nabla_\mu\rho_0\nabla_\mu s_{0,\nu}s_{0,\nu} + B_{01}^{\nabla\rho s}\ \nabla_\mu\rho_0\nabla_\mu s_{1,\nu}s_{1,\nu} + B_{10}^{\nabla\rho s}\ \nabla_\mu\rho_1\nabla_\mu s_{0,\nu}s_{1,\nu} \\
& + B_1^{\nabla\rho s}\ \nabla_\mu\rho_1\nabla_\mu s_{1,\nu}s_{0,\nu} + B_0^{j}\ j_{0,\mu}j_{0,\mu}\rho_0 + B_{10}^{j}\ j_{0,\mu}j_{1,\mu}\rho_1 \\
& + B_1^{j}\ j_{1,\mu}j_{1,\mu}\rho_0 + B_0^{J}\ J_{0,\mu\nu}J_{0,\mu\nu}\rho_0 + B_{10}^{J}\ J_{0,\mu\nu}J_{1,\mu\nu}\rho_1 \\
& + B_1^{J}\ J_{1,\mu\nu}J_{1,\mu\nu}\rho_0 + B_0^{Js}\ j_{0,\mu}J_{0,\mu\nu}s_{0,\nu} + B_{01}^{Js}\ j_{0,\mu}J_{1,\mu\nu}s_{1,\nu} \\
& + B_{10}^{Js}\ j_{1,\mu}J_{0,\mu\nu}s_{1,\nu} + B_1^{Js}\ j_{1,\mu}J_{1,\mu\nu}s_{0,\nu} + B_0^{\nabla sJ}\ \epsilon_{abc}\nabla_\mu s_{0,a}J_{0,\mu b}s_{0,c} \\
& + B_{01}^{\nabla sJ}\ \epsilon_{abc}\nabla_\mu s_{0,a}J_{1,\mu b}s_{1,c} + B_{10}^{\nabla sJ}\ \epsilon_{abc}\nabla_\mu s_{1,a}J_{0,\mu b}s_{1,c} + B_1^{\nabla sJ}\ \epsilon_{abc}\nabla_\mu s_{1,a}J_{1,\mu b}s_{0,c} \Big\} .
\end{aligned}
$$

where the functional coefficients are related to those of the pseudo-potential given in input according to TABS. {C.3-C.4}. For practical reason one might want to use the time-even part of the functional only given by

$$
E^{\rho\rho\rho} = \int d\vec{r} \Big\{ + B_0^{\rho}\ \rho_0\rho_0\rho_0 + B_1^{\rho}\ \rho_0\rho_1\rho_1 + B_0^{\tau}\ \tau_0\rho_0\rho_0 + B_{10}^{\tau}\ \tau_0\rho_1\rho_1
$$

$Func\backslash Int$	u_0	u_1	u_1y_1	u_2	u_2y_{21}	u_2y_{22}
$B^{s_1s_1\rho_2} =$	$-\frac{3}{4}$	$+0$	$+0$	$+0$	$+0$	$+0$
$B^{T_1s_1\rho_2} =$	$+0$	$-\frac{1}{4}$	$+\frac{1}{16}$	$+\frac{1}{8}$	$+\frac{1}{8}$	$+\frac{1}{4}$
$B^{T_1s_2\rho_1} =$	$+0$	$+0$	$+\frac{1}{16}$	$+0$	$+\frac{1}{8}$	$+\frac{1}{4}$
$B^{\tau_1s_1s_1} =$	$+0$	$+0$	$+0$	$-\frac{3}{16}$	$-\frac{3}{16}$	$+\frac{3}{16}$
$B^{\tau_1s_1s_2} =$	$+0$	$+0$	$-\frac{1}{16}$	$+0$	$+0$	$+\frac{3}{8}$
$B^{\tau_1s_2s_2} =$	$+0$	$-\frac{1}{8}$	$-\frac{1}{16}$	$-\frac{1}{8}$	$-\frac{1}{16}$	$+\frac{1}{16}$
$B^{\nabla s_1\nabla s_1\rho_1} =$	$+0$	$+0$	$+0$	$-\frac{3}{64}$	$-\frac{3}{64}$	$+\frac{3}{64}$
$B^{\nabla s_1\nabla s_1\rho_2} =$	$+0$	$-\frac{5}{32}$	$+\frac{1}{16}$	$-\frac{1}{16}$	$-\frac{3}{64}$	$-\frac{3}{64}$
$B^{\nabla s_1\nabla s_2\rho_1} =$	$+0$	$+0$	$+\frac{1}{16}$	$+0$	$-\frac{1}{32}$	$+\frac{1}{32}$
$B^{\nabla\rho_1\nabla s_1s_1} =$	$+0$	$+0$	$+0$	$+\frac{3}{32}$	$+\frac{3}{32}$	$-\frac{3}{32}$
$B^{\nabla\rho_1\nabla s_1s_2} =$	$+0$	$+0$	$+0$	$+0$	$-\frac{1}{32}$	$-\frac{5}{32}$
$B^{\nabla\rho_1\nabla s_2s_1} =$	$+0$	$+0$	$-\frac{1}{16}$	$+0$	$+\frac{1}{32}$	$-\frac{1}{32}$
$B^{\nabla\rho_1\nabla s_2s_2} =$	$+0$	$-\frac{5}{16}$	$-\frac{1}{16}$	$+\frac{1}{16}$	$+\frac{1}{32}$	$-\frac{1}{32}$
$B^{j_1J_1s_1} =$	$+0$	$+0$	$+0$	$+\frac{3}{8}$	$+\frac{3}{8}$	$-\frac{3}{8}$
$B^{j_1J_1s_2} =$	$+0$	$+0$	$+0$	$+0$	$-\frac{1}{8}$	$-\frac{5}{8}$
$B^{j_1J_2s_1} =$	$+0$	$+0$	$+\frac{1}{8}$	$+0$	$+\frac{1}{8}$	$-\frac{1}{8}$
$B^{j_1J_2s_2} =$	$+0$	$+\frac{1}{4}$	$+\frac{1}{8}$	$+\frac{1}{4}$	$+\frac{1}{8}$	$-\frac{1}{8}$
$B^{\nabla s_1J_1s_1} =$	$+0$	$+0$	$+0$	$-\frac{3}{16}$	$-\frac{3}{16}$	$+\frac{3}{16}$
$B^{\nabla s_1J_1s_2} =$	$+0$	$+0$	$-\frac{1}{16}$	$+0$	$-\frac{1}{16}$	$+\frac{1}{16}$
$B^{\nabla s_1J_2s_1} =$	$+0$	$+0$	$-\frac{1}{16}$	$+0$	$-\frac{1}{16}$	$+\frac{1}{16}$
$B^{\nabla s_1J_2s_2} =$	$+0$	$+0$	$+\frac{1}{8}$	$+0$	$-\frac{1}{16}$	$+\frac{1}{16}$
$B^{j_1j_1\rho_1} =$	$+0$	$+0$	$+0$	$-\frac{3}{16}$	$-\frac{3}{16}$	$+\frac{3}{16}$
$B^{j_1j_1\rho_2} =$	$+0$	$-\frac{1}{8}$	$+\frac{1}{8}$	$-\frac{1}{2}$	$-\frac{7}{16}$	$-\frac{11}{16}$
$B^{j_1j_2\rho_1} =$	$+0$	$-\frac{1}{4}$	$-\frac{1}{8}$	$-\frac{1}{4}$	$-\frac{1}{8}$	$+\frac{1}{8}$

Table C.2: Time-odd functional coefficients in neutron-proton representation expressed in terms of pseudo-potential parameters.

$$+ B_1^{\tau}\,\tau_1\rho_0\rho_1 + B_0^{\nabla\rho}\,\nabla_\mu\rho_0\nabla_\mu\rho_0\rho_0 + B_{10}^{\nabla\rho}\,\nabla_\mu\rho_0\nabla_\mu\rho_1\rho_1 + B_1^{\nabla\rho}\,\nabla_\mu\rho_1\nabla_\mu\rho_1\rho_0$$
$$\left. + B_0^{J}\,J_{0,\mu\nu}J_{0,\mu\nu}\rho_0 + B_{10}^{J}\,J_{0,\mu\nu}J_{1,\mu\nu}\rho_1 + B_1^{J}\,J_{1,\mu\nu}J_{1,\mu\nu}\rho_0 \right\} .$$

C.3 Functional derivatives

The one-body fields obtained through functional derivatives read

$$U_q \equiv \frac{\delta\mathcal{E}}{\delta\rho_q} = + 2B^{\rho_1\rho_1\rho_2}\rho_q\rho_{\bar{q}} + B^{\rho_1\rho_1\rho_2}\rho_{\bar{q}}\rho_{\bar{q}} + B^{s_1s_1\rho_2}s_{\bar{q},\nu}s_{\bar{q},\nu}$$
$$+ 2B^{\tau_1\rho_1\rho_1}\tau_q\rho_q + B^{\tau_1\rho_1\rho_2}\tau_q\rho_{\bar{q}} + B^{\tau_1\rho_1\rho_2}\tau_{\bar{q}}\rho_{\bar{q}}$$

$Func\backslash Int$	u_0	u_1	u_1y_1	u_2	u_2y_{21}	u_2y_{22}
$B_0^{\rho} =$	$+\frac{3}{16}$	$+0$	$+0$	$+0$	$+0$	$+0$
$B_1^{\rho} =$	$-\frac{3}{16}$	$+0$	$+0$	$+0$	$+0$	$+0$
$B_0^{\tau} =$	$+0$	$+\frac{3}{32}$	$+0$	$+\frac{15}{64}$	$+\frac{3}{16}$	$+\frac{3}{32}$
$B_{10}^{\tau} =$	$+0$	$-\frac{1}{32}$	$+\frac{1}{32}$	$-\frac{5}{64}$	$-\frac{1}{16}$	$-\frac{7}{32}$
$B_1^{\tau} =$	$+0$	$-\frac{1}{16}$	$-\frac{1}{32}$	$+\frac{1}{32}$	$+\frac{1}{16}$	$-\frac{1}{16}$
$B_0^{\nabla\rho} =$	$+0$	$+\frac{15}{128}$	$+0$	$-\frac{15}{256}$	$-\frac{3}{64}$	$-\frac{3}{128}$
$B_{10}^{\nabla\rho} =$	$+0$	$-\frac{5}{64}$	$+\frac{1}{32}$	$+\frac{5}{128}$	$+\frac{1}{32}$	$+\frac{7}{64}$
$B_1^{\nabla\rho} =$	$+0$	$-\frac{5}{128}$	$-\frac{1}{32}$	$-\frac{7}{256}$	$-\frac{1}{32}$	$-\frac{5}{128}$
$B_0^{J} =$	$+0$	$+\frac{1}{32}$	$-\frac{1}{16}$	$-\frac{7}{64}$	$-\frac{1}{8}$	$+\frac{1}{32}$
$B_{10}^{J} =$	$+0$	$-\frac{1}{16}$	$+\frac{1}{16}$	$+\frac{1}{32}$	$+0$	$+\frac{3}{16}$
$B_1^{J} =$	$+0$	$+\frac{1}{32}$	$+0$	$-\frac{7}{64}$	$-\frac{1}{16}$	$-\frac{1}{32}$

Table C.3: Time-even functional coefficients in isoscalar-isovector representation expressed in terms of pseudo-potential parameters.

$$
\begin{aligned}
&+ 2B^{\tau_1\rho_2\rho_2}\tau_{\bar{q}}\rho_q + B^{T_1s_1\rho_2}T_{\bar{q},\nu}s_{\bar{q},\nu} + B^{T_1s_2\rho_1}T_{q,\nu}s_{\bar{q},\nu} \\
&- 2B^{\nabla\rho_1\nabla\rho_1\rho_1}\Delta\rho_q\rho_q - 2B^{\nabla\rho_1\nabla\rho_1\rho_1}\nabla_\mu\rho_q\nabla_\mu\rho_q + B^{\nabla\rho_1\nabla\rho_1\rho_1}\nabla_\mu\rho_q\nabla_\mu\rho_q \\
&- 2B^{\nabla\rho_1\nabla\rho_1\rho_2}\Delta\rho_q\rho_{\bar{q}} - 2B^{\nabla\rho_1\nabla\rho_1\rho_2}\nabla_\mu\rho_q\nabla_\mu\rho_{\bar{q}} + B^{\nabla\rho_1\nabla\rho_1\rho_2}\nabla_\mu\rho_{\bar{q}}\nabla_\mu\rho_{\bar{q}} \\
&- B^{\nabla\rho_1\nabla\rho_2\rho_1}\Delta\rho_{\bar{q}}\rho_q - B^{\nabla\rho_1\nabla\rho_2\rho_1}\Delta\rho_{\bar{q}}\rho_{\bar{q}} - B^{\nabla\rho_1\nabla\rho_2\rho_1}\nabla_\mu\rho_{\bar{q}}\nabla_\mu\rho_q \\
&- B^{\nabla\rho_1\nabla\rho_2\rho_1}\nabla_\mu\rho_{\bar{q}}\nabla_\mu\rho_{\bar{q}} + B^{\nabla\rho_1\nabla\rho_2\rho_1}\nabla_\mu\rho_q\nabla_\mu\rho_{\bar{q}} + B^{\nabla s_1\nabla s_1\rho_1}\nabla_\mu s_{q,\nu}\nabla_\mu s_{q,\nu} \\
&+ B^{\nabla s_1\nabla s_1\rho_2}\nabla_\mu s_{\bar{q},\nu}\nabla_\mu s_{\bar{q},\nu} + B^{\nabla s_1\nabla s_2\rho_1}\nabla_\mu s_{q,\nu}\nabla_\mu s_{\bar{q},\nu} - B^{\nabla\rho_1\nabla s_1s_1}\Delta s_{q,\nu}s_{q,\nu} \\
&- B^{\nabla\rho_1\nabla s_1s_1}\nabla_\mu s_{q,\nu}\nabla_\mu s_{q,\nu} - B^{\nabla\rho_1\nabla s_1s_2}\Delta s_{q,\nu}s_{\bar{q},\nu} - B^{\nabla\rho_1\nabla s_1s_2}\nabla_\mu s_{q,\nu}\nabla_\mu s_{\bar{q},\nu} \\
&- B^{\nabla\rho_1\nabla s_2s_1}\Delta s_{\bar{q},\nu}s_{q,\nu} - B^{\nabla\rho_1\nabla s_2s_1}\nabla_\mu s_{\bar{q},\nu}\nabla_\mu s_{q,\nu} - B^{\nabla\rho_1\nabla s_2s_2}\Delta s_{\bar{q},\nu}s_{\bar{q},\nu} \\
&- B^{\nabla\rho_1\nabla s_2s_2}\nabla_\mu s_{\bar{q},\nu}\nabla_\mu s_{\bar{q},\nu} + B^{j_1j_1\rho_1}j_{q,\mu}j_{q,\mu} + B^{j_1j_1\rho_2}j_{\bar{q},\mu}j_{\bar{q},\mu} \\
&+ B^{j_1j_2\rho_1}j_{q,\mu}j_{\bar{q},\mu} + B^{J_1J_1\rho_1}J_{q,\mu\nu}J_{q,\mu\nu} + B^{J_1J_1\rho_2}J_{\bar{q},\mu\nu}J_{\bar{q},\mu\nu} \\
&+ B^{J_1J_2\rho_1}J_{q,\mu\nu}J_{\bar{q},\mu\nu} \ , \\
S_{q,\nu} \equiv \frac{\delta\mathcal{E}}{\delta s_{q,\mu}} =& + 2B^{s_1s_1\rho_2}s_{q,\nu}\rho_{\bar{q}} + B^{T_1s_1\rho_2}T_{q,\nu}\rho_{\bar{q}} + B^{T_1s_2\rho_1}T_{\bar{q},\nu}\rho_{\bar{q}} \\
&+ 2B^{\tau_1s_1s_1}\tau_q s_{q,\nu} + B^{\tau_1s_1s_2}\tau_q s_{\bar{q},\nu} + B^{\tau_1s_1s_2}\tau_{\bar{q}}s_{\bar{q},\nu} \\
&+ 2B^{\tau_1s_2s_2}\tau_{\bar{q}}s_{q,\nu} - 2B^{\nabla s_1\nabla s_1\rho_1}\Delta s_{q,\nu}\rho_q - 2B^{\nabla s_1\nabla s_1\rho_1}\nabla_\mu s_{q,\nu}\nabla_\mu\rho_q \\
&- 2B^{\nabla s_1\nabla s_1\rho_2}\Delta s_{q,\nu}\rho_{\bar{q}} - 2B^{\nabla s_1\nabla s_1\rho_2}\nabla_\mu s_{q,\nu}\nabla_\mu\rho_{\bar{q}} - B^{\nabla s_1\nabla s_2\rho_1}\Delta s_{\bar{q},\nu}\rho_q \\
&- B^{\nabla s_1\nabla s_2\rho_1}\Delta s_{\bar{q},\nu}\rho_{\bar{q}} - B^{\nabla s_1\nabla s_2\rho_1}\nabla_\mu s_{\bar{q},\nu}\nabla_\mu\rho_q - B^{\nabla s_1\nabla s_2\rho_1}\nabla_\mu s_{\bar{q},\nu}\nabla_\mu\rho_{\bar{q}} \\
&- B^{\nabla\rho_1\nabla s_1s_1}\Delta\rho_q s_{q,\nu} - B^{\nabla\rho_1\nabla s_1s_1}\nabla_\mu\rho_q\nabla_\mu s_{q,\nu} + B^{\nabla\rho_1\nabla s_1s_1}\nabla_\mu\rho_q\nabla_\mu s_{q,\nu} \\
&- B^{\nabla\rho_1\nabla s_1s_2}\Delta\rho_q s_{\bar{q},\nu} - B^{\nabla\rho_1\nabla s_1s_2}\nabla_\mu\rho_q\nabla_\mu s_{\bar{q},\nu} + B^{\nabla\rho_1\nabla s_1s_2}\nabla_\mu\rho_{\bar{q}}\nabla_\mu s_{\bar{q},\nu} \\
&- B^{\nabla\rho_1\nabla s_2s_1}\Delta\rho_{\bar{q}}s_{\bar{q},\nu} - B^{\nabla\rho_1\nabla s_2s_1}\nabla_\mu\rho_{\bar{q}}\nabla_\mu s_{\bar{q},\nu} + B^{\nabla\rho_1\nabla s_2s_1}\nabla_\mu\rho_q\nabla_\mu s_{\bar{q},\nu} \\
&- B^{\nabla\rho_1\nabla s_2s_2}\Delta\rho_{\bar{q}}s_{q,\nu} - B^{\nabla\rho_1\nabla s_2s_2}\nabla_\mu\rho_{\bar{q}}\nabla_\mu s_{q,\nu} + B^{\nabla\rho_1\nabla s_2s_2}\nabla_\mu\rho_{\bar{q}}\nabla_\mu s_{q,\nu} \\
&+ B^{j_1J_1s_1}j_{q,\mu}J_{q,\mu\nu} + B^{j_1J_1s_2}j_{\bar{q},\mu}J_{\bar{q},\mu\nu} + B^{j_1J_2s_1}j_{q,\mu}J_{\bar{q},\mu\nu}
\end{aligned}
$$

$Func\backslash Int$	u_0	u_1	u_1y_1	u_2	u_2y_{21}	u_2y_{22}
$B_0^s =$	$-\frac{3}{16}$	$+0$	$+0$	$+0$	$+0$	$+0$
$B_{10}^s =$	$+\frac{3}{8}$	$+0$	$+0$	$+0$	$+0$	$+0$
$B_1^s =$	$-\frac{3}{16}$	$+0$	$+0$	$+0$	$+0$	$+0$
$B_0^T =$	$+0$	$-\frac{1}{16}$	$+\frac{1}{32}$	$+\frac{1}{32}$	$+\frac{1}{16}$	$+\frac{1}{8}$
$B_{10}^T =$	$+0$	$+\frac{1}{16}$	$-\frac{1}{32}$	$-\frac{1}{32}$	$-\frac{1}{16}$	$-\frac{1}{8}$
$B_{01}^T =$	$+0$	$+\frac{1}{16}$	$+0$	$-\frac{1}{32}$	$+0$	$+0$
$B_1^T =$	$+0$	$-\frac{1}{16}$	$+0$	$+\frac{1}{32}$	$+0$	$+0$
$B_0^{\tau s} =$	$+0$	$-\frac{1}{32}$	$-\frac{1}{32}$	$-\frac{5}{64}$	$-\frac{1}{16}$	$+\frac{5}{32}$
$B_{10}^{\tau s} =$	$+0$	$-\frac{1}{32}$	$+0$	$-\frac{5}{64}$	$-\frac{1}{16}$	$-\frac{1}{32}$
$B_1^{\tau s} =$	$+0$	$+\frac{1}{16}$	$+\frac{1}{32}$	$-\frac{1}{32}$	$-\frac{1}{16}$	$+\frac{1}{16}$
$B_0^{\nabla s} =$	$+0$	$-\frac{5}{128}$	$+\frac{1}{32}$	$-\frac{7}{256}$	$-\frac{1}{32}$	$+\frac{1}{128}$
$B_{10}^{\nabla s} =$	$+0$	$+\frac{5}{64}$	$-\frac{1}{32}$	$+\frac{1}{128}$	$+0$	$+\frac{3}{64}$
$B_1^{\nabla s} =$	$+0$	$-\frac{5}{128}$	$+0$	$-\frac{7}{256}$	$-\frac{1}{64}$	$-\frac{1}{128}$
$B_0^{\nabla \rho s} =$	$+0$	$-\frac{5}{64}$	$-\frac{1}{32}$	$+\frac{5}{128}$	$+\frac{1}{32}$	$-\frac{5}{64}$
$B_{01}^{\nabla \rho s} =$	$+0$	$-\frac{5}{64}$	$+0$	$+\frac{5}{128}$	$+\frac{1}{32}$	$+\frac{1}{64}$
$B_{10}^{\nabla \rho s} =$	$+0$	$+\frac{5}{64}$	$+0$	$+\frac{1}{128}$	$+\frac{1}{32}$	$+\frac{1}{64}$
$B_1^{\nabla \rho s} =$	$+0$	$+\frac{5}{64}$	$+\frac{1}{32}$	$+\frac{1}{128}$	$+0$	$-\frac{3}{64}$
$B_0^{Js} =$	$+0$	$+\frac{1}{16}$	$+\frac{1}{16}$	$+\frac{5}{32}$	$+\frac{1}{8}$	$-\frac{5}{16}$
$B_{01}^{Js} =$	$+0$	$+\frac{1}{16}$	$+0$	$+\frac{5}{32}$	$+\frac{1}{8}$	$+\frac{1}{16}$
$B_{10}^{Js} =$	$+0$	$-\frac{1}{16}$	$+0$	$+\frac{1}{32}$	$+\frac{1}{8}$	$+\frac{1}{16}$
$B_1^{Js} =$	$+0$	$-\frac{1}{16}$	$-\frac{1}{16}$	$+\frac{1}{32}$	$+0$	$-\frac{3}{16}$
$B_0^{\nabla sJ} =$	$+0$	$+0$	$+0$	$-\frac{3}{64}$	$-\frac{3}{32}$	$+\frac{3}{32}$
$B_{01}^{\nabla sJ} =$	$+0$	$+0$	$+\frac{1}{16}$	$-\frac{3}{64}$	$-\frac{1}{32}$	$+\frac{1}{32}$
$B_{10}^{\nabla sJ} =$	$+0$	$+0$	$-\frac{1}{32}$	$-\frac{3}{64}$	$-\frac{1}{32}$	$+\frac{1}{32}$
$B_1^{\nabla sJ} =$	$+0$	$+0$	$-\frac{1}{32}$	$-\frac{3}{64}$	$-\frac{1}{32}$	$+\frac{1}{32}$
$B_0^j =$	$+0$	$-\frac{3}{32}$	$+0$	$-\frac{15}{64}$	$-\frac{3}{16}$	$-\frac{3}{32}$
$B_{10}^j =$	$+0$	$+\frac{1}{16}$	$-\frac{1}{16}$	$+\frac{5}{32}$	$+\frac{1}{8}$	$+\frac{7}{16}$
$B_1^j =$	$+0$	$+\frac{1}{32}$	$+\frac{1}{16}$	$-\frac{7}{64}$	$-\frac{1}{8}$	$-\frac{5}{32}$

Table C.4: Time-odd functional coefficients in isoscalar-isovector representation expressed in terms of pseudo-potential parameters.

$$
\begin{aligned}
&+ B^{j_1 J_2 s_2} j_{\bar{q},\mu} J_{q,\mu\nu} - B^{\nabla s_1 J_1 s_1} \epsilon_{abc} \nabla_\mu J_{q,\mu b} s_{q,c} - B^{\nabla s_1 J_1 s_1} \epsilon_{abc} J_{q,\mu b} \nabla_\mu s_{q,c} \\
&+ B^{\nabla s_1 J_1 s_1} \epsilon_{abc} \nabla_\mu s_{q,a} J_{q,\mu b} - B^{\nabla s_1 J_1 s_2} \epsilon_{abc} \nabla_\mu J_{q,\mu b} s_{\bar{q},c} - B^{\nabla s_1 J_1 s_2} \epsilon_{abc} J_{q,\mu b} \nabla_\mu s_{\bar{q},c} \\
&+ B^{\nabla s_1 J_1 s_2} \epsilon_{abc} \nabla_\mu s_{\bar{q},a} J_{\bar{q},\mu b} - B^{\nabla s_1 J_2 s_1} \epsilon_{abc} \nabla_\mu J_{\bar{q},\mu b} s_{q,c} - B^{\nabla s_1 J_2 s_1} \epsilon_{abc} J_{\bar{q},\mu b} \nabla_\mu s_{q,c} \\
&+ B^{\nabla s_1 J_2 s_1} \epsilon_{abc} \nabla_\mu s_{q,a} J_{\bar{q},\mu b} - B^{\nabla s_1 J_2 s_2} \epsilon_{abc} \nabla_\mu J_{\bar{q},\mu b} s_{\bar{q},c} - B^{\nabla s_1 J_2 s_2} \epsilon_{abc} J_{\bar{q},\mu b} \nabla_\mu s_{\bar{q},c} \\
&+ B^{\nabla s_1 J_2 s_2} \epsilon_{abc} \nabla_\mu s_{\bar{q},a} J_{q,\mu b} \ ,
\end{aligned}
$$

$$
\begin{aligned}
B_q \equiv \frac{\delta \mathcal{E}}{\delta \tau_q} =& + B^{\tau_1 \rho_1 \rho_1} \rho_q \rho_q + B^{\tau_1 \rho_1 \rho_2} \rho_q \rho_{\bar{q}} + B^{\tau_1 \rho_2 \rho_2} \rho_{\bar{q}} \rho_{\bar{q}} \\
&+ B^{\tau_1 s_1 s_1} s_{q,\nu} s_{q,\nu} + B^{\tau_1 s_1 s_2} s_{q,\nu} s_{\bar{q},\nu} + B^{\tau_1 s_2 s_2} s_{\bar{q},\nu} s_{\bar{q},\nu} \ , \\
C_{q,\nu} \equiv \frac{\delta \mathcal{E}}{\delta T_{q,\nu}} =& + B^{T_1 s_1 \rho_2} s_{q,\nu} \rho_{\bar{q}} + B^{T_1 s_2 \rho_1} s_{\bar{q},\nu} \rho_q \ , \\
A_{q,\nu} \equiv \frac{\delta \mathcal{E}}{\delta j_{q,\mu}} =& + 2B^{j_1 j_1 \rho_1} j_{q,\mu} \rho_q + 2B^{j_1 j_1 \rho_2} j_{q,\mu} \rho_{\bar{q}} + B^{j_1 j_2 \rho_1} j_{\bar{q},\mu} \rho_q \\
&+ B^{j_1 j_2 \rho_1} j_{\bar{q},\mu} \rho_{\bar{q}} + B^{j_1 J_1 s_1} J_{q,\mu\nu} s_{q,\nu} + B^{j_1 J_1 s_2} J_{q,\mu\nu} s_{\bar{q},\nu} \\
&+ B^{j_1 J_2 s_1} J_{\bar{q},\mu\nu} s_{q,\nu} + B^{j_1 J_2 s_2} J_{\bar{q},\mu\nu} s_{\bar{q},\nu} \ , \\
W_{q,\mu\nu} \equiv \frac{\delta \mathcal{E}}{\delta J_{q,\mu\nu}} =& + 2B^{J_1 J_1 \rho_1} J_{q,\mu\nu} \rho_q + 2B^{J_1 J_1 \rho_2} J_{q,\mu\nu} \rho_{\bar{q}} + B^{J_1 J_2 \rho_1} J_{\bar{q},\mu\nu} \rho_q \\
&+ B^{J_1 J_2 \rho_1} J_{\bar{q},\mu\nu} \rho_{\bar{q}} + B^{j_1 J_1 s_1} j_{q,\mu} s_{q,\nu} + B^{j_1 J_1 s_2} j_{q,\mu} s_{\bar{q},\nu} \\
&+ B^{j_1 J_2 s_1} j_{\bar{q},\mu} s_{\bar{q},\nu} + B^{j_1 J_2 s_2} j_{\bar{q},\mu} s_{q,\nu} + B^{\nabla s_1 J_1 s_1} \epsilon_{abc} \nabla_\mu s_{q,a} s_{q,c} \\
&+ B^{\nabla s_1 J_1 s_2} \epsilon_{abc} \nabla_\mu s_{q,a} s_{\bar{q},c} + B^{\nabla s_1 J_2 s_1} \epsilon_{abc} \nabla_\mu s_{\bar{q},a} s_{\bar{q},c} + B^{\nabla s_1 J_2 s_2} \epsilon_{abc} \nabla_\mu s_{\bar{q},a} s_{q,c} \ ,
\end{aligned}
$$

where $\bar{q} \equiv -q$.

C.4 Infinite Nuclear Matter

The code also computes a set of infinite nuclear matter properties. The four basic degrees of freedom of homogeneous INM are the isoscalar scalar density ρ_0, the isovector scalar density ρ_1, the isoscalar vector density s_0, and the isovector vector density s_1. Each of them can be written as a function of the scalar isoscalar density following

$$
\begin{aligned}
\rho_1 &\equiv \rho_0 I_\tau \ , \\
s_0 &\equiv \rho_0 I_\sigma \ , \\
s_1 &\equiv \rho_0 I_{\sigma\tau} \ ,
\end{aligned}
$$

where I_τ is the relative isospin excess, I_σ is the relative spin excess, and $I_{\sigma\tau}$ is the relative spin-isospin excess, with $-1 \leq I_i \leq 1$. Moreover, Fermi momentum is related to isoscalar density through

$$
\rho_0 = \frac{2}{3\pi^2} k_F^3 \ .
$$

Matter and spin kinetic densities are then given by

$$\tau_0 = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \rho_0^{\frac{5}{3}} F^{(0)}_{5/3}(I_\tau, I_\sigma, I_{\sigma\tau}) \ ,$$
$$\tau_1 = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \rho_0^{\frac{5}{3}} F^{(\tau)}_{5/3}(I_\tau, I_\sigma, I_{\sigma\tau}) \ ,$$
$$T_0 = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \rho_0^{\frac{5}{3}} F^{(\sigma)}_{5/3}(I_\tau, I_\sigma, I_{\sigma\tau}) \ ,$$
$$T_1 = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \rho_0^{\frac{5}{3}} F^{(\sigma\tau)}_{5/3}(I_\tau, I_\sigma, I_{\sigma\tau}) \ ,$$

where $F^{(0)}, F^{(\tau)}, F^{(\sigma)}$ and $F^{(\sigma\tau)}$ are defined as

$$\begin{aligned}
F^{(0)}_m(I_\tau, I_\sigma, I_{\sigma\tau}) \equiv & \frac{1}{4}\Big[(1+I_\tau+I_\sigma+I_{\sigma\tau})^m + (1+I_\tau-I_\sigma-I_{\sigma\tau})^m \\
& + (1-I_\tau+I_\sigma-I_{\sigma\tau})^m + (1-I_\tau-I_\sigma+I_{\sigma\tau})^m\Big] \ , \\
F^{(\tau)}_m(I_\tau, I_\sigma, I_{\sigma\tau}) \equiv & \frac{1}{4}\Big[(1+I_\tau+I_\sigma+I_{\sigma\tau})^m + (1+I_\tau-I_\sigma-I_{\sigma\tau})^m \\
& - (1-I_\tau+I_\sigma-I_{\sigma\tau})^m - (1-I_\tau-I_\sigma+I_{\sigma\tau})^m\Big] \ , \\
F^{(\sigma)}_m(I_\tau, I_\sigma, I_{\sigma\tau}) \equiv & \frac{1}{4}\Big[(1+I_\tau+I_\sigma+I_{\sigma\tau})^m - (1+I_\tau-I_\sigma-I_{\sigma\tau})^m \\
& + (1-I_\tau+I_\sigma-I_{\sigma\tau})^m - (1-I_\tau-I_\sigma+I_{\sigma\tau})^m\Big] \ , \\
F^{(\sigma\tau)}_m(I_\tau, I_\sigma, I_{\sigma\tau}) \equiv & \frac{1}{4}\Big[(1+I_\tau+I_\sigma+I_{\sigma\tau})^m - (1+I_\tau-I_\sigma-I_{\sigma\tau})^m \\
& - (1-I_\tau+I_\sigma-I_{\sigma\tau})^m + (1-I_\tau-I_\sigma+I_{\sigma\tau})^m\Big] \ .
\end{aligned}$$

All others one-body local densities are null in homogenous nuclear matter. Note that the properties given below is just the contribution coming from the three-body potential given in input, it then have to be added to the properties coming from the others potential one wants to used.

C.4.1 Spin and isospin Symmetric Nuclear Matter

Spin and isospin symmetric nuclear matter is defined by $\rho_1 = I_\tau = 0$ and $I_\sigma = I_{\sigma\tau} = 0$. The equation of state is given in this case by

$$\frac{E}{A} = +\, B_0^\rho\, \rho_0^2 + \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^\tau\, \rho_0^{\frac{8}{3}} \ ,$$

while the pressure, from which the saturation density is obtained, is expressed as

$$P = +\, 2B_0^\rho\, \rho_0^3 + \frac{8}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^\tau\, \rho_0^{\frac{11}{3}} \ .$$

The incompressibility writes as

$$K = +\, 36B_0^\rho\, \rho_0^2 + \frac{144}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^\tau\, \rho_0^{\frac{8}{3}} + 18B_0^\rho\, \rho_0^2 + 24\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^\tau\, \rho_0^{\frac{8}{3}} \ ,$$

such that at the saturation point one finds that

$$K_\infty = +\, 18B_0^\rho\, \rho_0^2 + 24\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^\tau\, \rho_0^{\frac{8}{3}} \ .$$

C.4.2 Isospin Asymmetric Nuclear Matter

Isospin asymmetric nuclear matter is characterized by $I_\tau \neq 0$. The equation of state is given by

$$\frac{E}{A} = + B_0^\rho\ \rho_0^2 + B_1^\rho\ \rho_0^2 I_\tau^2 + \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^\tau\ \rho_0^{\frac{8}{3}} F_{5/3}^{(0)}(I_\tau,0,0) + \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_{10}^\tau\ \rho_0^{\frac{8}{3}} F_{5/3}^{(0)}(I_\tau,0,0) I_\tau^2 + \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^\tau\ \rho_0^{\frac{8}{3}} F_{5/3}^{(\tau)}(I_\tau,0,0) I_\tau\ .$$

The pressure, is expressed as

$$P = + 2B_0^\rho\ \rho_0^3 + 2B_1^\rho\ \rho_0^3 I_\tau^2 + \frac{8}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^\tau\ \rho_0^{\frac{11}{3}} F_{5/3}^{(0)}(I_\tau,0,0) + \frac{8}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_{10}^\tau\ \rho_0^{\frac{11}{3}} F_{5/3}^{(0)}(I_\tau,0,0) I_\tau^2 + \frac{8}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^\tau\ \rho_0^{\frac{11}{3}} F_{5/3}^{(\tau)}(I_\tau,0,0) I_\tau\ .$$

The critical value of the isospin for which the saturation point disappears is obtained thanks to

$$\frac{\partial P}{\partial \rho} = + 6B_0^\rho\ \rho_0^2 + 6B_1^\rho\ \rho_0^2 I_\tau^2 + \frac{88}{15}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^\tau\ \rho_0^{\frac{8}{3}} F_{5/3}^{(0)}(I_\tau,0,0) + \frac{88}{15}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_{10}^\tau\ \rho_0^{\frac{8}{3}} F_{5/3}^{(0)}(I_\tau,0,0) I_\tau^2 + \frac{88}{15}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^\tau\ \rho_0^{\frac{8}{3}} F_{5/3}^{(\tau)}(I_\tau,0,0) I_\tau\ ,$$

$$\frac{\partial^2 P}{\partial \rho^2} = + 12B_0^\rho\ \rho_0 + 12B_1^\rho\ \rho_0 I_\tau^2 + \frac{704}{45}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^\tau\ \rho_0^{\frac{5}{3}} F_{5/3}^{(0)}(I_\tau,0,0) + \frac{704}{45}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_{10}^\tau\ \rho_0^{\frac{5}{3}} F_{5/3}^{(0)}(I_\tau,0,0) I_\tau^2 + \frac{704}{45}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^\tau\ \rho_0^{\frac{5}{3}} F_{5/3}^{(\tau)}(I_\tau,0,0) I_\tau\ .$$

The symmetry energy is

$$\begin{aligned} S = &+ B_1^\rho\ \rho_0^2 + \frac{1}{3}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^\tau\ \rho_0^{\frac{8}{3}} F_{-1/3}^{(0)}(I_\tau,0,0) \\ &+ \frac{1}{3}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_{10}^\tau\ \rho_0^{\frac{8}{3}} F_{-1/3}^{(0)}(I_\tau,0,0) I_\tau^2 + 1\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_{10}^\tau\ \rho_0^{\frac{8}{3}} F_{2/3}^{(\tau)}(I_\tau,0,0) I_\tau \\ &+ 1\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_{10}^\tau\ \rho_0^{\frac{8}{3}} F_{2/3}^{(\tau)}(I_\tau,0,0) I_\tau + \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_{10}^\tau\ \rho_0^{\frac{8}{3}} F_{5/3}^{(0)}(I_\tau,0,0) \\ &+ \frac{1}{3}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^\tau\ \rho_0^{\frac{8}{3}} F_{-1/3}^{(\tau)}(I_\tau,0,0) I_\tau + \frac{1}{2}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^\tau\ \rho_0^{\frac{8}{3}} F_{2/3}^{(0)}(I_\tau,0,0) \\ &+ \frac{1}{2}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^\tau\ \rho_0^{\frac{8}{3}} F_{2/3}^{(0)}(I_\tau,0,0)\ , \end{aligned}$$

such that the symmetry coefficient reads

$$a_I = + B_1^\rho\ \rho_0^2 + \frac{1}{3}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^\tau\ \rho_0^{\frac{8}{3}} + \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_{10}^\tau\ \rho_0^{\frac{8}{3}} + \frac{1}{2}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^\tau\ \rho_0^{\frac{8}{3}} + \frac{1}{2}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^\tau\ \rho_0^{\frac{8}{3}}\ .$$

The coefficient L is

$$L = + 6B_1^\rho\ \rho_0^2 + \frac{8}{3}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^\tau\ \rho_0^{\frac{8}{3}} + \frac{24}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_{10}^\tau\ \rho_0^{\frac{8}{3}} + 4\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^\tau\ \rho_0^{\frac{8}{3}} + 4\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^\tau\ \rho_0^{\frac{8}{3}}\ .$$

The symmetry incompressibility is obtained through

$$K_{sym} = +18B_1^\rho\ \rho_0^2 + \frac{40}{3}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^\tau\ \rho_0^{\frac{8}{3}} + 24\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_{10}^\tau\ \rho_0^{\frac{8}{3}} + 20\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^\tau\ \rho_0^{\frac{8}{3}} + 20\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^\tau\ \rho_0^{\frac{8}{3}}\ .$$

C.4.3 Pure Neutron Matter

For $I_\tau = 1$ the infinite nuclear matter is composed uniquely of neutrons. The equation of state is given by

$$\frac{E}{A} = +B_0^\rho\ \rho_0^2 + B_1^\rho\ \rho_0^2 + \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} 2^{\frac{2}{3}} B_0^\tau\ \rho_0^{\frac{8}{3}} + \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} 2^{\frac{2}{3}} B_{10}^\tau\ \rho_0^{\frac{8}{3}} + \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} 2^{\frac{2}{3}} B_1^\tau\ \rho_0^{\frac{8}{3}}\ .$$

C.4.4 Spin-isospin polarized nuclear matter

The most general equation of state is

$$\begin{aligned}
\frac{E}{A} =& + B_0^\rho\ \rho_0^2 + B_1^\rho\ \rho_0^2 I_\tau^2 \\
&+ B_0^s\ \rho_0^2 I_\sigma^2 + B_{10}^s\ \rho_0^2 I_\tau I_{\sigma\tau} \\
&+ B_1^s\ \rho_0^2 I_{\sigma\tau}^2 + \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^\tau\ \rho_0^{\frac{8}{3}} F_{5/3}^{(0)}(I_\tau, I_\sigma, I_{\sigma\tau}) \\
&+ \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_{10}^\tau\ \rho_0^{\frac{8}{3}} F_{5/3}^{(0)}(I_\tau, I_\sigma, I_{\sigma\tau}) I_\tau^2 + \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^\tau\ \rho_0^{\frac{8}{3}} F_{5/3}^{(\tau)}(I_\tau, I_\sigma, I_{\sigma\tau}) I_\tau \\
&+ \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^T\ \rho_0^{\frac{8}{3}} F_{5/3}^{(\sigma)}(I_\tau, I_\sigma, I_{\sigma\tau}) I_\sigma + \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_{10}^T\ \rho_0^{\frac{8}{3}} F_{5/3}^{(\sigma)}(I_\tau, I_\sigma, I_{\sigma\tau}) I_\tau I_{\sigma\tau} \\
&+ \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_{01}^T\ \rho_0^{\frac{8}{3}} F_{5/3}^{(\sigma\tau)}(I_\tau, I_\sigma, I_{\sigma\tau}) I_\sigma I_\tau + \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^T\ \rho_0^{\frac{8}{3}} F_{5/3}^{(\sigma\tau)}(I_\tau, I_\sigma, I_{\sigma\tau}) I_{\sigma\tau} \\
&+ \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_0^{\tau s}\ \rho_0^{\frac{8}{3}} F_{5/3}^{(0)}(I_\tau, I_\sigma, I_{\sigma\tau}) I_\sigma^2 + \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_{10}^{\tau s}\ \rho_0^{\frac{8}{3}} F_{5/3}^{(0)}(I_\tau, I_\sigma, I_{\sigma\tau}) I_{\sigma\tau}^2 \\
&+ \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} B_1^{\tau s}\ \rho_0^{\frac{8}{3}} F_{5/3}^{(\tau)}(I_\tau, I_\sigma, I_{\sigma\tau}) I_\sigma I_{\sigma\tau}\ .
\end{aligned}$$

C.4.5 Landau parameters

The Landau parameters are calculated from the residual interaction, i.e. using the following second derivatives of the energy functional

$$\begin{aligned}
V_0^{\rho\rho} &\equiv \frac{\partial^2 \mathcal{E}}{\partial\rho_0 \partial\rho_0} = +6B_0^\rho\ \rho_0 + 2B_0^\tau\ \tau_0\ , \\
V_1^{\rho\rho} &\equiv \frac{\partial^2 \mathcal{E}}{\partial\rho_1 \partial\rho_1} = +2B_1^\rho\ \rho_0 + 2B_{10}^\tau\ \tau_0\ , \\
V_0^{ss} &\equiv \frac{\partial^2 \mathcal{E}}{\partial s_0 \partial s_0} = +2B_0^s\ \rho_0 + 2B_0^{\tau s}\ \tau_0\ , \\
V_1^{ss} &\equiv \frac{\partial^2 \mathcal{E}}{\partial s_1 \partial s_1} = +2B_1^s\ \rho_0 + 2B_{10}^{\tau s}\ \tau_0\ ,
\end{aligned}$$

$$
\begin{aligned}
V_0^{\tau\rho} &\equiv \frac{\partial^2\mathcal{E}}{\partial\tau_0\partial\rho_0} = +\,2B_0^{\tau}\ \rho_0\ , \\
V_1^{\tau\rho} &\equiv \frac{\partial^2\mathcal{E}}{\partial\tau_1\partial\rho_1} = +\,B_1^{\tau}\ \rho_0\ , \\
V_0^{Ts} &\equiv \frac{\partial^2\mathcal{E}}{\partial T_0\partial s_0} = +\,B_0^{T}\ \rho_0\ , \\
V_1^{Ts} &\equiv \frac{\partial^2\mathcal{E}}{\partial T_1\partial s_1} = +\,B_1^{T}\ \rho_0\ , \\
V_0^{jj} &\equiv \frac{\partial^2\mathcal{E}}{\partial j_0\partial j_0} = +\,2B_0^{j}\ \rho_0\ , \\
V_1^{jj} &\equiv \frac{\partial^2\mathcal{E}}{\partial j_1\partial j_1} = +\,2B_1^{j}\ \rho_0\ , \\
V_0^{JJ} &\equiv \frac{\partial^2\mathcal{E}}{\partial J_0\partial J_0} = +\,2B_0^{J}\ \rho_0\ , \\
V_1^{JJ} &\equiv \frac{\partial^2\mathcal{E}}{\partial J_1\partial J_1} = +\,2B_1^{J}\ \rho_0\ , \\
V_0^{\nabla\rho\nabla\rho} &\equiv \frac{\partial^2\mathcal{E}}{\partial\nabla\rho_0\partial\nabla\rho_0} = +\,2B_0^{\nabla\rho}\ \rho_0\ , \\
V_1^{\nabla\rho\nabla\rho} &\equiv \frac{\partial^2\mathcal{E}}{\partial\nabla\rho_1\partial\nabla\rho_1} = +\,2B_1^{\nabla\rho}\ \rho_0\ , \\
V_0^{\nabla s\nabla s} &\equiv \frac{\partial^2\mathcal{E}}{\partial\nabla s_0\partial\nabla s_0} = +\,2B_0^{\nabla s}\ \rho_0\ , \\
V_1^{\nabla s\nabla s} &\equiv \frac{\partial^2\mathcal{E}}{\partial\nabla s_1\partial\nabla s_1} = +\,2B_1^{\nabla s}\ \rho_0\ .
\end{aligned}
$$

The Landau parameters are then given by

$$
\begin{aligned}
F_l &= N_0 f_l\ , \\
F_l' &= N_0 f_l'\ , \\
G_l &= N_0 g_l\ , \\
G_l' &= N_0 g_l'\ ,
\end{aligned}
$$

where $N_0 = \dfrac{2m_0^*}{\pi^2\hbar^2}k_F$, with m_0^* the isocalar effective mass, and

$$
\begin{aligned}
f_0 &= V_0^{\rho\rho} + 2k_F^2 V_0^{\rho\tau} = +6B_0^{\rho}\ \rho_0 + 2B_0^{\tau}\ \tau_0 + 4B_0^{\tau}\ k_F^2\rho_0\ , \\
f_0' &= V_1^{\rho\rho} + 2k_F^2 V_1^{\rho\tau} = +2B_1^{\rho}\ \rho_0 + 2B_{10}^{\tau}\ \tau_0 + 2B_1^{\tau}\ k_F^2\rho_0\ , \\
g_0 &= V_0^{ss} + 2k_F^2 V_0^{sT} = +2B_0^{s}\ \rho_0 + 2B_0^{\tau s}\ \tau_0 + 2B_0^{T}\ k_F^2\rho_0\ , \\
g_0' &= V_1^{ss} + 2k_F^2 V_1^{sT} = +2B_1^{s}\ \rho_0 + 2B_{10}^{\tau s}\ \tau_0 + 2B_1^{T}\ k_F^2\rho_0\ , \\
f_1 &= k_F^2 V_0^{jj} = +2B_0^{j}\ k_F^2\rho_0\ , \\
f_1' &= k_F^2 V_1^{jj} = +2B_1^{j}\ k_F^2\rho_0\ , \\
g_1 &= k_F^2 V_0^{JJ} = +2B_0^{J}\ k_F^2\rho_0\ , \\
g_1' &= k_F^2 V_1^{JJ} = +2B_1^{J}\ k_F^2\rho_0\ ,
\end{aligned}
$$

Appendix D

Angular momentum definitions and conventions

Abstract: Angular momentum conventions used in Appendix E are introduced in the present appendix and are based on [86, 159]. In particular definitions about angular momentum operators, Clebsch-Gordan coefficients, $3j$ symbols, spherical harmonics, Wigner D-functions, irreductible tensors and Wigner-Eckart theorem are provided.

Contents

D.1 Angular momentum operators

A quantum mechanical wave-function is characterized by quantum numbers which are the eigenvalues of a complete set of commuting operators. For a system displaying rotational invariance, it is convenient to use the square of the angular momentum, $\hat{J}^2$, and the projection of the angular momentum onto a quantization axis, $\hat{J}_z$. Thus, we define the ket $|jm\rangle$ satisfying

$$\hat{J}^2\,|jm\rangle = \hbar^2 j(j+1)|jm\rangle \qquad ; \qquad \hat{J}_z|jm\rangle = m\hbar\,|jm\rangle \ , \tag{D.1}$$

where j is a positive half-integer or integer and m is a half-integer or integer such that $|m| \leq j$. Moreover the three components $\hat{J}_i$ of the vector operator $\hat{\vec{J}}$ satisfy a SU(2) algebra

$$\left[\hat{J}_i, \hat{J}_j\right] = i\hbar\epsilon_{ijk}\hat{J}_k \ , \tag{D.2}$$

and are hermitian operators. It is useful to introduce the operators

$$\hat{J}_\pm \equiv \hat{J}_x \pm i\hat{J}_y \ , \tag{D.3}$$

that act on $|jm\rangle$ as

$$\hat{J}_\pm\,|jm\rangle \ = \ \sqrt{j(j+1) - m(m\pm 1)}\,\hbar\,|jm\pm 1\rangle \ . \tag{D.4}$$

Noting that

$$\hat{J}_\pm^\dagger = \hat{J}_\mp \ , \tag{D.5}$$

one has

$$\langle jm|\hat{J}_\pm = \langle jm\mp 1|\sqrt{j(j+1) - m(m\mp 1)}\hbar \ . \tag{D.6}$$

One can recover the eigenvalues of $\hat{J}^2$ through those of $\hat{J}_\pm$ and $\hat{J}_z$, thanks to

$$\begin{aligned}
\hat{J}^2 &= \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 \\
&= \hat{J}_x^2 + \hat{J}_y^2 + i\hat{J}_x\hat{J}_y - i\hat{J}_y\hat{J}_x - i\left[\hat{J}_x, \hat{J}_y\right] + \hat{J}_z^2 \\
&= \left(\hat{J}_x - i\hat{J}_y\right)\left(\hat{J}_x + i\hat{J}_y\right) - i\left[\hat{J}_x, \hat{J}_y\right] + \hat{J}_z^2 \\
&= \hat{J}_-\hat{J}_+ + \hbar\hat{J}_z + \hat{J}_z^2 \ ,
\end{aligned} \tag{D.7}$$

and

$$\begin{aligned}
\hat{J}^2|jm\rangle &= \hat{J}_-\hat{J}_+|jm\rangle + \hbar\hat{J}_z|jm\rangle + \hat{J}_z^2|jm\rangle \\
j(j+1)\hbar^2|jm\rangle &= \left[j(j+1) - m(m+1)\right]\hbar^2|jm\rangle + m\hbar^2|jm\rangle + m^2\hbar^2|jm\rangle \\
j(j+1)\hbar^2|jm\rangle &= \hbar^2\,j(j+1)|jm\rangle \ ,
\end{aligned} \tag{D.8}$$

D.2 Clebsch-Gordan coefficients

D.2.1 Definition

Let $\vec{j}_1$ and $\vec{j}_2$ be two angular momenta with projections m_1 and m_2 on the quantization axis. A Clebsch-Gordan coefficient represents the probability amplitude that $\vec{j}_1$ and $\vec{j}_2$ couple to a resulting angular momentum $\vec{j}$ with projection m. In the following expression

$$|j_1 j_2 j m\rangle \equiv \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} |j_1 m_1\rangle |j_2 m_2\rangle \langle j_1 m_1 j_2 m_2 | j m\rangle \ , \tag{D.9}$$

Clebsch-Gordan coefficients are denoted as $\langle j_1 m_1 j_2 m_2 | j m\rangle$. In accordance with the vector addition rules $\vec{j}_1 \oplus \vec{j}_2 = \vec{j}$, Clebsch-Gordan coefficients vanish unless the triangular condition is fulfilled

$$|j_1 - j_2| \leq j \leq j_1 + j_2 \ , \tag{D.10}$$

and the requirement

$$m_1 + m_2 = m \ , \tag{D.11}$$

is satisfied. It can also be shown that arguments of the Clebsch-Gordan coefficients satisfy the following conditions

- j_1, j_2, j are non-negative integers or half-integers
- m_1, m_2, m are integers or half-integers
- $|m_1| \leq j_1$, $|m_2| \leq j_2$, $|m| \leq j$
- $j_1 + m_1$, $j_2 + m_2$, $j + m$, $j_1 + j_2 + j$ are non-negative integers.

Clebsch-Gordan coefficients are also written under the form

$$\langle j_1 m_1 j_2 m_2 | j m\rangle \equiv C^{jm}_{j_1 m_1 j_2 m_2} \ . \tag{D.12}$$

D.2.2 Orthogonality relations

Clebsch-Gordan coefficients fulfill

$$\sum_{m_1 m_2} C^{jm}_{j_1 m_1 j_2 m_2} C^{j'm'}_{j_1 m_1 j_2 m_2} = \delta_{jj'}\delta_{mm'} \ , \tag{D.13a}$$

$$\sum_{jm} C^{jm}_{j_1 m_1 j_2 m_2} C^{jm}_{j_1 m'_1 j_2 m'_2} = \delta_{m_1 m'_1}\delta_{m_2 m'_2} \ . \tag{D.13b}$$

D.2.3 Symmetry properties

Clebsch-Gordan coefficients fulfill

$$\langle j_1 m_1 j_2 m_2 | j m\rangle = \langle j m | j_1 m_1 j_2 m_2\rangle \tag{D.14a}$$

$$= (-1)^{j_1+j_2-j} \langle j_2 m_2 j_1 m_1 | j m\rangle \tag{D.14b}$$

$$= (-1)^{j_1+j_2-j} \langle j_1 - m_1 j_2 - m_2 | j - m\rangle \tag{D.14c}$$

$$= (-1)^{j_1+m_1} \sqrt{\frac{2j+1}{2j_2+1}} \langle j_1 m_1 j - m | j_2 - m_2\rangle \tag{D.14d}$$

$$= (-1)^{j_2+m_2} \sqrt{\frac{2j+1}{2j_1+1}} \langle j - m j_2 m_2 | j_1 - m_1\rangle \ . \tag{D.14e}$$

Using Eq. D.14b, one finds

$$\langle j_1 m_1 j_1 m_1 | j m\rangle = (-1)^{j_1+j_1-j} \langle j_1 m_1 j_1 m_1 | j m\rangle \ , \tag{D.15}$$

such that, the Clebsch-Gordan coefficient $\langle j_1 m_1 j_1 m_1 | j m\rangle$ is non-zero only if j is even. In the same spirit using Eq. D.14c, one has

$$\langle j_1 0 j_2 0 | j 0\rangle = (-1)^{j_1+j_2-j}\langle j_1 0 j_2 0 | j 0\rangle \ , \tag{D.16}$$

such that, the Clebsch-Gordan coefficient $\langle j_1 0 j_2 0 | j 0\rangle$ is non-zero only if $j_1 + j_2 - j$ is even.

D.2.4 Specific values

For $j = 0$, Clebsch-Gordan coefficients give

$$\langle j_1 m_1 j_2 m_2 | 0 0\rangle = \delta_{j_1 j_2}\delta_{m_1 -m_2}\frac{(-1)^{j_1-m_1}}{\sqrt{2j_2+1}} \ , \tag{D.17a}$$

$$\langle j_1 m_1 0 0 | j_2 m_2\rangle = \delta_{j_1 j_2}\delta_{m_1 m_2} \ , \tag{D.17b}$$

whereas for $j = j_1 + j_2$ and $m = j$

$$\langle j_1 j_1 j_2 j_2 | j_1 + j_2 j_1 + j_2\rangle = 1 \tag{D.18}$$

D.2.5 Sum of products of the Clebsch-Gordan coefficients

The following relation will be used in this document

$$\sum_{m_1 m_2 m_3 m_4} C^{l_{12}m_{12}}_{l_1 m_1 l_2 m_2} C^{l_{34}m_{34}}_{l_3 m_3 l_4 m_4} C^{l_{13}m_{13}}_{l_1 m_1 l_3 m_3} C^{l_{24}m_{24}}_{l_2 m_2 l_4 m_4}$$

$$= \Pi_{l_{12}l_{34}l_{13}l_{24}} \sum_{\mu\nu} C^{\mu\nu}_{l_{12}m_{12}l_{34}m_{34}} C^{\mu\nu}_{l_{13}m_{13}l_{24}m_{24}} \begin{Bmatrix} l_4 & l_3 & l_{34} \\ l_2 & l_1 & l_{12} \\ l_{24} & l_{13} & \mu \end{Bmatrix} \ , \tag{D.19}$$

where $\Pi_{l_{12}l_{34}l_{13}l_{24}} = \sqrt{(2l_{12}+1)(2l_{34}+1)(2l_{13}+1)(2l_{24}+1)}$ and where we make use of the $9j$ symbols, Sec. D.4. Let us add another relation that comes from this expression and from Eq. D.13a

$$\sum_{m_{12}m_{34}} C^{LM}_{l_{12}m_{12}l_{34}m_{34}} \sum_{m_1 m_2 m_3 m_4} C^{l_{12}m_{12}}_{l_1 m_1 l_2 m_2} C^{l_{34}m_{34}}_{l_3 m_3 l_4 m_4} C^{l_{13}m_{13}}_{l_1 m_1 l_3 m_3} C^{l_{24}m_{24}}_{l_2 m_2 l_4 m_4}$$

$$= \Pi_{l_{12}l_{34}l_{13}l_{24}} C^{LM}_{l_{13}m_{13}l_{24}m_{24}} \begin{Bmatrix} l_4 & l_3 & l_{34} \\ l_2 & l_1 & l_{12} \\ l_{24} & l_{13} & L \end{Bmatrix} \ . \tag{D.20}$$

D.3 $3j$ symbols

D.3.1 Definition

The Wigner $3j$ symbols are defined by

$$\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix} = \frac{(-1)^{j_1-j_2-m}}{\sqrt{2j+1}}\langle j_1 m_1 j_2 m_2 | j -m\rangle \ , \tag{D.21}$$

and satisfy the same conditions as Clebsch-Gordan coefficients except that here $m_1+m_2+m = 0$.

D.3.2 Symmetry properties

The $3j$ symbols have the following symmetries

$$\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix} = \begin{pmatrix} j & j_1 & j_2 \\ m & m_1 & m_2 \end{pmatrix} , \tag{D.22a}$$

$$= \begin{pmatrix} j_2 & j & j_1 \\ m_2 & m & m_1 \end{pmatrix} , \tag{D.22b}$$

$$= (-1)^{j_1+j_2+j} \begin{pmatrix} j_2 & j_1 & j \\ m_2 & m_1 & m \end{pmatrix} , \tag{D.22c}$$

$$= (-1)^{j_1+j_2+j} \begin{pmatrix} j_1 & j_2 & j \\ -m_1 & -m_2 & -m \end{pmatrix} . \tag{D.22d}$$

D.4 $9j$ symbols

D.4.1 Definition

Let us consider an addition of four angular momenta $\vec{j}_1$, $\vec{j}_2$, $\vec{j}_3$ and $\vec{j}_4$ to form a resultant angular momentum $\vec{j}$ with projection m. There exist different coupling schemes of these angular momenta, for instance

$$\text{i)} \qquad \vec{j}_1 + \vec{j}_2 = \vec{j}_{12} , \qquad \vec{j}_3 + \vec{j}_4 = \vec{j}_{34} , \qquad \vec{j}_{12} + \vec{j}_{34} = \vec{j} ; \tag{D.23a}$$

$$\text{ii)} \qquad \vec{j}_1 + \vec{j}_3 = \vec{j}_{13} , \qquad \vec{j}_2 + \vec{j}_4 = \vec{j}_{24} , \qquad \vec{j}_{13} + \vec{j}_{24} = \vec{j} . \tag{D.23b}$$

Let $|j_1 j_2 (j_{12}) j_3 j_4 (j_{34}) jm\rangle$ be the ket for the scheme i), this ket may be written as

$$|j_1 j_2 (j_{12}) j_3 j_4 (j_{34}) jm\rangle \tag{D.24}$$
$$= \sum_{m_1 m_2 m_3 m_4 m_{12} m_{34}} C^{jm}_{j_{12} m_{12} j_{34} m_{34}} C^{j_{12} m_{12}}_{j_1 m_1 j_2 m_2} C^{j_{34} m_{34}}_{j_3 m_3 j_4 m_4} |j_1 m_1 j_2 m_2 j_3 m_3 j_4 m_4\rangle .$$

For the scheme ii) one has

$$|j_1 j_3 (j_{13}) j_2 j_4 (j_{24}) jm\rangle \tag{D.25}$$
$$= \sum_{m_1 m_2 m_3 m_4 m_{13} m_{24}} C^{jm}_{j_{13} m_{13} j_{24} m_{24}} C^{j_{13} m_{13}}_{j_1 m_1 j_3 m_3} C^{j_{24} m_{24}}_{j_2 m_2 j_4 m_4} |j_1 m_1 j_2 m_2 j_3 m_3 j_4 m_4\rangle .$$

The Wigner $9j$ symbols are related to coefficients of the transformation between kets in schemes i) and ii) by

$$\langle j_1 j_2 (j_{12}) j_3 j_4 (j_{34}) jm | j_1 j_3 (j_{13}) j_2 j_4 (j_{24}) j' m'\rangle \tag{D.26}$$
$$= \delta_{jj'} \delta_{mm'} \Pi_{j_{12} j_{34} j_{13} j_{24}} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{Bmatrix} .$$

In accordance with the quantum mechanical rules of angular momentum addition, arguments of the $9j$ symbol

$$\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & j \end{Bmatrix} , \tag{D.27}$$

satisfy the following conditions. (i) arguments $a, b, c, \cdots, j$ are integer or half-integer non-negative numbers (ii) a $9j$ symbol vanishes unless the triangular conditions (Sec. D.1) are fulfill for triads (abc), (def), (ghj), (adg), (beh), (cfj).

D.5 Spherical harmonics

D.5.1 Definition

The spherical harmonic $Y_l^m(\theta,\phi)$ is the eigenfunction of the orbital angular momentum operators $\hat{L}^2$ and $\hat{L}_z$ expressed in spherical coordinates

$$\hat{L}^2\, Y_l^m(\theta,\phi) = l(l+1)\hbar^2 Y_l^m(\theta,\phi) \ , \tag{D.28a}$$
$$\hat{L}_z\, Y_l^m(\theta,\phi) = m\hbar Y_l^m(\theta,\phi) \ , \tag{D.28b}$$

with $l \in \mathbb{N}$, $m \in \mathbb{Z}$ and $|m| \leq l$. The integral over total solid angle gives

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \; Y_l^m(\theta,\phi) = \sqrt{4\pi}\, \delta_{l0}\, \delta_{m0} \ , \tag{D.29}$$

whereas

$$Y_l^{m*}(\theta,\phi) = (-1)^m Y_l^{-m}(\theta,\phi) \ , \tag{D.30}$$

that is the Condon-Shortley phase convention.

D.5.2 Normalization, orthogonality and completeness relations

The completeness relation for spherical harmonics is given by

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_l^{m*}(\theta,\phi) Y_l^m(\theta',\phi') = \delta(\phi-\phi')\delta(\cos\theta - \cos\theta') \ , \tag{D.31}$$

whereas their orthogonality and normalization read

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta\, Y_l^{m*}(\theta,\phi)\; Y_{l'}^{m'}(\theta,\phi) = \delta_{ll'}\; \delta_{mm'} \ . \tag{D.32}$$

Furthermore, the spherical harmonics satisfy the following relations

$$\sum_{m=-l}^{l} (-1)^m\, Y_l^m(\theta,\phi)\, Y_l^{-m}(\theta,\phi) = \frac{2l+1}{4\pi} \ , \tag{D.33}$$

D.5.3 Symmetry properties

Spherical harmonics fulfill several symmetry properties as

$$Y_l^{m*}(\theta,\phi) = (-1)^m Y_l^{-m}(\theta,\phi) \ , \tag{D.34}$$

for complex conjugation, and

$$Y_l^m(-\theta,\phi) = (-1)^m Y_l^m(\theta,\phi) \ , \tag{D.35a}$$
$$Y_l^m(-\theta,-\phi) = Y_l^{-m}(\theta,\phi) \ , \tag{D.35b}$$

for changing the arguments sign.

D.5.4 Specific values

Spherical harmonics are related to Legendre polynomials P_l^m through

$$Y_l^m(\theta,\phi) = e^{im\phi}\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta) \ , \tag{D.36}$$

such that, in particular,

$$Y_l^0(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}}P_l^0(\cos\theta) \ , \tag{D.37a}$$

$$Y_l^0(0,0) = \sqrt{\frac{2l+1}{4\pi}} \ . \tag{D.37b}$$

The inverse vector $-\vec{r}$ of vector $\vec{r}$ with angles θ and ϕ has angles $\theta' = \pi - \theta$ and $\phi' = \pi + \phi$. For this particular case it is interesting to introduce the relation

$$Y_l^m(\pi-\theta,\pi+\phi) = (-1)^l\, Y_l^m(\theta,\phi) \ . \tag{D.38}$$

D.5.5 Clebsch-Gordan series

We add the two following relations

$$Y_{l_1}^{m_1}(\theta,\phi)\, Y_{l_2}^{m_2}(\theta,\phi) = \sum_{LM}\sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2L+1)}}\, C^{L0}_{l_1 0\, l_2 0}\, C^{LM}_{l_1 m_1\, l_2 m_2}\, Y_L^M(\theta,\phi) \ , \tag{D.39}$$

and

$$\begin{aligned} &Y_{l_1}^{m_1}(\theta,\phi)\, Y_{l_2}^{m_2}(\theta,\phi)\, Y_{l_3}^{m_3}(\theta,\phi) \\ &\quad = \sum_{LML'M'}\sqrt{\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{(4\pi)^2(2L+1)}}\, C^{L'0}_{l_1 0\, l_2 0}\, C^{L0}_{L'0\, l_3 0}\, C^{L'M'}_{l_1 m_1\, l_2 m_2}\, C^{LM}_{L'M'\, l_3 m_3}\, Y_L^M(\theta,\phi) \ , \end{aligned} \tag{D.40}$$

One finds through integration

$$\begin{aligned} &\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin(\theta) Y_{l_1}^{m_1}(\theta,\phi) Y_{l_2}^{m_2}(\theta,\phi) Y_{l_3}^{m_3}(\theta,\phi) \\ &\qquad = \sqrt{\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi}} C^{l_3 0}_{l_1 0\, l_2 0}\, C^{l_3 m_3}_{l_1 m_1\, l_2 m_2} \ . \end{aligned} \tag{D.41}$$

D.5.6 Bipolar spherical harmonics

For this section, we are going to use irreductible tensors presented in Sec. D.8. In some applications one has to deal with functions which depend on two vector directions. Thus, bipolar spherical harmonics are given by irreducible tensor product of the spherical harmonics with different arguments

$$\Big[Y_{l_1}(\theta_1,\phi_1)\otimes Y_{l_2}(\theta_2,\phi_2)\Big]_{l_3 m_3} = \sum_{m_1 m_2} C^{l_3 m_3}_{l_1 m_1 l_2 m_2} Y_{l_1}^{m_1}(\theta_1,\phi_1) Y_{l_2}^{m_2}(\theta_2,\phi_2) \ . \tag{D.42}$$

The orthogonality and normalization relation for these harmonics is given by

$$\begin{aligned} &\int\int\int\int d\theta_1 d\theta_2 d\phi_1 d\phi_2 \Big[Y_{l_1}(\theta_1,\phi_1)\otimes Y_{l_2}(\theta_2,\phi_2)\Big]_{l_3 m_3} \Big[Y_{l_1'}(\theta_1,\phi_1)\otimes Y_{l_2'}(\theta_2,\phi_2)\Big]^*_{l_3' m_3'} \\ &\qquad = \delta_{l_1 l_1'}\delta_{l_2 l_2'}\delta_{l_3 l_3'}\delta_{m_3 m_3'} \ . \end{aligned} \tag{D.43}$$

The completeness condition has the form

$$\sum_{l_1 l_2 l_3 m_3} \Big[Y_{l_1}(\theta_1,\phi_1) \otimes Y_{l_2}(\theta_2,\phi_2) \Big]_{l_3 m_3} \Big[Y_{l_1'}(\theta_1',\phi_1') \otimes Y_{l_2}(\theta_2',\phi_2') \Big]^*_{l_3 m_3} \tag{D.44}$$
$$= \delta(\cos\theta_1 - \cos\theta_1')\delta(\phi_1 - \phi_1')\delta(\cos\theta_2 - \cos\theta_2')\delta(\phi_2 - \phi_2') \ .$$

For the important special case $L = 0$ a bipolar harmonic is reduced to a scalar product of the spherical harmonics (Eq. D.96)

$$\Big[Y_{l_1}(\theta_1,\phi_1) \otimes Y_{l_2}(\theta_2,\phi_2) \Big]_{00} = \frac{(-1)^{l_1}}{\sqrt{2l_1+1}} \Big(Y_{l_1}(\theta_1,\phi_1) \cdot Y_{l_2}(\theta_2,\phi_2) \Big) \delta_{l_1 l_2} \ , \tag{D.45}$$

where in accordance with Sec. D.8.6 the scalar product is defined through

$$\Big(Y_l(\theta_1,\phi_1) \cdot Y_l(\theta_2,\phi_2) \Big) = \sum_m Y_l^{m*}(\theta_1,\phi_1) Y_l^m(\theta_2,\phi_2) \ . \tag{D.46}$$

The expansions of the scalar product in terms of the Legendre polynomials is

$$\Big(Y_l(\theta_1,\phi_1) \cdot Y_l(\theta_2,\phi_2) \Big) = \frac{2l+1}{4\pi} P_l(\cos\omega_{12}) \ , \tag{D.47}$$

where ω_{12} is the angle between $\vec{r}_1$, of polar coordinates (r_1,θ_1,ϕ_1), and $\vec{r}_2$, of polar coordinates (r_2,θ_2,ϕ_2).

D.6 Rotation

D.6.1 Definition

An arbitrary rotation of a coordinate system about the origin is completely specified by three real parameters. The most useful description of rotation is that in terms of the Euler angles α,β,γ. Any rotation of the coordinate system may be performed by three successive rotations about the coordinate axes (Fig. D.1) (i) rotation about the z-axis by an angle α $(0 \le \alpha < 2\pi)$, (ii) rotation about the new v-axis by an angle β $(0 \le \beta \le \pi)$ and (iii) rotation about the new z'-axis by an angle γ $(0 \le \gamma < 2\pi)$.
The relative orientations of initial and final coordinate axes are shown in Fig. D.2. In spherical coordinates a vector $\vec{v}$ is determine by the norm v and the polar angles θ,ϕ. The norm of a vector $\vec{v}$ is invariant under rotations, but the polar angles θ,ϕ, which determine the vector direction, change. The relations between angles θ,ϕ and θ',ϕ', which specify vector directions in the initial and final coordinate systems, are given by

$$\cos\theta' = \cos\theta\cos\beta + \sin\theta\sin\beta\cos(\phi-\alpha) \ , \tag{D.48a}$$
$$\cot(\phi'+\gamma) = \cot(\phi-\alpha)\cos\beta - \frac{\cot\theta\sin\beta}{\sin(\phi-\alpha)} \ , \tag{D.48b}$$

where α,β,γ are the Euler angles.

D.6.2 Rotation operator

Under the rotation of a coordinate system, quantum-mechanical quantities are transformed by the rotation operator $\hat{D}(\alpha,\beta,\gamma)$. The state $|\psi'\rangle$ and the operator $\hat{O}'$ in the rotated coordinate system are related to the state $|\psi\rangle$ and the operator $\hat{O}$ in the initial coordinate system by

$$|\psi'\rangle = \hat{D}(\alpha,\beta,\gamma)|\psi\rangle \ , \qquad \hat{O}' = \hat{D}(\alpha,\beta,\gamma)\,\hat{O}\,\Big[\hat{D}(\alpha,\beta,\gamma)\Big]^{-1} \ . \tag{D.49}$$

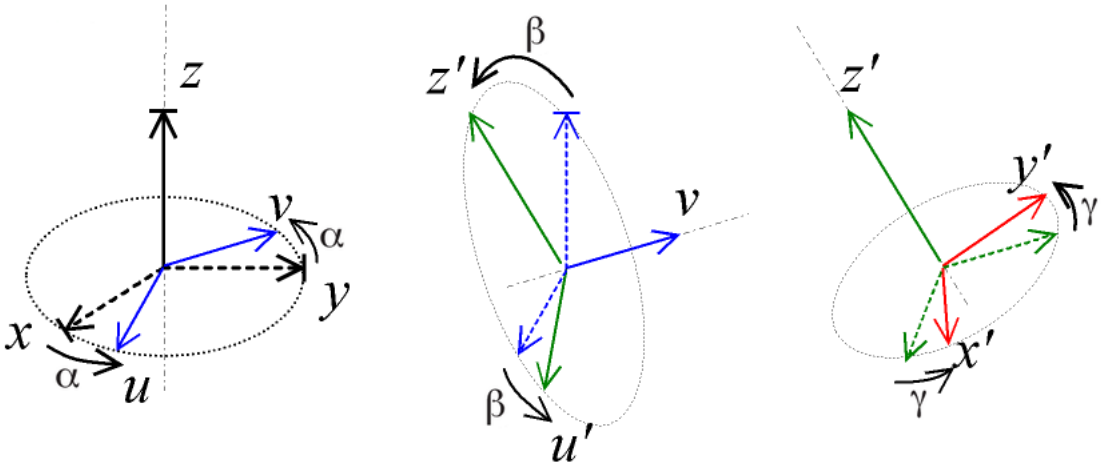

Figure D.1: Succession of rotation of a coordinate system.

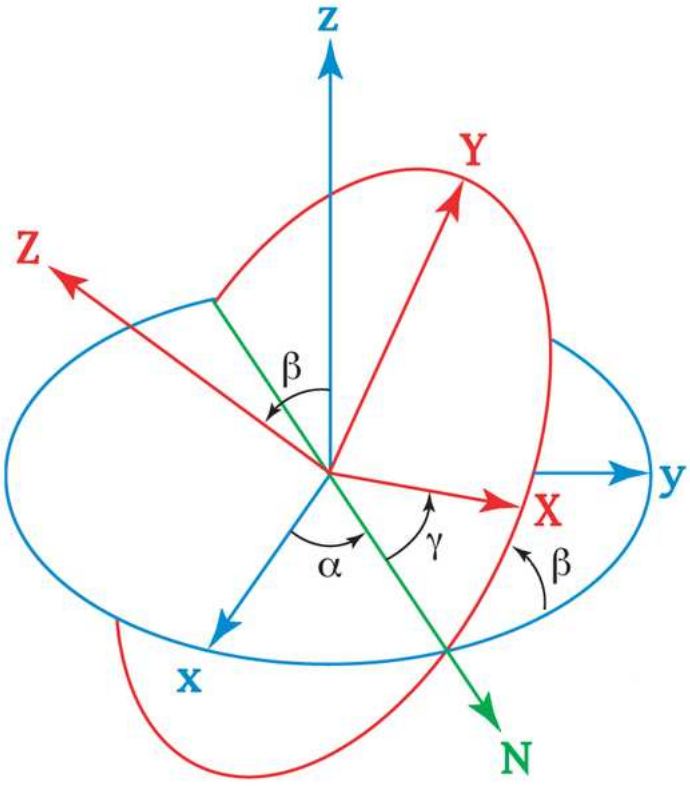

Figure D.2: Euler angles α, β, γ.

The rotation operator $\hat{D}(\alpha,\beta,\gamma)$ may be written as

$$\hat{D}(\alpha,\beta,\gamma) = e^{-i\gamma\hat{J}_{z'}}\, e^{-i\beta\hat{J}_v}\, e^{-i\alpha\hat{J}_z} \ , \tag{D.50}$$

where $\hat{J}_i$ is the projection of the total angular momentum operator on the i-axis. The rotation operator is a unitary operator and thus

$$\hat{D}^\dagger(\alpha,\beta,\gamma) = \left[\hat{D}(\alpha,\beta,\gamma)\right]^{-1} \ . \tag{D.51}$$

D.6.3 Addition of rotations

Considering two successive rotations of the coordinate system, the first with Euler angles $(\alpha_1,\beta_1,\gamma_1)$ and the second with Euler angles $(\alpha_2,\beta_2,\gamma_2)$, the resulting rotation is described by Euler angles (α,β,γ). One can write the operator of the resulting rotation as

$$\hat{D}(\alpha,\beta,\gamma) \equiv \hat{D}(\alpha_1,\beta_1,\gamma_1)\hat{D}(\alpha_2,\beta_2,\gamma_2) \ . \tag{D.52}$$

where (α,β,γ) are expressed in terms of $(\alpha_1,\beta_1,\gamma_1)$ and $(\alpha_2,\beta_2,\gamma_2)$ through

$$\cot(\alpha-\alpha_1) = \cos(\beta_1)\cot(\alpha_2+\gamma_1) + \cot(\beta_2)\frac{\sin(\beta_1)}{\sin(\alpha_2+\gamma_1)} \ , \tag{D.53a}$$

$$\cos(\beta) = \cos(\beta_2)\cos(\beta_1) - \sin(\beta_2)\sin(\beta_1)\cos(\alpha_2+\gamma_1) \ , \tag{D.53b}$$

$$\cot(\gamma-\gamma_2) = \cos(\beta_2)\cot(\alpha_2+\gamma_1) + \cot(\beta_1)\frac{\sin(\beta_2)}{\sin(\alpha_2+\gamma_1)} \ . \tag{D.53c}$$

D.7 Wigner D-functions

D.7.1 Definition

The Wigner D-functions $D^j_{mm'}(\alpha,\beta,\gamma)$ are defined as the matrix elements of the rotation operator $\hat{D}(\alpha,\beta,\gamma)$ in the jm-representation

$$\langle jm|\hat{D}(\alpha,\beta,\gamma)|j'm'\rangle \equiv \delta_{jj'}D^j_{mm'}(\alpha,\beta,\gamma) \ . \tag{D.54}$$

From this definition, one can express the rotation of a ket $|jm\rangle$ as

$$\begin{aligned}\hat{D}(\alpha,\beta,\gamma)|jm\rangle &= \sum_{j'm'}|j'm'\rangle\langle j'm'|\hat{D}(\alpha,\beta,\gamma)|jm\rangle \\ &= \sum_{m'}|jm'\rangle D^j_{m'm}(\alpha,\beta,\gamma) \ ,\end{aligned} \tag{D.55}$$

and of a wavefunction in spherical coordinate $\langle\theta\phi|jm\rangle = Y^m_j(\theta,\phi)$

$$\langle\theta\phi|\hat{D}(\alpha,\beta,\gamma)|jm\rangle = \sum_{m'} D^j_{m'm}(\alpha,\beta,\gamma)\,\langle\theta\phi|jm'\rangle \ , \tag{D.56a}$$

$$\langle\theta'\phi'|jm\rangle = Y^m_j(\theta',\phi') = \sum_{m'} D^j_{m'm}(\alpha,\beta,\gamma)\,Y^{m'}_j(\theta,\phi) \ . \tag{D.56b}$$

D.7.2 Unitary condition

The unitary condition for the Wigner D-functions may be written as

$$\sum_{m=-j}^{j} D^j_{mm'}(\alpha,\beta,\gamma)D^{j*}_{mm''}(\alpha,\beta,\gamma) = \delta_{m'm''} \ , \tag{D.57a}$$

$$\sum_{m=-j}^{j} D^{j*}_{m''m}(\alpha,\beta,\gamma)D^j_{m'm}(\alpha,\beta,\gamma) = \delta_{m''m'} \ . \tag{D.57b}$$

D.7.3 Orthogonality condition

The D-functions with different j are mutually orthogonal with respect to integration over the volume of the 3-dimensional rotation group (if j_1 and j_2 are both either integer or half-integer)

$$\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin\beta \int_0^{2\pi} d\gamma \, D^{j_2 *}_{m_2 m_2'}(\alpha,\beta,\gamma) D^{j_1}_{m_1 m_1'}(\alpha,\beta,\gamma) = \frac{8\pi^2}{2j_1+1} \delta_{j_1 j_2} \delta_{m_1 m_2} \delta_{m_1' m_2'} \ . \quad \text{(D.58)}$$

D.7.4 Symmetry properties

The matrix of the inverse rotation satisfies the equation

$$\left[D^{-1}(\alpha,\beta,\gamma)\right]^j_{mm'} = D^{j\dagger}_{mm'}(\alpha,\beta,\gamma) \quad \text{(D.59a)}$$

$$= D^{j*}_{m'm}(\alpha,\beta,\gamma) \quad \text{(D.59b)}$$

$$= D^{j}_{mm'}(-\gamma,-\beta,-\alpha) \quad \text{(D.59c)}$$

The D-functions fulfill the following symmetry properties

$$D^j_{mm'}(\alpha,\beta,\gamma) = (-1)^{m'-m} D^{j*}_{-m-m'}(\alpha,\beta,\gamma) \quad \text{(D.60a)}$$

$$= D^j_{-m-m'}(-\alpha,-\beta,-\gamma) \quad \text{(D.60b)}$$

$$= (-1)^{m'-m} D^j_{m'm}(\gamma,\beta,\alpha) \ , \quad \text{(D.60c)}$$

and several others [86].

D.7.5 Adjoint, cogredience and contragredience

The ket $|jm\rangle$, which fulfill Eqs. (D.1,D.4) transforms under rotation as in Eq. D.55 is thus said to transform cogrediently [159]. On the other hand, the bra $\langle jm|$, which fulfill the equations

$$\langle jm|\,\hat{J}_z = \langle jm|\,m\hbar \quad , \quad \langle jm|\hat{J}_\pm = \langle jm\mp 1|\sqrt{l(l+1)-m(m\mp 1)}\hbar \ , \quad \text{(D.61)}$$

transform under rotation, thanks to Eq. D.60, as

$$\begin{aligned} \langle jm|\hat{D}^\dagger(\alpha,\beta,\gamma) &= \sum_{m'} \langle jm'|D^{j\dagger}_{mm'}(\alpha,\beta,\gamma) \\ &= \sum_{m'} \langle jm'|D^{j*}_{m'm}(\alpha,\beta,\gamma) \\ &= \sum_{m'} \langle jm'|(-1)^{m'-m} D^j_{-m'-m}(\alpha,\beta,\gamma) \ . \end{aligned} \quad \text{(D.62)}$$

As a result, $\langle jm|$ transforms as $(-1)^m|j-m\rangle$ since

$$\begin{aligned} \hat{D}(\alpha,\beta,\gamma)(-1)^m|j-m\rangle &= \sum_{m'} (-1)^m D^j_{m'-m}(\alpha,\beta,\gamma)\,|jm'\rangle \\ &= \sum_{m'} (-1)^{m-m'} D^j_{-m'-m}(\alpha,\beta,\gamma)\,(-1)^{m'}\,|j-m'\rangle \ , \end{aligned} \quad \text{(D.63)}$$

i.e. $\langle jm|$ is said to transform contragrediently [159].

D.7.6 Specific values

The D-functions have the following boundary condition

$$D^j_{mm'}(0,0,0) = \delta_{mm'} \ , \tag{D.64}$$

whereas the phase convention corresponds to the condition

$$D^j_{mm'}(0,\pi,0) = (-1)^{j+m}\delta_{m-m'} \ . \tag{D.65}$$

An important particular value is given by

$$D^j_{00}(\alpha,\beta,\gamma) = P_l(\cos\beta) \ , \tag{D.66}$$

only valid for integer value of j.

D.7.7 Addition theorem

The addition theorem reads

$$\sum_{m''=-j}^{j} D^j_{mm''}(\alpha_1,\beta_1,\gamma_1)\, D^j_{m''m'}(\alpha_2,\beta_2,\gamma_2) \ = \ D^j_{mm'}(\alpha,\beta,\gamma) \ , \tag{D.67}$$

where (α,β,γ) are related to $(\alpha_1,\beta_1,\gamma_1)$ and $(\alpha_2,\beta_2,\gamma_2)$ through Eqs. (D.53a,D.53b,D.53c).

D.7.8 Clebsch-Gordan series

The product of two D-functions with the same arguments may be expanded in the following series

$$D^{j_1}_{m_1m'_1}(\alpha,\beta,\gamma)D^{j_2}_{m_2m'_2}(\alpha,\beta,\gamma) = \sum_j \sum_{mm'} C^{jm}_{j_1m_1j_2m_2} D^j_{mm'}(\alpha,\beta,\gamma)\, C^{jm'}_{j_1m'_1j_2m'_2} \tag{D.68}$$

Another interesting relation is

$$\sum_{n_1n_2} D^{j_1}_{m_1n_1}(\alpha,\beta,\gamma)D^{j_2}_{m_2n_2}(\alpha,\beta,\gamma)\, C^{jn}_{j_1n_1j_2n_2} = \sum_m C^{jm}_{j_1m_1j_2m_2} D^j_{mn}(\alpha,\beta,\gamma) \tag{D.69}$$

D.7.9 Relation with spherical harmonics

The D-funtions are related to spherical harmonics through

$$D^l_{m0}(\alpha,\beta,\gamma) \ = \ (-1)^m\sqrt{\frac{4\pi}{2l+1}}Y_l^{-m}(\beta,\alpha) = \sqrt{\frac{4\pi}{2l+1}}Y_l^{m*}(\beta,\alpha) \ , \tag{D.70a}$$

$$D^l_{0m}(\alpha,\beta,\gamma) \ = \ \sqrt{\frac{4\pi}{2l+1}}Y_l^{-m}(\beta,\gamma) = (-1)^m\sqrt{\frac{4\pi}{2l+1}}Y_l^{m*}(\beta,\gamma) \ . \tag{D.70b}$$

D.7.10 Integral of three or more Wigner matrices

First the integral of three Wigner matrices gives

$$\int d\Omega\ D^{j_3*}_{m_3n_3}(\Omega)D^{j_2}_{m_2n_2}(\Omega)D^{j_1}_{m_1n_1}(\Omega) \ = \ \frac{8\pi^2}{2j_3+1}C^{j_3m_3}_{j_1m_1j_2m_2}C^{j_3n_3}_{j_1n_1j_2n_2} \tag{D.71a}$$

$$\int d\Omega\ D^{j_3}_{m_3n_3}(\Omega)D^{j_2*}_{m_2n_2}(\Omega)D^{j_1*}_{m_1n_1}(\Omega) \ = \ \frac{8\pi^2}{2j_3+1}C^{j_3m_3}_{j_1m_1j_2m_2}C^{j_3n_3}_{j_1n_1j_2n_2} \tag{D.71b}$$

For more than three Wigner matrices one has to use first Eq. D.68 and thus,

$$\int d\Omega\; D^{j_4*}_{m_4n_4}(\Omega) D^{j_3}_{m_3n_3}(\Omega) D^{j_2}_{m_2n_2}(\Omega) D^{j_1}_{m_1n_1}(\Omega) \tag{D.72a}$$
$$= \frac{8\pi^2}{2j_3+1} \sum_{j_{12}m_{12}n_{12}} C^{j_4m_4}_{j_3m_3j_{12}m_{12}} C^{j_4n_4}_{j_3n_3j_{12}n_{12}} C^{j_{12}m_{12}}_{j_1m_1j_2m_2} C^{j_{12}n_{12}}_{j_1n_1j_2n_2}$$

$$\int d\Omega\; D^{j_4}_{m_4n_4}(\Omega) D^{j_3*}_{m_3n_3}(\Omega) D^{j_2*}_{m_2n_2}(\Omega) D^{j_1*}_{m_1n_1}(\Omega) \tag{D.72b}$$
$$= \frac{8\pi^2}{2j_3+1} \sum_{j_{12}m_{12}n_{12}} C^{j_4m_4}_{j_3m_3j_{12}m_{12}} C^{j_4n_4}_{j_3n_3j_{12}n_{12}} C^{j_{12}m_{12}}_{j_1m_1j_2m_2} C^{j_{12}n_{12}}_{j_1n_1j_2n_2}$$

D.8 Irreductible tensor and Wigner Eckart theorem

D.8.1 Definition

An irreductible spherical tensor $\mathcal{M}_j$ of rank j (with j integer or half-integer) is defined as a set of $2j+1$ functions (components) $\mathcal{M}_{jm}$ (where $m = -j, -j+1, \cdots, j-1, j$) which satisfy the following relation under rotation of the coordinate system

$$\mathcal{M}_{jm}(X') \equiv \hat{D}(\alpha,\beta,\gamma)\, \mathcal{M}_{jm}(X) \left[\hat{D}(\alpha,\beta,\gamma)\right]^{-1} = \sum_{m'} \mathcal{M}_{jm'}(X) D^{j}_{m'm}(\alpha,\beta,\gamma) \ . \tag{D.73}$$

where X and X' denote the sets of arguments of the tensor in the initial and final coordinate systems, respectively. This relation with $\hat{D}$ representing an infinitesimal rotation leads to commutation laws of the components of the angular momentum $\hat{J}$ with the components of $\mathcal{M}_j$. Let $\hat{D}(\alpha)$ be the infinitesimal rotation

$$\hat{D}(\alpha) = e^{-i\alpha\hat{J}_\lambda} \simeq 1 - i\alpha\hat{J}_\lambda \ , \tag{D.74}$$

where $\hat{J}_\lambda = \hat{J}_z$ or $\hat{J}_\lambda = \hat{J}_\pm$. From Eq. D.54, one has

$$D^{j}_{m'm}(\alpha) = \langle jm'|1 - i\alpha\hat{J}_\lambda|jm\rangle \ = \ \delta_{m'm} \ - \ i\alpha\langle jm'|\hat{J}_\lambda|jm\rangle \ . \tag{D.75}$$

Under such a rotation, Eq. D.73 becomes at first order in α

$$\begin{aligned} (1 - i\alpha\hat{J}_\lambda)\, \mathcal{M}_{jm}\, (1 + i\alpha\hat{J}_\lambda) \ &= \ \sum_{m'} \mathcal{M}_{jm'}\, D^{j}_{m'm}(\alpha) \\ \hat{J}_\lambda\, \mathcal{M}_{jm} \ - \ \mathcal{M}_{jm}\, \hat{J}_\lambda \ &= \ \sum_{m'} \mathcal{M}_{jm'}\, \langle jm'|\hat{J}_\lambda|jm\rangle \ . \end{aligned} \tag{D.76}$$

Using matrix elements of $\hat{J}_z$ and $\hat{J}_\pm$ (Sec. D.1), one obtains

$$\left[\hat{J}_z, \mathcal{M}_{jm}\right] \ = \ m\,\hbar\,\mathcal{M}_{jm} \ , \tag{D.77a}$$
$$\left[\hat{J}_\pm, \mathcal{M}_{jm}\right] \ = \ \sqrt{j(j+1) - m(m\pm1)}\,\hbar\,\mathcal{M}_{jm\pm1} \ , \tag{D.77b}$$

and consequently,

$$\left[\hat{J}^2, \mathcal{M}_{jm}\right] = j(j+1)\,\hbar^2\,\mathcal{M}_{jm} \ , \tag{D.78}$$

Such commutation rules can be taken as a definition of irreductible spherical tensors.

D.8.2 Adjoint and hermitian tensor operator

Given that for two operators A and B one has $(AB)^\dagger = B^\dagger A^\dagger$, one proves that

$$[A,B]^\dagger \;=\; [B^\dagger, A^\dagger] \;=\; -[A^\dagger, B^\dagger] \;. \tag{D.79}$$

Thus, the commutation laws of the components of $\hat{J}$ with the components of $\mathcal{M}_j^\dagger$ are

$$\Big[\hat{J}_z, \mathcal{M}^\dagger_{jm}\Big] \;=\; -\Big[\hat{J}_z, \mathcal{M}_{jm}\Big]^\dagger = -m\,\hbar\,\mathcal{M}^\dagger_{jm} \tag{D.80a}$$

$$\Big[\hat{J}_\pm, \mathcal{M}^\dagger_{jm}\Big] \;=\; -\Big[\hat{J}_\mp, \mathcal{M}_{jm}\Big]^\dagger = -\sqrt{j(j+1)-m(m\mp 1)}\,\hbar\,\mathcal{M}^\dagger_{jm\mp 1} \;. \tag{D.80b}$$

Thus $\mathcal{M}_j^\dagger$ transforms contragrediently (Sec. D.7.5). Defining the operator $\bar{\mathcal{M}}_{jm}$ as

$$\bar{\mathcal{M}}_{jm} \;\equiv\; (-1)^{p-m}\mathcal{M}^\dagger_{j-m} \;, \tag{D.81}$$

one can use Eqs. (D.80a,D.80b) to prove that the $2j+1$ components of $\bar{\mathcal{M}}_{jm}$ transform as a tensor operator of rank j through [1]

$$\Big[\hat{J}_z, \bar{\mathcal{M}}_{jm}\Big] \;=\; (-1)^{p-m}\Big[\hat{J}_z, \mathcal{M}^\dagger_{j-m}\Big] \;=\; (-1)^{p-m}\Big(-(-m)\hbar\mathcal{M}^\dagger_{j-m}\Big) \;=\; m\hbar\,\bar{\mathcal{M}}_{jm} \;, \tag{D.82}$$

and

$$\begin{aligned}
\Big[\hat{J}_\pm, \bar{\mathcal{M}}_{jm}\Big] \;&=\; (-1)^{p-m}\Big[\hat{J}_\pm, \mathcal{M}^\dagger_{j-m}\Big] \\
&=\; (-1)^{p-m}\Big(-\sqrt{j(j+1)+m(-m\mp 1)}\hbar\,\mathcal{M}^\dagger_{j-m\mp 1}\Big) \\
&=\; (-1)^{p-(m\pm 1)}\sqrt{j(j+1)-m(m\pm 1)}\hbar\,\mathcal{M}^\dagger_{j-(m\pm 1)} \\
&=\; \sqrt{j(j+1)-m(m\pm 1)}\,\hbar\,\bar{\mathcal{M}}_{jm\pm 1} \;,
\end{aligned} \tag{D.83}$$

using the fact that $(-1)^{\pm 1} = -1$. One interesting consequence is that only the $m = 0$ component of a spherical tensor operator can be hermitian. However, it is possible to extend the notion of hermitian operator to cover tensor operator by defining a "hermitian tensor operator" as one with the property

$$\mathcal{M}_{jm} \;=\; (-1)^{p-m}\mathcal{M}^\dagger_{j-m} \;. \tag{D.84}$$

The choice of phase p is arbitrary and we choose here $p = 0$ that is compatible with the Condon-Shortley phase convention for spherical harmonics.

D.8.3 Wigner-Eckart theorem

According to Wigner-Eckart theorem, the dependence of matrix elements of a spherical tensor operator on the orientation of coordinate axes, i.e. on quantum numbers m which determine the projections of angular momenta, is contained in a Clebsch-Gordan coefficient, i.e.

$$\langle j_2 m_2|\hat{\mathcal{M}}_{jm}|j_1 m_1\rangle \equiv C^{j_2 m_2}_{j_1 m_1 jm}\frac{\langle j_2||\hat{\mathcal{M}}_j||j_1\rangle}{\sqrt{2j_2+1}} \;, \tag{D.85}$$

where $\langle j_2||\hat{\mathcal{M}}_j||j_1\rangle$ is an invariant factor called a reduced matrix element. This theorem is a direct consequence of the definition of irreductible tensor operators.

1. p is an arbitrary integer or half integer depending on whether j is integral or half integral.

D.8.4 Transformation under rotation

The standard definition of an irreductible spherical tensor Eq. D.73 can be recovered using the fact that $\mathcal{M}_{jm}$ satisfies the Wigner-Eckart theorem (Eq. D.85). Let us start by writing

$$\langle X|\hat{D}(\alpha,\beta,\gamma)\,\mathcal{M}_{jm}\left[\hat{D}(\alpha,\beta,\gamma)\right]^{-1}|X\rangle = \langle X'|\mathcal{M}_{jm}|X'\rangle \equiv \mathcal{M}_{jm}(X')\ , \tag{D.86}$$

where $|X'\rangle = \left[\hat{D}(\alpha,\beta,\gamma)\right]^{-1}|X\rangle$ and by inserting four closure relations

$$\begin{aligned}\langle X|\hat{D}(\alpha,\beta,\gamma)\,\mathcal{M}_{jm}\left[\hat{D}(\alpha,\beta,\gamma)\right]^{-1}|X\rangle \;=\; &\sum_{\{j\},\{m\}}\langle X|j_1m_1\rangle\langle j_1m_1|\hat{D}(\alpha,\beta,\gamma)|j_2m_2\rangle \\ &\langle j_2m_2|\mathcal{M}_{jm}|j_3m_3\rangle\langle j_3m_3|\left[\hat{D}(\alpha,\beta,\gamma)\right]^{-1}|j_4m_4\rangle\langle j_4m_4|X\rangle\ ,\end{aligned} \tag{D.87}$$

where $\{j\} = j_1, j_2, j_3, j_4$ and $\{m\} = m_1, m_2, m_3, m_4$. Using Wigner Eckart theorem (Eq. D.85) and Eq. D.59

$$\begin{aligned}\mathcal{M}_{jm}(X') \;=\; &\sum_{j_1,j_3,\{m\}}\langle X|j_1m_1\rangle\, D^{j_1}_{m_1m_2}(\alpha,\beta,\gamma)\, C^{j_1m_2}_{j_3m_3jm} \\ &\frac{1}{\sqrt{2j_1+1}}\langle j_1||\mathcal{M}_j||j_3\rangle\, D^{j_3*}_{m_4m_3}(\alpha,\beta,\gamma)\langle j_3m_4|X\rangle\ ,\end{aligned} \tag{D.88}$$

and with Eqs. (D.14c,D.14d,D.60)

$$\begin{aligned}\mathcal{M}_{jm}(X') \;=\; &\sum_{j_1j_3}\sum_{\{m\}}\langle X|j_1m_1\rangle\, D^{j_1}_{m_1m_2}(\alpha,\beta,\gamma)\, C^{jm}_{j_3-m_3j_1m_2} \\ &(-1)^{m_4+j_1+j}\frac{1}{\sqrt{2j+1}}\langle j_2||\mathcal{M}_j||j_3\rangle\, D^{j_3}_{-m_4-m_3}(\alpha,\beta,\gamma)\langle j_3m_4|X\rangle\ .\end{aligned} \tag{D.89}$$

Using Eq. D.69, one has

$$\begin{aligned}\mathcal{M}_{jm}(X') \;=\; &\sum_{j_1j_3}\sum_{nm_1m_4}\langle X|j_1m_1\rangle\, C^{jn}_{j_3-m_4j_1m_1} \\ &D^{j}_{nm}(\alpha,\beta,\gamma)(-1)^{m_4+j_2+j}\frac{1}{\sqrt{2j+1}}\langle j_2||\mathcal{M}_j||j_3\rangle\,\langle j_3m_4|X\rangle\ .\end{aligned} \tag{D.90}$$

Using Eqs. (D.14c,D.14d) and Eq. D.85, one finally finds

$$\begin{aligned}\mathcal{M}_{jm}(X') \;&=\; \sum_{j_1j_3}\sum_{nm_1m_4}\langle X|j_1m_1\rangle\, D^{j}_{nm}(\alpha,\beta,\gamma)\langle j_1m_1|\mathcal{M}_{jn}|j_3m_4\rangle\,\langle j_3m_4|X\rangle \\ &=\; \sum_{n} D^{j}_{nm}(\alpha,\beta,\gamma)\,\langle X|\mathcal{M}_{jn}|X\rangle \\ &=\; \sum_{m'} D^{j}_{m'm}(\alpha,\beta,\gamma)\,\mathcal{M}_{jm'}(X)\ .\end{aligned} \tag{D.91}$$

D.8.5 Direct and irreductible tensor products

An irreductible tensor product $\mathcal{L}_j$ of two irreductible tensors $\mathcal{M}_{j_1}$ and $\mathcal{N}_{j_2}$ is defined as the tensor of rank j whose components $\mathcal{L}_{jm}$ can be expressed in terms of $\mathcal{M}_{j_1m_1}$ and $\mathcal{N}_{j_2m_2}$ according to

$$\mathcal{L}_{jm} = \sum_{m_1m_2} C^{jm}_{j_1m_1j_2m_2}\mathcal{M}_{j_1m_1}\mathcal{N}_{j_2m_2}\ . \tag{D.92}$$

The irreductible tensor product is usually denoted as

$$\mathcal{L}_j \equiv \Big[\mathcal{M}_{j_1} \otimes \mathcal{N}_{j_2}\Big]_j \ . \tag{D.93}$$

The direct product of two irreductible tensors $\mathcal{M}_{j_1}$ and $\mathcal{N}_{j_2}$ can be represented as a sum of irreducible tensors $\mathcal{L}_{jm}$

$$\mathcal{M}_{j_1 m_1}\mathcal{N}_{j_2 m_2} = \sum_j C^{jm}_{j_1 m_1 j_2 m_2}\mathcal{L}_{jm} \ . \tag{D.94}$$

D.8.6 Scalar product

The scalar product of two irreductible tensors $\mathcal{M}_j$ and $\mathcal{N}_j$ of the same rank is defined as

$$\Big(\mathcal{M}_j \cdot \mathcal{N}_j\Big) \equiv \sum_m (-1)^{-m}\mathcal{M}_{jm}\cdot\mathcal{N}_{j-m} = \sum_m \mathcal{M}_{jm}\cdot\mathcal{N}^\dagger_{jm} \ , \tag{D.95}$$

and differ from the irreductible tensor product of rank zero only by a numerical factor

$$\Big[\mathcal{M}_j \otimes \mathcal{N}_j\Big]_{00} = \sum_{m_1 m_2} C^{00}_{jm_1 jm_2}\mathcal{M}_{jm_1}\cdot\mathcal{N}_{jm_2} = \frac{1}{\sqrt{2j+1}}\sum_m (-1)^{j-m}\mathcal{M}_{jm}\cdot\mathcal{N}_{j-m} \ . \tag{D.96}$$

D.9 Center of mass and relative coordinates

The present section deals with the change of variables from vectors $\vec{r}_1$ and $\vec{r}_2$ to center of mass $\vec{R}$ and relative $\vec{r}$, position vectors through

$$\vec{R} = \frac{\vec{r}_1 + \vec{r}_2}{2} \ , \tag{D.97a}$$

$$\vec{r} = \vec{r}_1 - \vec{r}_2 \ , \tag{D.97b}$$

$$\vec{r}_1 = \vec{R} + \frac{\vec{r}}{2} \ , \tag{D.97c}$$

$$\vec{r}_2 = \vec{R} - \frac{\vec{r}}{2} \ . \tag{D.97d}$$

Polar coordinates of vectors $\vec{R}(R,\Theta,\Phi)$ and $\vec{r}(r,\theta,\phi)$ are related to those of vectors $\vec{r}_1(r_1,\theta_1,\phi_1)$ and $\vec{r}_2(r_2,\theta_2,\phi_2)$ by

$$R = \frac{r_1^2 + r_2^2 + 2r_1 r_2\cos\omega_{12}}{4} \ , \tag{D.98a}$$

$$\cos\Theta = \frac{r_1\cos\theta_1 + r_2\cos\theta_2}{\sqrt{r_1^2 + r_2^2 + 2r_1 r_2\cos\omega_{12}}} \ , \tag{D.98b}$$

$$\tan\Phi = \frac{r_1\sin\theta_1\sin\phi_1 + r_2\sin\theta_2\sin\phi_2}{r_1\sin\theta_1\cos\phi_1 + r_2\sin\theta_2\cos\phi_2} \ , \tag{D.98c}$$

$$r = r_1^2 + r_2^2 - 2r_1 r_2\cos\omega_{12} \ , \tag{D.98d}$$

$$\cos\theta = \frac{r_1\cos\theta_1 - r_2\cos\theta_2}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2\cos\omega_{12}}} \ , \tag{D.98e}$$

$$\tan\phi = \frac{r_1\sin\theta_1\sin\phi_1 - r_2\sin\theta_2\sin\phi_2}{r_1\sin\theta_1\cos\phi_1 - r_2\sin\theta_2\cos\phi_2} \ , \tag{D.98f}$$

where ω_{12} is the angle between $\vec{r}_1$ and $\vec{r}_2$, i.e.

$$\cos\omega_{12} = \cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\cos(\phi_1 - \phi_2) \ . \tag{D.99}$$

Appendix E

Breaking and restoring symmetries

Abstract: The angular context of the one- and two-body density matrices is pinned down. These results are used to assess Eq. 2.27 and the angular momentum content of a general tensor operator density.

Contents

E.1 Density matrices

E.1.1 Introduction

E.1.1.1 Problematic

The aim of the present section is to characterize the angular-momentum [1] content of the matrix element of the one-body density matrix $\hat{\rho}^{[1]}(\vec{r},\vec{r}')$ and two-body density matrix $\hat{\rho}^{[2]}(\vec{r},\vec{r}')$ operators between states $\langle LM|$ and $|L'M'\rangle$. Taking the local density $\rho_{LM}(\vec{r})$ of a state with good angular momentum as an example and the fact that it can be expanded under the form

$$\rho_{LM}(\vec{r}) \equiv \langle LM|\hat{\rho}^{[1]}(\vec{r},\vec{r}')|LM\rangle = \sum_{lm} f_l^{LM}(r) Y_l^m(\hat{\vec{r}}) \ , \tag{E.1}$$

the aim is typically to characterize for which values of l the form factor f_l is non zero.

E.1.1.2 One-body density matrix operator

The one-body density matrix operator is defined as [2]

$$\hat{\rho}^{[1]}(\vec{r}_1,\vec{r}_2) \equiv a^\dagger(\vec{r}_2)a(\vec{r}_1) \ , \tag{E.2}$$

where $a^\dagger(\vec{r})$ ($a(\vec{r})$) creates (annihilates) a particle at position $\vec{r}$. One can perform a change of basis through

$$a^\dagger(\vec{r}) = \sum_i \varphi_i^*(\vec{r}) a_i^\dagger \quad , \quad a(\vec{r}) = \sum_i \varphi_i(\vec{r}) a_i \ , \tag{E.3}$$

with $i = nlm$, i.e. $\{\varphi_i\}$ is a spherical basis. Thus, Eq. E.2 becomes

$$\hat{\rho}^{[1]}(\vec{r}_1,\vec{r}_2) = \sum_{n_1l_1m_1} \sum_{n_2l_2m_2} \varphi^*_{n_1l_1m_1}(\vec{r}_2)\varphi_{n_2l_2m_2}(\vec{r}_1)\, a^\dagger_{n_1l_1m_1} a_{n_2l_2m_2} \ . \tag{E.4}$$

E.1.1.3 Two-body density matrix operator

The two-body density matrix operator is defined as [3].

$$\hat{\rho}^{[2]}(\vec{r}_1,\vec{r}_2) \equiv a^\dagger(\vec{r}_2)a^\dagger(\vec{r}_1)a(\vec{r}_1)a(\vec{r}_2) \ , \tag{E.5}$$

and read in a spherical basis as

$$\begin{aligned}\hat{\rho}^{[2]}(\vec{r}_1,\vec{r}_2) = \sum_{\{n,l,m\}} & \varphi^*_{n_1l_1m_1}(\vec{r}_2)\, \varphi^*_{n_2l_2m_2}(\vec{r}_1)\, \varphi_{n_3l_3m_3}(\vec{r}_1)\, \varphi_{n_4l_4m_4}(\vec{r}_2) \\ & a^\dagger_{n_1l_1m_1} a^\dagger_{n_2l_2m_2} a_{n_3l_3m_3} a_{n_4l_4m_4} \ ,\end{aligned} \tag{E.6}$$

where $\{n,l,m\} = n_1,n_2,n_3,n_4;l_1,l_2,l_3,l_4;m_1,m_2,m_3,m_4$.

1. We omit the spin at this point and only deal with the orbital angular momentum.
2. In addition to omitting spin, we also omit the isospin quantum number for simplicity.
3. We take into account only the diagonal part of the two-body density matrix, i.e. the two nucleons are created at the same point that they are annihilated. This comes from the fact that we will use a local two-body central interaction for which $\langle\vec{r}_1\vec{r}_2|V|\vec{r}_3\vec{r}_4\rangle = v(|\vec{r}_1-\vec{r}_2|)\delta(\vec{r}_1-\vec{r}_3)\delta(\vec{r}_2-\vec{r}_4)$.

E.1.1.4 Notations

We define shorthand notations

$$\begin{aligned}
\{nlm\} &= n_1, n_2, n_3, n_4, l_1, l_2, l_3, l_4, m_1, m_2, m_3, m_4 \ , && \text{(E.7a)}\\
\Pi_{ab\cdots z} &= \sqrt{(2a+1)\,(2b+1)\,\cdots\,(2z+1)} \ , && \text{(E.7b)}\\
\{l_{1-2}\} &= l_2, l_1 \ , && \text{(E.7c)}\\
\{l_{1-2Rr}\} &= l_{2R}, l_{2r}, l_{1R}, l_{1r} \ , && \text{(E.7d)}\\
\{l_{1-4Rr}\} &= l_{4R}, l_{4r}, l_{3R}, l_{3r}, l_{2R}, l_{2r}, l_{1R}, l_{1r} \ , && \text{(E.7e)}\\
\{m_{1-2Rr}\} &= m_{2R}, m_{2r}, m_{1R}, m_{1r} \ , && \text{(E.7f)}\\
\{m_{1-4Rr}\} &= m_{4R}, m_{4r}, m_{3R}, m_{3r}, m_{2R}, m_{2r}, m_{1R}, m_{1r} \ , && \text{(E.7g)}\\
\{lm_{1-4Rr}\} &= \{l_{1-4Rr}\}, \{m_{1-4Rr}\} \ , && \text{(E.7h)}\\
\{L_{12,34Rr}\} &= L_{12R}, L_{12r}, L_{34R}, L_{34r} \ , && \text{(E.7i)}\\
\{M_{12,34Rr}\} &= M_{12R}, M_{12r}, M_{34R}, M_{34r} \ , && \text{(E.7j)}\\
\{LM_{12,34Rr}\} &= \{L_{12,34Rr}\}, \{M_{12,34Rr}\} \ , && \text{(E.7k)}\\
A^{\{l_{1-4Rr}\}}_{\{l_{1-4}\}}(R,r) &= A^{l_{1R}l_{1r}}_{l_1}(R,r) A^{l_{2R}l_{2r}}_{l_2}(R,r) A^{l_{3R}l_{3r}}_{l_3}(R,r) A^{l_{4R}l_{4r}}_{l_4}(R,r) \ , && \text{(E.7l)}\\
C^{\{L_{12,34Rr}\}0}_{\{l_{1-4Rr}\}0} &= C^{L_{12R}0}_{l_{1R}0l_{2R}0} C^{L_{12r}0}_{l_{1r}0l_{2r}0} C^{L_{34R}0}_{l_{3R}0l_{4R}0} C^{L_{34r}0}_{l_{3r}0l_{4r}0} \ , && \text{(E.7m)}
\end{aligned}$$

that will be useful in the following.

E.1.2 Wave-functions

E.1.2.1 Expansion

The expansion [160–162]

$$\phi_{nlm}(\alpha_1\vec{r}_1 + \alpha_2\vec{r}_2) = \sum_{l_1 l_2} A^{l_1 l_2}_{l}(r_1, r_2) \sum_{m_1 m_2} C^{lm}_{l_1 m_1 l_2 m_2} Y^{m_1}_{l_1}(\theta_1, \phi_1) Y^{m_2}_{l_2}(\theta_2, \phi_2) \ , \qquad \text{(E.8)}$$

will be used to separate center of mass and relative coordinates in a wave-function carrying good (l, m) quantum numbers. In Eq. E.8, one has

$$A^{l_1 l_2}_{l}(r_1, r_2) = \frac{\Pi_{l_1 l_2}}{\sqrt{4\pi}\Pi_l} 8(-i)^{l_1 - l_2 - l} C^{l0}_{l_1 0 l_2 0} \int k^2 dk j_{l_1}(\alpha k r_1) j_{l_2}(\beta k r_2) \int r^2 dr j_l(kr) \phi_l(r) \ , \qquad \text{(E.9)}$$

where $j_l(x)$ are spherical Bessel functions of the first kind.

E.1.2.2 Separation of center of mass and relative coordinates

Using center of mass and relative coordinates Eq. E.8 can be used to expand $\varphi_{n_1 l_1 m_1}(\vec{r}_2)$ as

$$\varphi_{n_1 l_1 m_1}(\vec{R} - \frac{\vec{r}}{2}) = \sum_{l_{1R} l_{1r}} A^{l_{1R} l_{1r}}_{l_1}(R, r) \sum_{m_{1R} m_{1r}} C^{l_1 m_1}_{l_{1R} m_{1R} l_{1r} m_{1r}} Y^{m_{1R}}_{l_{1R}}(\hat{R}) Y^{m_{1r}}_{l_{1r}}(-\hat{r}) \ , \qquad \text{(E.10)}$$

where $\hat{R} = (\Theta, \Phi)$, $-\hat{r} = (\pi - \theta, \pi + \phi)$ and

$$A^{l_{1R} l_{1r}}_{l_1}(R, r) = \frac{\Pi_{l_{1R} l_{1r}}}{\sqrt{4\pi}\Pi_{l_1}} 8(-i)^{l_{1R} - l_{1r} - l_1} C^{l_1 0}_{l_{1R} 0 l_{1r} 0} \int k^2 dk j_{l_{1R}}(kR) j_{l_{1r}}(\frac{kr}{2}) \int s^2 dr j_{l_1}(ks) \varphi_l(s) \ . \qquad \text{(E.11)}$$

Angles $\theta' = \pi - \theta$ and $\phi' = \pi + \phi$ are those of vector $-\vec{r}$ in spherical coordinates, whenever θ and ϕ are those of $\vec{r}$. The same expansion applied to $\varphi_{n_2 l_2 m_2}(\vec{r}_1)$ gives

$$\varphi_{n_2 l_2 m_2}(\vec{R}+\frac{\vec{r}}{2}) = \sum_{l_{2R} l_{2r}} A_{l_2}^{l_{2R} l_{2r}}(R,r) \sum_{m_{2R} m_{2r}} C^{l_2 m_2}_{l_{2R} m_{2R} l_{2r} m_{2r}} Y_{l_{2R}}^{m_{2R}}(\hat{R}) Y_{l_{2r}}^{m_{2r}}(\hat{r}) \ . \tag{E.12}$$

It is useful to note that

$$A_l^{l_R l_r *}(R,r) = (-1)^{l_R+l_r+l} A_l^{l_R l_r}(R,r) \ . \tag{E.13}$$

E.1.2.3 Product of two wave functions

Below, we will need to consider the product of two wave-functions for various choices of coordinates. Using Eqs. (E.10,E.12), Eq. D.30 to evaluate the complex conjugate of spherical harmonics, Eq. D.38 to evaluate the spherical harmonic at $-\hat{r}$, Eq. D.39 to couple two spherical harmonics with the same argument and Eq. D.14c, one finds

$$\begin{aligned}
\varphi^*_{n_1 l_1 m_1}(\vec{r}_1)\varphi_{n_2 l_2 m_2}(\vec{r}_1) &= (-1)^{-m_1} \sum_{\{l_{1-2Rr}\}\{m_{1-2Rr}\}} A_{l_1}^{l_{1R} l_{1r}}(R,r) A_{l_2}^{l_{2R} l_{2r}}(R,r) \sum_{L_R L_r M_R M_r} \frac{\Pi_{l_{1R} l_{1r} l_{2R} l_{2r}}}{4\pi \Pi_{L_R L_r}} \\
&\quad C^{L_R 0}_{l_{1R} 0 l_{2R} 0} C^{L_r 0}_{l_{1r} 0 l_{2r} 0} C^{l_1 - m_1}_{l_{1R} - m_{1R} l_{1r} - m_{1r}} C^{l_2 m_2}_{l_{2R} m_{2R} l_{2r} m_{2r}} \\
&\quad C^{L_R M_R}_{l_{1R} - m_{1R} l_{2R} m_{2R}} C^{L_r M_r}_{l_{1r} - m_{1r} l_{2r} m_{2r}} Y_{L_R}^{M_R}(\hat{R}) Y_{L_r}^{M_r}(\hat{r}) \ . \qquad \text{(E.14a)} \\
\varphi^*_{n_1 l_1 m_1}(\vec{r}_2)\varphi_{n_2 l_2 m_2}(\vec{r}_2) &= (-1)^{-m_1} \sum_{\{l_{1-2Rr}\}\{m_{1-2Rr}\}} A_{l_1}^{l_{1R} l_{1r}}(R,r) A_{l_2}^{l_{2R} l_{2r}}(R,r) \sum_{L_R L_r M_R M_r} \frac{\Pi_{l_{1R} l_{1r} l_{2R} l_{2r}}}{4\pi \Pi_{L_R L_r}} \\
&\quad C^{L_R 0}_{l_{1R} 0 l_{2R} 0} C^{L_r 0}_{l_{1r} 0 l_{2r} 0} (-1)^{l_{1r}+l_{2r}} C^{l_1 - m_1}_{l_{1R} - m_{1R} l_{1r} - m_{1r}} C^{l_2 m_2}_{l_{2R} m_{2R} l_{2r} m_{2r}} \\
&\quad C^{L_R M_R}_{l_{1R} - m_{1R} l_{2R} m_{2R}} C^{L_r M_r}_{l_{1r} - m_{1r} l_{2r} m_{2r}} Y_{L_R}^{M_R}(\hat{R}) Y_{L_r}^{M_r}(\hat{r}) \ . \qquad \text{(E.14b)} \\
\varphi^*_{n_1 l_1 m_1}(\vec{r}_1)\varphi_{n_2 l_2 m_2}(\vec{r}_2) &= (-1)^{-m_1} \sum_{\{l_{1-2Rr}\}\{m_{1-2Rr}\}} A_{l_1}^{l_{1R} l_{1r}}(R,r) A_{l_2}^{l_{2R} l_{2r}}(R,r) \sum_{L_R L_r M_R M_r} \frac{\Pi_{l_{1R} l_{1r} l_{2R} l_{2r}}}{4\pi \Pi_{L_R L_r}} \\
&\quad C^{L_R 0}_{l_{1R} 0 l_{2R} 0} C^{L_r 0}_{l_{1r} 0 l_{2r} 0} (-1)^{l_{2r}} C^{l_1 - m_1}_{l_{1R} - m_{1R} l_{1r} - m_{1r}} C^{l_2 m_2}_{l_{2R} m_{2R} l_{2r} m_{2r}} \\
&\quad C^{L_R M_R}_{l_{1R} - m_{1R} l_{2R} m_{2R}} C^{L_r M_r}_{l_{1r} - m_{1r} l_{2r} m_{2r}} Y_{L_R}^{M_R}(\hat{R}) Y_{L_r}^{M_r}(\hat{r}) \ . \qquad \text{(E.14c)} \\
\varphi^*_{n_1 l_1 m_1}(\vec{r}_2)\varphi_{n_2 l_2 m_2}(\vec{r}_1) &= (-1)^{-m_1} \sum_{\{l_{1-2Rr}\}\{m_{1-2Rr}\}} A_{l_1}^{l_{1R} l_{1r}}(R,r) A_{l_2}^{l_{2R} l_{2r}}(R,r) \sum_{L_R L_r M_R M_r} \frac{\Pi_{l_{1R} l_{1r} l_{2R} l_{2r}}}{4\pi \Pi_{L_R L_r}} \\
&\quad C^{L_R 0}_{l_{1R} 0 l_{2R} 0} C^{L_r 0}_{l_{1r} 0 l_{2r} 0} (-1)^{l_{1r}} C^{l_1 - m_1}_{l_{1R} - m_{1R} l_{1r} - m_{1r}} C^{l_2 m_2}_{l_{2R} m_{2R} l_{2r} m_{2r}} \\
&\quad C^{L_R M_R}_{l_{1R} - m_{1R} l_{2R} m_{2R}} C^{L_r M_r}_{l_{1r} - m_{1r} l_{2r} m_{2r}} Y_{L_R}^{M_R}(\hat{R}) Y_{L_r}^{M_r}(\hat{r}) \ . \qquad \text{(E.14d)}
\end{aligned}$$

E.1.2.4 Product of four wave functions

We are here interested in the product $\varphi^*_{n_1 l_1 m_1}(\vec{r}_2)\, \varphi^*_{n_2 l_2 m_2}(\vec{r}_1)\, \varphi_{n_3 l_3 m_3}(\vec{r}_1)\, \varphi_{n_4 l_4 m_4}(\vec{r}_2)$, which is noted φ^4 for convenience. Using Eqs. (E.10,E.12), one finds

$$\begin{aligned}
\varphi^4 &= (-1)^{-m_1-m_2} \sum_{\{l_{1-4Rr}\}\{m_{1-4Rr}\}} A_{l_1}^{l_{1R} l_{1r}}(R,r) A_{l_2}^{l_{2R} l_{2r}}(R,r) A_{l_3}^{l_{3R} l_{3r}}(R,r) A_{l_4}^{l_{4R} l_{4r}}(R,r) \\
&\quad (-1)^{l_{1r}} C^{l_1 - m_1}_{l_{1R} - m_{1R} l_{1r} - m_{1r}} C^{l_2 - m_2}_{l_{2R} - m_{2R} l_{2r} - m_{2r}} Y_{l_{1R}}^{-m_{1R}}(\hat{R}) Y_{l_{1r}}^{-m_{1r}}(\hat{r}) Y_{l_{2R}}^{-m_{2R}}(\hat{R}) Y_{l_{2r}}^{-m_{2r}}(\hat{r}) \\
&\quad (-1)^{l_{4r}} C^{l_3 m_3}_{l_{3R} m_{3R} l_{3r} m_{3r}} C^{l_4 m_4}_{l_{4R} m_{4R} l_{4r} m_{4r}} Y_{l_{3R}}^{m_{3R}}(\hat{R}) Y_{l_{3r}}^{m_{3r}}(\hat{r}) Y_{l_{4R}}^{m_{4R}}(\hat{R}) Y_{l_{4r}}^{m_{4r}}(\hat{r}) \ , \qquad \text{(E.15)}
\end{aligned}$$

where properties of Clebsch-Gordan coefficients have been used to obtain $-m_2 = m_{2R} + m_{2r}$ and $-m_1 = m_{1R} + m_{1r}$, as well as to change the sign of the two first Clebsch-Gordan coefficients. Note

that the factor $(-1)^{l_{1R}+l_{1r}+l_1+l_{2R}+l_{2r}+l_2}$ coming from the sign change in the two first Clebsch-Gordan coefficients, cancel with the factor coming from the evaluation of $A_l^{l_R l_r *}(R,r)$. Using Eq. D.39 twice to couple pairs of spherical harmonics with the same argument and Eq. D.14c, one finally obtain

$$\begin{aligned}\varphi^4 &= (-1)^{-m_1-m_2}\sum_{\{lm_{1-4Rr}\}} A^{\{l_{1-4Rr}\}}_{\{l_{1-4}\}}(R,r)\sum_{\{LM_{12,34Rr}\}}\sum_{L_RM_RL_rM_r}\frac{\Pi_{\{l_{1-4Rr}\}}}{64\pi^3\Pi_{L_RL_r}}C^{\{L_{12,34Rr}\}0}_{\{l_{1-4Rr}\}0}\\ &\quad C^{L_R0}_{L_{12R}0L_{34R}0}C^{L_r0}_{L_{12r}0L_{34r}0}(-1)^{l_{1r}}\,C^{l_1-m_1}_{l_{1R}-m_1Rl_{1r}-m_{1r}}C^{l_2-m_2}_{l_{2R}-m_2Rl_{2r}-m_{2r}}C^{L_{12R}M_{12R}}_{l_{1R}-m_1Rl_{2R}-m_{2R}}\\ &\quad C^{L_{12r}M_{12r}}_{l_{1r}-m_{1r}l_{2r}-m_{2r}}(-1)^{l_{4r}}\,C^{l_3m_3}_{l_{3R}m_{3R}l_{3r}m_{3r}}C^{l_4m_4}_{l_{4R}m_{4R}l_{4r}m_{4r}}C^{L_{34R}M_{34R}}_{l_{3R}m_{3R}l_{4R}m_{4R}}\\ &\quad C^{L_{34r}M_{34r}}_{l_{3r}m_{3r}l_{4r}m_{4r}}C^{L_RM_R}_{L_{12R}M_{12R}L_{34R}M_{34R}}C^{L_rM_r}_{L_{12r}M_{12r}L_{34r}M_{34r}}\,Y^{M_R}_{L_R}(\hat{R})\,Y^{M_r}_{L_r}(\hat{r})\ . \end{aligned} \tag{E.16}$$

E.1.3 Operators

E.1.3.1 Recoupling of creation and annihilation operators

Let us first prove that creation and annihilation operators associated with a single-particle basis $|lm\rangle$ are irreductible tensors. This can be done by proving that such operators fulfill conditions (D.77a,D.77b). Let us begin with creation operator $a^\dagger_{lm}$. Using results from Sec. D.1, one finds

$$\left[\hat{J}_z, a^\dagger_{nlm}\right]|0\rangle = m\,\hbar\,a^\dagger_{nlm}|0\rangle\ , \tag{E.17a}$$

$$\left[\hat{J}_\pm, a^\dagger_{nlm}\right]|0\rangle = \sqrt{l(l+1)-m(m\pm1)}\,\hbar\,a^\dagger_{nlm\pm1}|0\rangle\ , \tag{E.17b}$$

which proves that $a^\dagger_{nlm}$ is an irreductible tensor that we denote as $\mathcal{A}_{nlm}$. As for the annihilation operator a_{nlm} we first prove, using results from Sec. D.1, that

$$\langle 0|\left[\hat{J}_z, a_{nlm}\right] = -m\,\hbar\,\langle 0|a_{nlm}\ , \tag{E.18a}$$

$$\langle 0|\left[\hat{J}_\pm, a_{nlm}\right] = -\sqrt{l(l+1)-m(m\mp1)}\,\hbar\,\langle 0|a_{nlm\mp1}\ , \tag{E.18b}$$

i.e. a_{nlm} transforms contragrediently to $a^\dagger_{nlm}$. Using the result of Sec. D.8.2, we thus obtain that

$$\bar{\mathcal{A}}_{nlm} \equiv (-1)^m a_{nl-m} = (-1)^m \mathcal{A}^\dagger_{nl-m}\ . \tag{E.19}$$

is a tensor operator of rank l. Finally, applying Eq. D.94 leads to

$$a^\dagger_{n'l'm'}a_{nlm} \equiv \mathcal{A}_{n'l'm'}(-1)^m\bar{\mathcal{A}}_{nl-m} = (-1)^m\sum_{L'}C^{L'M'}_{l'm'l-m}\left[\mathcal{A}_{n'l'}\otimes\bar{\mathcal{A}}_{nl}\right]_{L'M'}\ , \tag{E.20}$$

which we will rather write

$$a^\dagger_{n'l'm'}a_{nlm} \equiv (-1)^m\sum_{L'}C^{L'M'}_{l'm'l-m}\left[a^\dagger_{n'l'}a_{nl}\right]_{L'M'}\ , \tag{E.21}$$

where $\left[a^\dagger_{n'l'}a_{nl}\right]_{L'}$ is an irreductible spherical tensor of rank L'. A similar derivation can be done for $a^\dagger_{n'l'm'}a^\dagger_{nlm}$

$$a^\dagger_{n'l'm'}a^\dagger_{nlm} \equiv \sum_{L'}C^{L'M'}_{l'm'lm}\left[a^\dagger_{n'l'}a^\dagger_{nl}\right]_{L'M'}\ , \tag{E.22}$$

and for $a_{n'l'm'}a_{nlm}$,

$$a_{n'l'm'}a_{nlm} \equiv (-1)^{m+m'}\sum_{L'}C^{L'M'}_{l'-m'l-m}\left[a_{n'l'}a_{nl}\right]_{L'M'}\ ,\ . \tag{E.23}$$

E.1.3.2 Product of two operators

Applying Wigner-Eckart theorem (Eq. D.85) to Eq. E.21, one finds

$$\langle LM|a^\dagger_{n_1l_1m_1}a_{n_2l_2m_2}|L'M'\rangle \;=\; (-1)^{m_2}\sum_J C^{JK}_{l_1m_1l_2-m_2}C^{LM}_{L'M'JK}\;\varrho^{[1]J}_{n_1l_1n_2l_2}(L,L')\;, \tag{E.24}$$

where the following notation has been introduced [4]

$$\varrho^{[1]J}_{n_1l_1n_2l_2}(L,L') \equiv \frac{1}{\sqrt{2L+1}}\langle L||\left[a^\dagger_{n_1l_1}a_{n_2l_2}\right]_J||L'\rangle\;, \tag{E.25}$$

for the reduced matrix element.

E.1.3.3 Product of four operators

Let us evaluate $\langle LM|a^\dagger_{n_1l_1m_1}a^\dagger_{n_2l_2m_2}a_{n_3l_3m_3}a_{n_4l_4m_4}|L'M'\rangle$, that we denote as $\langle a^\dagger a^\dagger aa\rangle$ for convenience. Using Eqs. (E.22,E.23) $\langle a^\dagger a^\dagger aa\rangle$ reduces to

$$\begin{aligned}\langle a^\dagger a^\dagger aa\rangle \;=\; (-1)^{m_3+m_4}\sum_{UV}\sum_{XY} & C^{UV}_{l_1m_1l_2m_2}C^{XY}_{l_3-m_3l_4-m_4} \\ & \langle LM|\left[a^\dagger_{n_1l_1}a^\dagger_{n_2l_2}\right]_{UV}\left[a_{n_3l_3}a_{n_4l_4}\right]_{XY}|L'M'\rangle\;.\end{aligned} \tag{E.26}$$

Using the direct product properties of irreductible tensor (Eq. D.94), one finds

$$\begin{aligned}\langle a^\dagger a^\dagger aa\rangle \;=\; (-1)^{m_3+m_4}\sum_{UV}\sum_{XY}\sum_{JK} & C^{UV}_{l_1m_1l_2m_2}C^{XY}_{l_3-m_3l_4-m_4}C^{JK}_{UVXY} \\ & \langle LM|\left[\left[a^\dagger_{n_1l_1}a^\dagger_{n_2l_2}\right]_U\left[a_{n_3l_3}a_{n_4l_4}\right]_X\right]_{JK}|L'M'\rangle\;,\end{aligned} \tag{E.27}$$

before applying the Wigner-Eckart theorem (Eq. D.85)

$$\begin{aligned}\langle a^\dagger a^\dagger aa\rangle \;=\; (-1)^{m_3+m_4}\sum_{UV}\sum_{XY}\sum_{JK} & C^{UV}_{l_1m_1l_2m_2}C^{XY}_{l_3-m_3l_4-m_4} \\ & C^{JK}_{UVXY}C^{LM}_{L'M'JK}\;\varrho^{[2]JUX}_{\{nl\}}(L,L')\;,\end{aligned} \tag{E.28}$$

where

$$\varrho^{[2]JUX}_{\{nl\}}(L,L') \equiv \frac{1}{\sqrt{2L+1}}\langle L||\left[\left[a^\dagger_{n_1l_1}a^\dagger_{n_2l_2}\right]_U\left[a_{n_3l_3}a_{n_4l_4}\right]_X\right]_J||L'\rangle\;, \tag{E.29}$$

denotes the reduced matrix element.

E.1.4 Matrix elements of $\hat{\rho}^{[1]}$

The matrix elements of the operator $\hat{\rho}^{[1]}$ are defined as

$$\rho^{[1]}_{LML'M'}(\vec{r}_1,\vec{r}_2) \equiv \langle LM|\hat{\rho}^{[1]}(\vec{r}_1,\vec{r}_2)|L'M'\rangle\;. \tag{E.30}$$

Starting from Eq. E.4 and applying Eqs. (E.14d,E.24), one finds

$$\begin{aligned}\rho^{[1]}_{LML'M'}(\vec{R},\vec{r}) \;=\; & \sum_{n_1l_1m_1}\sum_{n_2l_2m_2}(-1)^{-m_1+m_2}\sum_{\{l_{1-2R_r}\}\{m_{1-2R_r}\}}A^{l_{1R}l_{1r}}_{l_1}(R,r)A^{l_{2R}l_{2r}}_{l_2}(R,r) \\ & \sum_{L_RL_rM_RM_r}\frac{\Pi_{l_{1R}l_{1r}l_{2R}l_{2r}}}{4\pi\Pi_{L_RL_r}}C^{L_R0}_{l_{1R}0l_{2R}0}C^{L_r0}_{l_{1r}0l_{2r}0}(-1)^{l_{1r}}\,C^{l_1-m_1}_{l_{1R}-m_{1R}l_{1r}-m_{1r}}C^{l_2m_2}_{l_{2R}m_{2R}l_{2r}m_{2r}} \\ & C^{L_RM_R}_{l_{1R}-m_{1R}l_{2R}m_{2R}}C^{L_rM_r}_{l_{1r}-m_{1r}l_{2r}m_{2r}}\,Y^{M_R}_{L_R}(\hat{R})\,Y^{M_r}_{L_r}(\hat{r}) \\ & \sum_{JK}C^{JK}_{l_1m_1l_2-m_2}C^{LM}_{L'M'JK}\;\varrho^{[1]J}_{n_1l_1n_2l_2}(L,L')\;.\end{aligned} \tag{E.31}$$

4. The quantity $\varrho^{[1]0}_{nln'l'}(0,0)$ is positive.

Using properties of Clebsch-Gordan coefficients, it follows that $m_1 - m_2 = K = M - M'$ and $(-1)^{-m_1+m_2} = (-1)^{m_1-m_2} = (-1)^{M-M'}$. Using Eq. D.14c and Eq. D.20, one has

$$\begin{aligned}\rho^{[1]}_{LML'M'}(\vec{R},\vec{r}) &= \sum_{L_R L_r M_R M_r} \sum_{JK} (-1)^{M-M'} C^{J-K}_{L_R M_R L_r M_r} C^{LM}_{L'M'JK}\, Y^{M_R}_{L_R}(\hat{R}) \\ &\quad Y^{M_r}_{L_r}(\hat{r})\, \zeta^{[1]JL_RL_r}_{LL'}(R,r) \ , \end{aligned} \tag{E.32}$$

where

$$\zeta^{[1]JL_RL_r}_{LL'}(R,r) \equiv \sum_{n_1 l_1 n_2 l_2} \mathcal{F}^{[1]JL_RL_r}_{l_1 l_2}(R,r)\varrho^{[1]J}_{n_1 l_1 n_2 l_2}(L,L') \ , \tag{E.33}$$

and

$$\begin{aligned}\mathcal{F}^{[1]JL_RL_r}_{l_1 l_2}(R,r) &\equiv \sum_{\{l_{1-2Rr}\}} A^{l_{1R}l_{1r}}_{l_1}(R,r) A^{l_{2R}l_{2r}}_{l_2}(R,r) \frac{\Pi_{l_{1R}l_{1r}l_{2R}l_{2r}l_1 l_2}}{4\pi}\, C^{L_R 0}_{l_{1R}0 l_{2R}0} C^{L_r 0}_{l_{1r}0 l_{2r}0} \\ &\quad (-1)^{l_{1r}+l_1+l_2+J} \begin{Bmatrix} l_{2r} & l_{2R} & l_2 \\ l_{1r} & l_{1R} & l_1 \\ L_r & L_R & J \end{Bmatrix} \ . \end{aligned} \tag{E.34}$$

E.1.5 Matrix elements of $\hat{\rho}^{[2]}$

The matrix elements of the operator $\hat{\rho}^{[1]}$ is defined as

$$\rho^{[2]}_{LML'M'}(\vec{r}_1,\vec{r}_2) \equiv \langle LM|\hat{\rho}^{[2]}(\vec{r}_1,\vec{r}_2)|L'M'\rangle \tag{E.35}$$

Starting from Eq. E.6 and applying Eqs. (E.16,E.28), one finds

$$\begin{aligned}\rho^{[2]}_{LML'M'}(\vec{R},\vec{r}) &= \sum_{\{n,l,m\}\{lm_{1-4Rr}\}} \sum A^{\{l_{1-4Rr}\}}_{\{l_{1-4}\}}(R,r) \sum_{\{LM_{12,34Rr}\}} \sum_{L_R M_R L_r M_r} \frac{\Pi_{\{l_{1-4Rr}\}}}{64\pi^3 \Pi_{L_R L_r}} C^{\{L_{12,34Rr}\}0}_{\{l_{1-4Rr}\}0} \\ &\quad C^{L_R 0}_{L_{12R}0 L_{34R}0} C^{L_r 0}_{L_{12r}0 L_{34r}0} (-1)^{l_{1r}}\, C^{l_1-m_1}_{l_{1R}-m_{1R} l_{1r}-m_{1r}} C^{l_2-m_2}_{l_{2R}-m_{2R} l_{2r}-m_{2r}} \\ &\quad C^{L_{12R}M_{12R}}_{l_{1R}-m_{1R} l_{2R}-m_{2R}} C^{L_{12r}M_{12r}}_{l_{1r}-m_{1r} l_{2r}-m_{2r}} (-1)^{l_{4r}}\, C^{l_3 m_3}_{l_{3R}m_{3R} l_{3r}m_{3r}} C^{l_4 m_4}_{l_{4R}m_{4R} l_{4r}m_{4r}} \\ &\quad C^{L_{34R}M_{34R}}_{l_{3R}m_{3R} l_{4R}m_{4R}} C^{L_{34r}M_{34r}}_{l_{3r}m_{3r} l_{4r}m_{4r}} C^{L_R M_R}_{L_{12R}M_{12R} L_{34R}M_{34R}} C^{L_r M_r}_{L_{12r}M_{12r} L_{34r}M_{34r}} \\ &\quad Y^{M_R}_{L_R}(\hat{R})\, Y^{M_r}_{L_r}(\hat{r}) (-1)^{-m_1-m_2+m_3+m_4} \sum_{UV} \sum_{XY} \sum_{JK} C^{UV}_{l_1 m_1 l_2 m_2} C^{XY}_{l_3 - m_3 l_4 - m_4} \\ &\quad C^{JK}_{UVXY} C^{LM}_{L'M'JK}\, \varrho^{[2]JUX}_{\{nl\}}(L,L') \ . \end{aligned} \tag{E.36}$$

Using properties of Clebsch-Gordan coefficients, it follows that $m_1 + m_2 - m_3 - m_4 = V + Y = K = M - M'$ and $(-1)^{-m_1-m_2+m_3+m_4} = (-1)^{m_1+m_2-m_3-m_4} = (-1)^{M-M'}$, so that

$$\begin{aligned}\rho^{[2]}_{LML'M'}(\vec{R},\vec{r}) &= \sum_{\{n,l,m\}\{lm_{1-4Rr}\}} \sum A^{\{l_{1-4Rr}\}}_{\{l_{1-4}\}}(R,r) \sum_{\{LM_{12,34Rr}\}} \sum_{L_R M_R L_r M_r} \frac{\Pi_{\{l_{1-4Rr}\}}}{64\pi^3 \Pi_{L_R L_r}} C^{\{L_{12,34Rr}\}0}_{\{l_{1-4Rr}\}0} \\ &\quad C^{L_R 0}_{L_{12R}0 L_{34R}0} C^{L_r 0}_{L_{12r}0 L_{34r}0} (-1)^{l_{1r}}\, C^{l_1-m_1}_{l_{1R}-m_{1R} l_{1r}-m_{1r}} C^{l_2-m_2}_{l_{2R}-m_{2R} l_{2r}-m_{2r}} \\ &\quad C^{L_{12R}M_{12R}}_{l_{1R}-m_{1R} l_{2R}-m_{2R}} C^{L_{12r}M_{12r}}_{l_{1r}-m_{1r} l_{2r}-m_{2r}} (-1)^{l_{4r}}\, C^{l_3 m_3}_{l_{3R}m_{3R} l_{3r}m_{3r}} C^{l_4 m_4}_{l_{4R}m_{4R} l_{4r}m_{4r}} \\ &\quad C^{L_{34R}M_{34R}}_{l_{3R}m_{3R} l_{4R}m_{4R}} C^{L_{34r}M_{34r}}_{l_{3r}m_{3r} l_{4r}m_{4r}} C^{L_R M_R}_{L_{12R}M_{12R} L_{34R}M_{34R}} C^{L_r M_r}_{L_{12r}M_{12r} L_{34r}M_{34r}} \\ &\quad Y^{M_R}_{L_R}(\hat{R})\, Y^{M_r}_{L_r}(\hat{r}) (-1)^{M-M'} \sum_{UV} \sum_{XY} \sum_{JK} C^{UV}_{l_1 m_1 l_2 m_2} C^{XY}_{l_3 - m_3 l_4 - m_4} \\ &\quad C^{JK}_{UVXY} C^{LM}_{L'M'JK}\, \varrho^{[2]JUX}_{\{nl\}}(L,L') \ . \end{aligned} \tag{E.37}$$

Using Eq. D.14c, one has

$$\begin{aligned}\rho^{[2]}_{LML'M'}(\vec{R},\vec{r}) \;=\; & \sum_{\{n,l,m\}}\sum_{\{lm_{1-4Rr}\}} A^{\{l_{1-4Rr}\}}_{\{l_{1-4}\}}(R,r) \sum_{\{LM_{12,34Rr}\}}\sum_{L_RM_RL_rM_r} \frac{\Pi_{\{l_{1-4Rr}\}}}{64\pi^3\Pi_{L_RL_r}} C^{\{L_{12,34Rr}\}0}_{\{l_{1-4Rr}\}0} \\ & C^{L_R0}_{L_{12R}0L_{34R}0} C^{L_r0}_{L_{12r}0L_{34r}0} (-1)^{l_{1r}}\, C^{l_1-m_1}_{l_{1R}-m_{1R}l_{1r}-m_{1r}} C^{l_2-m_2}_{l_{2R}-m_{2R}l_{2r}-m_{2r}} \\ & C^{L_{12R}M_{12R}}_{l_{1R}-m_{1R}l_{2R}-m_{2R}} C^{L_{12r}M_{12r}}_{l_{1r}-m_{1r}l_{2r}-m_{2r}} (-1)^{l_{4r}}\, C^{l_3m_3}_{l_{3R}m_{3R}l_{3r}m_{3r}} C^{l_4m_4}_{l_{4R}m_{4R}l_{4r}m_{4r}} \\ & C^{L_{34R}M_{34R}}_{l_{3R}m_{3R}l_{4R}m_{4R}} C^{L_{34r}M_{34r}}_{l_{3r}m_{3r}l_{4r}m_{4r}} C^{L_RM_R}_{L_{12R}M_{12R}L_{34R}M_{34R}} C^{L_rM_r}_{L_{12r}M_{12r}L_{34r}M_{34r}} \\ & Y^{M_R}_{L_R}(\hat{R})\, Y^{M_r}_{L_r}(\hat{r}) (-1)^{M-M'}\, (-1)^{\{l_{1-4}\}+J} \sum_{UV}\sum_{XY}\sum_{JK} C^{U-V}_{l_1-m_1l_2-m_2} C^{X-Y}_{l_3m_3l_4m_4} \\ & C^{J-K}_{U-VX-Y} C^{LM}_{L'M'JK}\, \varrho^{[2]JUX}_{\{nl\}}(L,L') \;. \end{aligned} \tag{E.38}$$

Now one can use Eq. D.20 to find

$$\begin{aligned}\rho^{[2]}_{LML'M'}(\vec{R},\vec{r}) \;=\; & \sum_{\{n,l\}}\sum_{\{l_{1-4Rr}\}} A^{\{l_{1-4Rr}\}}_{\{l_{1-4}\}}(R,r) \sum_{\{L_{12,34Rr}\}}\sum_{L_RM_RL_rM_r} \frac{\Pi_{\{l_{1-4Rr}\}}}{64\pi^3\Pi_{L_RL_r}} C^{\{L_{12,34Rr}\}0}_{\{l_{1-4Rr}\}0} \\ & C^{L_R0}_{L_{12R}0L_{34R}0} C^{L_r0}_{L_{12r}0L_{34r}0} \sum_{UX}\sum_{JK} (-1)^{\{l_{1-4}\}+J+l_{1r}+l_{4r}}\, \Pi_{\{l_{1-4}\}\{L_{12,34Rr}\}} \\ & \begin{Bmatrix} l_{2r} & l_{2R} & l_2 \\ l_{1r} & l_{1R} & l_1 \\ L_{12r} & L_{12R} & U \end{Bmatrix} \begin{Bmatrix} l_{4r} & l_{4R} & l_4 \\ l_{3r} & l_{3R} & l_3 \\ L_{34r} & L_{34R} & X \end{Bmatrix} \sum_{VY} C^{J-K}_{U-VX-Y} \\ & \sum_{\{M_{12,34Rr}\}} C^{U-V}_{L_{12R}M_{12R}L_{12r}M_{12r}} C^{X-Y}_{L_{34R}M_{34R}L_{34r}M_{34r}} C^{L_RM_R}_{L_{12R}M_{12R}L_{34R}M_{34R}} \\ & C^{L_rM_r}_{L_{12r}M_{12r}L_{34r}M_{34r}} (-1)^{M-M'}\, Y^{M_R}_{L_R}(\hat{R})\, Y^{M_r}_{L_r}(\hat{r})\, C^{LM}_{L'M'JK}\, \varrho^{[2]JUX}_{\{nl\}}(L,L') \;. \end{aligned} \tag{E.39}$$

Applying Eq. D.20 to the resulting Clebsch-Gordan coefficients, one obtains

$$\begin{aligned}\rho^{[2]}_{LML'M'}(\vec{R},\vec{r}) \;=\; & \sum_{L_RM_RL_rM_r}\sum_{JK} (-1)^{M-M'}\, C^{J-K}_{L_RM_RL_rM_r}\, C^{LM}_{L'M'JK} \\ & Y^{M_R}_{L_R}(\hat{R})\, Y^{M_r}_{L_r}(\hat{r})\, \zeta^{[2]JL_RL_r}_{LL'}(R,r) \;, \end{aligned} \tag{E.40}$$

where

$$\zeta^{[2]JL_RL_r}_{LL'}(R,r) \equiv \sum_{\{n,l\}}\sum_{UX} \mathcal{F}^{[2]JL_RL_rUX}_{\{l_{1-4}\}}(R,r)\, \varrho^{[2]JUX}_{\{nl\}}(L,L') \;, \tag{E.41}$$

and

$$\begin{aligned}\mathcal{F}^{[2]JL_RL_rUX}_{\{l_{1-4}\}}(R,r) \;\equiv\; & \sum_{\{l_{1-4Rr}\}} A^{\{l_{1-4Rr}\}}_{\{l_{1-4}\}}(R,r) \sum_{\{L_{12,34Rr}\}} \frac{\Pi_{\{l_{1-4Rr}\}}}{64\pi^3} C^{\{L_{12,34Rr}\}0}_{\{l_{1-4Rr}\}0} \\ & C^{L_R0}_{L_{12R}0L_{34R}0} C^{L_r0}_{L_{12r}0L_{34r}0} (-1)^{l_{1r}+l_{4r}} (-1)^{\{l_{1-4}\}+J}\, \Pi_{\{l_{1-4}\}\{L_{12,34Rr}\}UX} \\ & \begin{Bmatrix} l_{2r} & l_{2R} & l_2 \\ l_{1r} & l_{1R} & l_1 \\ L_{12r} & L_{12R} & U \end{Bmatrix} \begin{Bmatrix} l_{4r} & l_{4R} & l_4 \\ l_{3r} & l_{3R} & l_3 \\ L_{34r} & L_{34R} & X \end{Bmatrix} \begin{Bmatrix} L_{34r} & L_{34R} & X \\ L_{12r} & L_{12R} & U \\ L_r & L_R & J \end{Bmatrix} \;. \end{aligned} \tag{E.42}$$

E.2 Matrix elements of operators

E.2.1 Introduction

A general two-body operator is defined, omitting spin and isospin degrees of freedom, as

$$\hat{O} \equiv \frac{1}{2}\int d\vec{r}_1 d\vec{r}_2 d\vec{r}_3 d\vec{r}_4 \, \langle 1:\vec{r}_1\, 2:\vec{r}_2|\hat{O}|1:\vec{r}_3\, 2:\vec{r}_4\rangle \; a^\dagger_{\vec{r}_1} a^\dagger_{\vec{r}_2} a_{\vec{r}_4} a_{\vec{r}_3} \quad . \tag{E.43}$$

In our application local operators are considered

$$\langle 1:\vec{r}_1\, 2:\vec{r}_2|\hat{O}|1:\vec{r}_3\, 2:\vec{r}_4\rangle \equiv O(\vec{r}_1,\vec{r}_2)\,\delta(\vec{r}_1-\vec{r}_3)\delta(\vec{r}_2-\vec{r}_4) \quad , \tag{E.44}$$

such that

$$\hat{O} = \frac{1}{2}\int d\vec{r}_1 d\vec{r}_2 \; O(\vec{r}_1,\vec{r}_2)\; a^\dagger_{\vec{r}_1} a^\dagger_{\vec{r}_2} a_{\vec{r}_2} a_{\vec{r}_1} \quad . \tag{E.45}$$

Matrix elements of such an operator between states with good orbital angular momenta read

$$\langle LM|\,\hat{O}\,|L'M'\rangle = \frac{1}{2}\int d\vec{r}_1 d\vec{r}_2 \; O(\vec{r}_1,\vec{r}_2)\; \rho^{[2]}_{LML'M'}(\vec{r}_2,\vec{r}_1) \quad . \tag{E.46}$$

E.2.2 Tensor operator local density

E.2.2.1 General case

Starting from a local tensor operator depending only on the relative coordinate $\vec{r}$

$$T^q_k(\vec{r}_1,\vec{r}_2) \equiv T(r) Y^q_k(\hat{r}) \quad , \tag{E.47}$$

we define the density $T^{LM}_{L'M'kq}(\vec{R})$ from the matrix element $\langle LM|\,\hat{T}^q_k\,|L'M'\rangle$ through

$$\langle LM|\,\hat{T}^q_k\,|L'M'\rangle \equiv \int d\vec{R}\; T^{LM}_{L'M'kq}(\vec{R}) \quad , \tag{E.48}$$

such that

$$\begin{aligned} T^{LM}_{L'M'kq}(\vec{R}) &= \frac{1}{2}\int d\vec{r}\, T(r) Y^q_k(\hat{r}) \sum_{L_R M_R L_r M_r} \sum_{JK} (-1)^{M-M'} C^{J-K}_{L_R M_R L_r M_r} C^{LM}_{L'M'JK} \\ &\qquad Y^{M_R}_{L_R}(\hat{R})\, Y^{M_r}_{L_r}(\hat{r})\, \zeta^{[2]L_R L_r}_{JLL'}(R,r) \quad . \end{aligned} \tag{E.49}$$

Using Eqs. (D.30,D.32)) and integrating over $\hat{r}$, one obtains

$$\begin{aligned} T^{LM}_{L'M'kq}(\vec{R}) &= \frac{1}{2}\sum_{L_R M_R L_r M_r}\sum_{JK}\int dr\; T(r)\; \zeta^{[2]JL_RL_r}_{LL'}(R,r) \\ &\qquad (-1)^{M-M'-q}\,\delta_{L_r k}\delta_{M_r -q} Y^{M_R}_{L_R}(\hat{R})\, C^{J-K}_{L_R M_R L_r M_r}\, C^{LM}_{L'M'JK} \quad , \end{aligned} \tag{E.50}$$

which reduces to

$$T^{LM}_{L'M'kq}(\vec{R}) = \sum_{L_R M_R}\sum_{JK} \mathcal{T}^{JL_Rk}_{LL'}(R)\,(-1)^{M-M'-q}\, C^{J-K}_{L_R M_R k-q} C^{LM}_{L'M'JK} Y^{M_R}_{L_R}(\hat{R}) \quad , \tag{E.51}$$

where

$$\mathcal{T}^{JL_Rk}_{LL'}(R) \equiv \frac{1}{2}\int dr\; T(r)\; \zeta^{[2]JL_Rk}_{LL'}(R,r) \quad . \tag{E.52}$$

E.2.2.2 Local potential Energy density

Let us now calculate the potential energy density associated with a scalar operator V by replacing $T_k^q(\vec{r}_1,\vec{r}_2)$ by $V(\vec{r}_1,\vec{r}_2)=V(r)$ such that

$$\begin{aligned} V_{L'M'}^{LM}(\vec{R}) &= \sum_{L_RM_R}\sum_{JK} \mathcal{V}_{LL'}^{JL_R0}(R)\,(-1)^{M-M'}\,C_{L_RM_R00}^{J-K}\,C_{L'M'JK}^{LM}Y_{L_R}^{M_R}(\hat{R}) \\ &= \sum_{L_RM_R} \mathcal{V}_{LL'}^{L_RL_R0}(R)\,(-1)^{M-M'}\,C_{L'M'L_R-M_R}^{LM}Y_{L_R}^{M_R}(\hat{R})\ , \end{aligned} \tag{E.53}$$

where

$$\mathcal{V}_{LL'}^{L_RL_R0}(R) \equiv \frac{1}{2}\int dr\ V(r)\,\zeta_{LL'}^{[2]L_RL_R0}(R,r)\ . \tag{E.54}$$

In the case of a diagonal matrix elements, i.e. $L=L'$ and $M=M'$, one eventually obtain

$$V^{LM}(\vec{R}) = \sum_{L_R=0}^{2L} \mathcal{V}_{LL}^{L_RL_R0}(R)\ C_{LML_R0}^{LM}Y_{L_R}^{0}(\hat{R})\ , \tag{E.55}$$

which depends on M through the Clebsch-Gordan coefficients. Eq. E.55 constitutes the result presented in Eq. 2.27 and used in Chap. 2.

E.2.3 Tensor operator matrix elements

E.2.3.1 General case

To compute $\langle LM|\,\hat{T}_k^q\,|L'M'\rangle$, $T_{L'M'kq}^{LM}(\vec{R})$ must be integrated over $\vec{R}$

$$\begin{aligned} &\langle LM|\,\hat{T}_k^q\,|L'M'\rangle \\ &\quad= \int d\vec{R} \sum_{L_RM_R}\sum_{JK} \mathcal{T}_{LL'}^{JL_Rk}(R)\,(-1)^{M-M'-q}\,C_{L_RM_Rk-q}^{J-K}\,C_{L'M'JK}^{LM}Y_{L_R}^{M_R}(\hat{R})\ , \end{aligned} \tag{E.56}$$

which, thanks to Eq. D.29, reads

$$\langle LM|\,\hat{T}_k^q\,|L'M'\rangle = \sum_{JK}\int dR\ \mathcal{T}_{LL'}^{J0k}(R)\sqrt{4\pi}\,(-1)^{M-M'-q}\,C_{00k-q}^{J-K}\,C_{L'M'JK}^{LM}\ , \tag{E.57}$$

which reduces to

$$\langle LM|\,\hat{T}_k^q\,|L'M'\rangle = C_{L'M'kq}^{LM}\int dR\ \mathcal{T}_{LL'}^{k0k}(R)\sqrt{4\pi}\ , \tag{E.58}$$

where we have used that $M-M'-q=0$. Using Eqs. (E.29,E.41,E.52) one obtains

$$\langle LM|\,\hat{T}_k^q\,|L'M'\rangle \equiv C_{L'M'kq}^{LM}\frac{1}{\sqrt{2L+1}}\langle L||\tilde{T}_k||L'\rangle\ , \tag{E.59}$$

where

$$\begin{aligned} \langle L||\tilde{T}_k||L'\rangle = \sum_{\{n,l\}}\sum_{UX}\frac{1}{2}\int dR\int dr\ \mathcal{F}_{\{l_{1-4}\}}^{[2]0kkUX}(R,r)\,T(r)\,\sqrt{4\pi} \\ \langle L||\left[\left[a_{n_1l_1}^\dagger a_{n_2l_2}^\dagger\right]_U\left[a_{n_3l_3}a_{n_4l_4}\right]_X\right]_k||L'\rangle\ , \end{aligned} \tag{E.60}$$

which is nothing but the Wigner-Eckart theorem applied to the operator $\hat{T}_k^q$.

E.2.3.2 Potential energy

Let us now calculate the potential energy

$$\langle LM|\,\hat{V}\,|L'M'\rangle \quad = \quad C^{LM}_{L'M'00}\frac{1}{\sqrt{2L+1}}\langle L||\tilde{V}_0||L'\rangle \ , \tag{E.61}$$

and thus

$$V^L = \delta_{LL'}\delta_{MM'}\frac{1}{\sqrt{2L+1}}\langle L||\tilde{V}||L'\rangle \ , \tag{E.62}$$

which is independent of M.

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Résumé

La méthode dite de la fonctionnelle de la densité d'énergie (EDF) est l'outil théorique de référence pour l'étude systématique de la structure des noyaux atomiques de masse $A \gtrsim 20$. La méthode EDF est formulée en deux étapes successives consistant à briser puis à restaurer les symétries du Hamiltonien nucléaire sous-jacent. La technique de restauration des symétries n'est cependant rigoureusement formulée que si la fonctionnelle d'énergie dérive explicitement d'une interaction effective, i.e. d'un pseudo-potentiel, ce qui constitue un cas particulier de la méthode EDF plus générale. Ainsi, et comme cela a été démontré récemment, l'utilisation des paramétrisations existantes des fonctionnelles d'énergie conduit à l'obtention de résultats non physiques. Le pouvoir prédictif limité des fonctionnelles d'énergie existantes et leur inocuité relative à la restauration des symétries, nécessitent aujourd'hui de repenser leur méthode de construction. La première partie de ce travail a été dédié à l'analyse approfondie du problème associé à la restauration de symétrie et à l'identification de pistes permettant de contraindre la forme analytique des fonctionnelles d'énergie ne dérivant pas d'un pseudo-potentiel indépendant du système. La seconde partie a consisté à développer un pseudo-potentiel rendant la restauration des symétries automatiquement bien définie. Les difficultés de ce travail ont résidé dans (i) l'identification de la complexité minimale du pseudo-potentiel nécessaire à l'obtention d'une fonctionnelle d'énergie assez flexible pour égaler, et si possible améliorer, les performances des paramétrisations existantes, (ii) la dérivation analytique de la fonctionnelle et des champs à un corps découlant de celle ci, (iii) l'implémentation de ces derniers dans les codes de calculs, et dans (iv) le développement d'un protocole d'ajustement des paramètres adapté à la nouvelle fonctionnelle d'énergie ainsi développée. Les premiers résultats obtenus ont permis de valider l'approche en démontrant la flexibilité suffisante du pseudo-potentiel au niveau des calculs réalisés sans restauration des symétries.

Abstract

The theoretical tool of choice for the microscopic description of all medium- and heavy-mass nuclei is the Energy Density Functional (EDF) method. Such a method relies on the concept of spontaneous symmetry breaking and restoration. In that sense, it is intrinsically a two-step approach. However, the symmetry restoration procedure is only well-defined in the particular case where the energy functional derives from a pseudo-potential. Thereby and as it has been recently shown, existing parameterizations of the energy functional provides unphysical results. Such a problem as well as the lack of predictive power call for developing new families of functionals. The first part of the present work is devoted to a study of the symmetry restoration problem and to the identification of properties that could constrain the analytic form of energy functionals that do not derive from a pseudo-potential. The second part deals with the construction of an energy functional that derives from a pseudo potential. The difficulties of such work are (i) the identification of the minimal complexity of the pseudo-potential necessary to obtain an energy functional that is flexible enough to provide high-quality EDF parameterizations, (ii) the tedious analytical derivation of the functional and of the associated one-body fields, (iii) the implementation of the latter in existing codes, and (iv) the development of an efficient fitting procedure. Eventually, it seems possible to generate a parameterization that strictly derives from a pseudo-potential and that provides as good results as state-of-the-art (quasi) bilinear functionals.