Continuity equation and local gauge invariance for the N^3LO nuclear Energy Density Functionals

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Background: The next-to-next-to-next-to-leading order (N^3LO) nuclear energy density functional extends the standard Skyrme functional with new terms depending on higher-order derivatives of densities, introduced to gain better precision in the nuclear many-body calculations. A thorough study of the transformation properties of the functional with respect to different symmetries is required, as a step preliminary to the adjustment of the coupling constants.

Purpose: Determine to which extent the presence of higher-order derivatives in the functional can be compatible with the continuity equation. In particular, to study the relations between the validity of the continuity equation and invariance of the functional under gauge transformations.

Methods: Derive conditions for the validity of the continuity equation in the framework of time-dependent density functional theory. The conditions apply separately to the four spin-isospin channels of the one-body density matrix.

Results: We obtained four sets of constraints on the coupling constants of the N^3LO energy density functional that guarantee the validity of the continuity equation in all spin-isospin channels. In particular, for the scalar-isoscalar channel, the constraints are the same as those resulting from imposing the standard U(1) local-gauge-invariance conditions.

Conclusions: Validity of the continuity equation in the four spin-isospin channels is equivalent to the local-gauge invariance of the energy density functional. For vector and isovector channels, such validity requires the invariance of the functional under local rotations in the spin and isospin spaces.

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I. INTRODUCTION

In recent years, methods using energy density functionals (EDFs) [1] to describe nuclear properties are being developed in three complementary directions. First, the ideas of effective theories [2,3] are employed in determining the EDFs from first principles [4–7]. These developments are supplemented by a renewed interest in the density-matrix expansion (DME) methods [11,12], which allow for treating exchange correlations in terms of (quasi)local functionals. Second, the coupling constants of the well-known EDFs undergo a thorough scrutiny, including an advanced work on the readjustment of parameters [13,14] and study of inter-parameter correlations [15]. Finally, the standard functionals are extended by adding new terms [16–19], so as to gain increased precision of description and predictability, in quest for the spectroscopic-quality and universal [21] EDFs.

In the present work we study properties of EDFs [16] and pseudopotentials [18] extended by adding terms that depend on higher-order derivatives up to sixth, next-to-next-to-next-to-leading order (N^3LO). Such extensions lead to self-consistent mean-field Hamiltonians that are sixth-order differential operators [22], that is, they depend on up to sixth power of the momentum operator. This makes them unusual objects, in the sense that standard second-order one-body Hamiltonians contain only the Laplace operator in the kinetic-energy term and possibly the angular-momentum operator in the spin-orbit term. The main question we address here is whether the presence of higher powers of momenta is compatible with the continuity equation (CE).

The CE is a differential equation that describes a conservative transport of some physical quantity [23]. In quantum mechanics, it relates the time variation of the probability density to the probability current [24]. In our case, it appears when the N^3LO EDFs or pseudopotentials are employed within a time-dependent theory. For the standard Skyrme (NLO) functional, the validity of the CE has been checked explicitly [25]. Our goal here is to derive constraints on the coupling constant of the N^3LO EDF or parameters of the pseudopotential that would guarantee the validity of the CE. Apart from linking the CE to the local gauge symmetry [26], we also analyze the CEs in vector and isovector channels and link them to the local non-abelian gauge symmetries.

The paper is organized as follows. In Sec. II A we present the standard quantal CE for a single particle and introduce the vector CE. Then, in Sec. II B we discuss the CEs within the time-dependent density functional theory and in Sec. II C we specify the case to the N^3LO quasilocal functional. The main body of results obtained for the CEs in the four spin-isospin channels is presented in Sec. III and Appendices A–C. Finally in Sec. IV we formulate the conclusions of the present study.

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II. CONTINUITY EQUATION IN THE EDF APPROACH

A. Time evolution of a spin-$\frac{1}{2}$ particle

We begin by recalling the well-known CE for a single particle. The time evolution of a non-relativistic spin-$\frac{1}{2}$ particle moving in a local potential is given by the Schrödinger equation,

$$ih\frac{\partial}{\partial t}\psi(r,\sigma, t) = -\frac{\hbar^2}{2m}\nabla^2\psi(r,\sigma, t) + V_0(r, t)\psi(r,\sigma, t) + \sum_{\mu=x,y,z} V_{\mu}(r, t)\langle\sigma|\sigma_\mu|\sigma\rangle\psi(r,\sigma, t),$$  

where $V_0(r, t)$ and $V_{\mu}(r, t)$ are scalar and vector real-time-dependent potentials, respectively, and $\langle\sigma|\sigma_\mu|\sigma\rangle$ are the standard Pauli matrices. By multiplying Eq. (1) with $\psi^*(r,\sigma, t)$, summing up over $\sigma$, and taking the imaginary part, we obtain the standard CE for the probability density $\rho(r, t)$ in terms of the current $j(r, t)$,

$$\rho(r, t) = \sum_{\sigma} \langle\psi(r,\sigma, t)|\psi(r,\sigma, t)\rangle,$$

$$j(r, t) = \sum_{\sigma} \text{Im}\left(\psi^*(r,\sigma, t)\nabla\psi(r,\sigma, t)\right).$$

We see that the hermiticity of the local potential guarantees that the potential energy does not contribute to the CE of Eq. (2).

Similarly, by multiplying Eq. (1) with $\psi^*(r,\sigma', t)\langle\sigma'|\sigma_\mu|\sigma\rangle$, summing up over $\sigma'$ and $\sigma$, and taking the imaginary part, we obtain the CE for the spin density $s_\sigma(r, t)$ in terms of the spin current $J_\sigma(r, t)$,

$$\rho(r, t) = \sum_{\sigma} \langle\psi(r,\sigma, t)|\psi(r,\sigma, t)\rangle,$$

$$s_{\sigma}(r, t) = \sum_{\sigma'} \langle\psi^*(r,\sigma', t)\langle\sigma'|\sigma_\mu|\sigma\rangle\psi(r,\sigma, t)\rangle,$$

where

$$J_\sigma(r, t) = \sum_{\sigma'} \text{Im}\left(\psi^*(r,\sigma', t)\langle\sigma'|\sigma_\mu|\sigma\rangle\nabla\psi(r,\sigma, t)\right).$$

We see that the spin CE does depend on the vector potential, and the second term in Eq. (4) is responsible, e.g., for the spin precession in magnetic field.

It is interesting to note that when potential $V_1(r, t)$ is parallel to the spin density $s(r, t)$ (non-linear Schrödinger equation), all components of the spin density fulfill the CEs. In fact, this is exactly the case for the TDHF equation induced by a zero-range two-body interaction, see below. Another interesting case corresponds to the vector potential aligned along a fixed direction in space, say, along the $z$ axis, that is $V_1(r, t) = V_1(r, t)e_z$. In this case, the time evolutions of the spin-up and spin-down components decouple from one another, that is, $s(r, 0) = s(r, 0)e_z$ implies $s(r, t) = s(r, t)e_z$, and the spin-up and spin-down components individually obey the corresponding CEs.

We also note here that for a non-local potential-energy term,

$$\langle\psi^*(r,\sigma, t)\nabla\psi(r,\sigma, t)\rangle,$$

the time evolution does not, in general, lead to a CE.

B. Time-dependent density functional theory

In the framework of the time-dependent Hartree-Fock (TDHF) approximation or time-dependent density functional theory (TDDFT), the so-called memory effects are often neglected and it is assumed that the potential at time $t$ is just the static potential evaluated at the instantaneous density $\rho_0$. For these two time-dependent approaches, the starting point is the equation of motion for the one-body density matrix $\rho_{\alpha\beta}$,

$$ih\frac{d}{dt}\rho_{\alpha\beta} = [h, \rho],$$

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

$$h_{\alpha\beta} = \frac{\partial E(\rho)}{\partial \rho_{\beta\alpha}}.$$

In the present study we are concerned with the Kohn-Sham approach, whereby the total energy is the sum of the kinetic and potential-energy terms,

$$E(\rho) = E_k(\rho) + E_p(\rho),$$

where

$$E_k(\rho) = \frac{\hbar^2}{2m} \int d^3r \tau_0^0(r, t)$$

and $\tau_0^0(r, t) = \sum_{\sigma\tau} \nabla \cdot \nabla\rho(r,\sigma, r'\sigma', t)|_{r=r'}$ is the scalar-isoscalar kinetic density, see, e.g., Ref. [30] for definitions. The nonlocal density, can be defined in terms of either the fixed-basis orbitals, $\psi_\alpha(r,\sigma\tau)$, or instantaneous Kohn-Sham orbitals, $\phi_i(r,\sigma\tau, t)$,

$$\rho(r,\sigma, r'\sigma', t) = \sum_{i} \phi_i(r,\sigma\tau, t) \phi_i^*(r',\sigma'\tau', t),$$

or instantaneous Kohn-Sham orbitals, $\phi_i(r,\sigma\tau, t)$,

$$\rho(r,\sigma, r'\sigma', t) = \sum_{i=1}^{A} \phi_i(r,\sigma\tau, t) \phi_i^*(r',\sigma'\tau', t).$$
The mean-field Hamiltonian is the sum of kinetic and potential-energy terms, \( h_{\alpha\beta} = T_{\alpha\beta} + \Gamma_{\alpha\beta} \), where

\[
T_{\alpha\beta} = \int d^3r \sum_{i\tau} \psi^*_{\alpha}(r\sigma\tau) \frac{-i\hbar^2}{2m} \Delta \psi_{\beta}(r\sigma\tau),
\]

and

\[
\Gamma_{\alpha\beta} = \frac{\partial E_p\{\rho\}}{\partial \rho_{\beta\alpha}}.
\]

Let us now assume that the potential energy is invariant with respect to a unitary transformation of the density matrix \([20,28]\), \( U = \exp(i\eta G) \), that is, for all parameters \( \eta \) we have,

\[
E_p\{\rho\} = E_p\{U\rho U^+\},
\]

where \( G_{\alpha\beta} \) is the hermitian matrix of a one-body symmetry generator. Then, the first-order expansion in \( \eta \),

\[
E_p\{U\rho U^+\} \simeq E_p\{\rho\} + \eta \sum_{\beta\alpha} \left[ \frac{\partial E_p\{\rho\}}{\partial \rho_{\beta\alpha}} \frac{\partial (U\rho U^+)}{\partial \eta} \right]_{\eta=0},
\]

gives a condition for the energy to be invariant with respect to this unitary transformation, that is

\[
\text{Tr}[G, \rho] \equiv \text{Tr}[G, \rho] = 0,
\]

which allows us to derive the equation of motion for the average value of \( \langle G \rangle = \text{Tr}[G, \rho] \). Indeed, from the TDDFT equation we then have:

\[
\frac{i\hbar}{\partial t} \langle G \rangle = i\hbar \text{Tr}[h, \rho] = \text{Tr}[h, \rho] = \text{Tr}[T, \rho],
\]

that is, the time evolution of \( \langle G \rangle \) is governed solely by the kinetic term of the mean-field Hamiltonian.

1. Continuity equation for the scalar-isoscalar density

The CE now results from specifying \( \eta G \) to the local gauge transformation \([20,31]\) that is defined as

\[
\psi^*_{\alpha}(r\sigma\tau) \equiv \langle U\psi_{\alpha}\rangle(r\sigma\tau) = e^{i\gamma(r)} \psi_{\alpha}(r\sigma\tau).
\]

Then, Eq. (11) gives:

\[
\rho'(r\sigma\tau, r'\sigma'\tau', t) = e^{i(\gamma(r') - \gamma(r))} \rho(r\sigma\tau, r'\sigma'\tau', t).
\]

Matrix elements of the local-gauge angle \( \gamma(r) \) are given by local integrals,

\[
\gamma_{\alpha\beta} = \int d^3r \sum_{i\tau} \psi^*_{\alpha}(r\sigma\tau) \gamma(r) \psi_{\beta}(r\sigma\tau);
\]

therefore, from Eq. (11) again, the average value of the gauge angle, \( \langle \gamma \rangle = \text{Tr}[\gamma, \rho] \), depends on the scalar-isoscalar local density \( \rho^0_{\sigma\tau}(r, t) = \sum_{\sigma'} \rho(r\sigma\tau, r\sigma\tau', t) \), that is,

\[
\langle \gamma \rangle = \int d^3r \gamma(r) \rho^0_{\sigma\tau}(r, t).
\]

Now, the assumed local-gauge invariance of the potential energy implies the equation of motion for the average value \( \langle \gamma \rangle \), which from Eq. (15) reads

\[
\frac{d}{dt} \langle \gamma \rangle = -\frac{\hbar}{m} \int d^3r \gamma(r) \nabla \cdot J^0_{\tau\sigma\tau'}(r, t),
\]

where the standard scalar-isoscalar current is defined as

\[
J^0_{\tau\sigma\tau'}(r, t) = \sum_{\sigma'} \frac{1}{\hbar} \left[ (\nabla - \nabla') \rho(r\sigma\tau, r'\sigma'\tau', t) \right]_{\tau'=\tau}.
\]

We note here \([20,31]\), that the gauge invariance that corresponds to a specific dependence of the gauge angle on position, \( \gamma(r) = P_0 \cdot r \), represents the Galilean invariance of the potential energy for the system boosted to momentum \( P_0 \). Then, equation of motion (23) simply represents the classical equation for the center-of-mass velocity,

\[
\frac{d}{dt} \langle \rho \rangle = \frac{d}{dt} R_{\text{CM}} = \frac{\langle P \rangle}{\langle m \rangle} = \frac{-i\hbar \nabla}{m \langle m \rangle}.
\]

In the general case, that is, when the potential energy is gauge-invariant and the gauge angle \( \gamma(r) \) is an arbitrary function of \( r \), Eq. (23) gives the CE that reads

\[
\frac{d}{dt} \rho^0_{\sigma\tau}(r, t) = -\frac{\hbar}{m} \nabla \cdot J^0_{\tau\sigma\tau'}(r, t).
\]

Thus for a gauge-invariant potential energy density, the TDHF or TDDFT equation of motion implies the CE, that is, the gauge invariance is a sufficient condition for the validity of the CE. By proceeding in the opposite direction, we can prove that it is also a necessary condition. Indeed, the CE of Eq. (25) implies the first-order condition (17), and then the full gauge invariance stems from the fact that the gauge transformations form local U(1) groups.

2. Continuity equation for densities in spin-isospin channels

We can now repeat derivations presented in Eqs. (19)–(23) by considering the spin-isospin local-gauge groups, and derive CEs in other spin-isospin channels. To this end, we first express the nuclear one-body density matrix \([11,12]\) as a linear combination of nonlocal spin-isospin densities \( \rho^0_{\tau\sigma\sigma'}(r, r') \),

\[
\rho(r\sigma\tau, r'\sigma'\tau') = \frac{1}{4} \sum_{v=0,1} \sum_{t=0,1} \left( \sqrt{3} \right)^{v+t} \left[ \sigma^v_{\tau\sigma\tau'} [\tau^t_{\tau\sigma\tau'} \rho^0_{\tau'\sigma'}(r, r')]^0 \right],
\]

where the sums now run over the spin \((v = 0, 1)\) and isospin \((t = 0, 1)\) indices denoted by subscripts and superscripts, respectively, coupled to total scalar and isoscalar. Here and below we use the coupling of spherical tensors both for angular momentum and isospin tensors; therefore, in Eq. (26) the factor of \( \sqrt{3}^{v+t} \) was included so as to cancel the corresponding values of the Clebsch-Gordan coefficients, and to maintain the standard normalization.
of the spin-isospin densities. The spin-isospin densities can be conversely expressed as the following traces of the density matrix,

\[ \rho^t_v(r, r') = \sum_{\sigma, \sigma', \tau} \sigma^\tau_{\sigma, \sigma'} \rho(r \sigma \tau, r' \sigma' \tau'). \]  

(27)

The CEs for densities in the scalar-isoscalar \((v = 0, t = 0)\), scalar-isovector \((v = 0, t = 1)\), vector-isoscalar \((v = 1, t = 0)\), and vector-isovector \((v = 1, t = 1)\) channels,

\[ \frac{d}{dr} \rho^t_v(\mathbf{r}) = -\frac{\hbar}{m} \nabla \cdot \mathbf{J}^t_v(\mathbf{r}), \]

(28)

where \( \mathbf{J}^t_v(\mathbf{r}) = \frac{1}{2} (\nabla - \nabla') \rho^t_v(\mathbf{r}, \mathbf{r}')\big|_{\mathbf{r}'=\mathbf{r}} \) and \( \rho^t_v(\mathbf{r}) = \rho^t_v(\mathbf{r}, \mathbf{r}) \), are now equivalent to the four local spin-isospin groups:

\[ U^t_v(\mathbf{r}) = \exp\left(i \left[[\gamma^t_v(\mathbf{r}) \sigma^t_v(\mathbf{r})]_0 \tau^t_v\right]^0\right). \]

(29)

Of course, the standard CE derived in Sec. II.B corresponds to \( \gamma(\mathbf{r}) \equiv \gamma^0_0(\mathbf{r}) \). Note that the four gauge groups are different: \( U^0_0(\mathbf{r}) \) gives the standard abelian gauge group \( U(1) \), \( U^0_0(\mathbf{r}) \) and \( U^0_0(\mathbf{r}) \) form the non-abelian gauge groups \( SU(2) \), whereas \( U^0_0(\mathbf{r}) \) corresponds to the non-abelian gauge group \( SU(2) \times SU(2) \).

C. The \( N^3LO \) quasilocal functional

We are now in a position to discuss the CE for the \( N^3LO \) quasilocal functional introduced by Carlsson et al. [10]. By imposing on the functional the gauge-invariance conditions, we can then confirm and explicitly rederive the results of Sec. II.B. The explicit derivation will also allow us to discuss the CEs for densities in other spin-isospin channels analyzed in Sec. II.B.

Below we consider the EDF given in terms of a local integral of the energy density \( \mathcal{H}_E(\mathbf{r}) \),

\[ E(\rho) = \int d^3r \ \mathcal{H}_E(\mathbf{r}), \]

(30)

which is represented as a sum of the kinetic and potential energies conforming to Eq. (9),

\[ \mathcal{H}_E(\mathbf{r}) = \frac{\hbar^2}{2m} \rho^0_0(\mathbf{r}) + \sum_{t=0,1} \mathcal{H}^t(\mathbf{r}). \]

(31)

To lighten the notation and avoid confusion with the isospin index \( t = 0, 1 \), in this section we do not explicitly show the time argument of densities, which within the TDDFT all depend on time.

The quasilocal \( N^3LO \) EDF was constructed [10] by building the \( t = 0 \) and \( t = 1 \) potential-energy densities \( \mathcal{H}^t(\mathbf{r}) \) from isoscalar and isovector densities, respectively, and their derivatives up to sixth order. For clarity, we give here a brief summary of definitions and notations used in this construction.

The local higher-order primary densities are defined by the coupling of relative-momentum tensors \( K_{nL} \) with nonlocal densities \( \rho_{nL} \) to total angular momentum \( J \), that is,

\[ \rho_{nL,J}(\mathbf{r}) = \{ [K_{nL} \rho^t_v(\mathbf{r}, \mathbf{r}')]_{J=E} \}. \]

(32)

Then, a general term of the \( N^3LO \) functional can be written, in the language of the spherical tensors, as

\[ T_{mI,nL;J,J'}(\mathbf{r}) = \left[[\rho^t_v(\mathbf{r}, \mathbf{r}') D_{mI} \rho_{nL,J}(\mathbf{r})]_{J'}\right]_0^0(33) \]

where the local secondary densities, \( D_{mI} \rho_{nL,J}(\mathbf{r}) \), are obtained by acting with derivatives \( D_{mI} \) on primary densities and coupling them to total angular momentum \( J' \). Each term \( 33 \) is multiplied by the corresponding coupling constant \( C_{mI,nL,J,J'} \) that is denoted by the same set of indices as those in the term itself.

We note here that the definition of the isovector terms depends on whether one uses Cartesian or spherical representation of tensors in isospace. On the other hand, the use of the standard Cartesian representation, see, e.g., Refs. 14-50, implies that the isovector terms depend on products of differences of neutron and proton densities. On the other hand, the use of the spherical representation, which was assumed in Ref. [18] and is also used in the present study, involves the coupling of two isovectors to a scalar, whereby there appears a Clebsch-Gordan coefficient of \( (\sqrt{3})^{-1} \). Therefore, for the isospace spherical representation, the isovector coupling constants are by the factor of \( (\sqrt{3}) \) larger than those for the Cartesian representation.

In the remaining part of this section, we employ the compact notation introduced in Ref. 22, whereby the grouped indices, such as the Greek indices \( \alpha = \{n_\alpha I_\alpha \} \) and the Roman indices \( a = \{m_\alpha L_\alpha \} \), denote all the quantum numbers of the local \( \rho_{nL}(\mathbf{r}) \) and derivative operators \( D_{\alpha} \), respectively. In this notation, the \( N^3LO \) potential-energy density of Eq. (31) reads

\[ \mathcal{H}^t(\mathbf{r}) = \sum_{\alpha \alpha' \beta} C_{\alpha \alpha' \beta}^{I \alpha} T_{\alpha \alpha' \beta}^{3,3}(\mathbf{r}). \]

(34)

Our following discussion of the CE is mainly focused on the one-body potential-energy term, defined in Eq. (14) as the variation of the potential energy with respect to the density matrix. For the \( N^3LO \) functional, this term was derived in Ref. 22, where it was shown that in space coordinates it has the form of a one-body pseudopotential,

\[ \hat{\Gamma}^{t \sigma \tau'}_{\sigma' \tau'}(\mathbf{r}) = \sum_{\gamma, t} \left[[U^t_{\gamma}(\mathbf{r}) D_{\gamma \gamma} \sigma^t_{\gamma \tau'}]_{J=0} \tau^t_{\sigma' \tau'}\right]. \]

(35)

An equivalent form of the one-body pseudopotential, which can be obtained by recoupling spherical tensors
within a scalar, and which separates out the spin Pauli matrices, reads
\[
\hat{\Gamma}_{\tau'\tau}^{\sigma'\sigma}(r) = \sum_{\gamma,t} \left[ \left( U_{\gamma}^{t}(r) D_{\gamma,\gamma} \right)_{v_{\gamma},v_{\gamma}} \sigma_{v_{\gamma}v_{\gamma}}^{\sigma'\sigma} \right]_{0}^{\tau'\tau} 0. \tag{36}
\]

In turn, potentials \( U^{t}_{\gamma}(r) \) were derived as linear combinations of the secondary densities,
\[
U^{t}_{\gamma}(r) = \sum_{\alpha\beta}\sum_{\delta} C^{\beta,t}_{\alpha\gamma} D^{\delta}_{\beta}(r) J_{\gamma}, \tag{37}
\]
where \( C^{\beta,t}_{\alpha\gamma} \) are numerical coefficients. We call the one-body operator \( \hat{\Gamma}_{\tau'\tau}^{\sigma'\sigma}(r) \) pseudopotential, because it is defined in terms of potentials \( U^{t}_{\gamma}(r) \) and differential operators \( D_{\gamma,\gamma} \) acting on single-particle wave functions. We note here, that in Eqs. (35) and (36), potentials always appear to the left of all derivatives; nonetheless, the one-body pseudopotential is a hermitian operator, which is guaranteed by specific conditions obeyed by potentials \( U^{t}_{\gamma}(r) \), which were derived in Ref. [22].

For the one-body pseudopotential (34), the Schrödinger equation that gives the time evolution of single-particle Kohn-Sham wave functions in space coordinates reads,
\[
\hbar \frac{\partial}{\partial t} \phi_{i}(r,\sigma,\tau, t) = -\hbar^{2} \frac{\Delta \phi_{i}(r,\sigma,\tau, t)}{2m} + \sum_{\sigma',\tau'} \hat{\Gamma}_{\tau'\tau}^{\sigma'\sigma}(r) \phi_{i}(r,\sigma',\tau', t). \tag{38}
\]

By multiplying the Schrödinger equation with the complex-conjugated wave function, \( \phi_{i}^{*}(r,\sigma',\tau', t) \) and summing over the single-particle index \( i \) we obtain the time-evolution equation of the density matrix (12), that is,
\[
\hbar \frac{\partial}{\partial t} \rho(r,\sigma,\tau', \sigma',\tau', t) = -\hbar^{2} \frac{\Delta - \Delta'}{2m} \rho(r,\sigma,\tau, \sigma',\tau', t) + \sum_{\sigma''\tau''} \left( \hat{\Gamma}_{\tau''\tau'}^{\sigma''\sigma'''}(r) \rho(r,\sigma''\tau'', \sigma',\tau', t) - \hat{\Gamma}_{\tau''\tau'}^{\sigma''\sigma'''}(r') \rho(r,\sigma,\tau, \sigma''\tau'', t) \right). \tag{39}
\]

Before we proceed, we must first consider the complex-conjugated pseudopotential \( \hat{\Gamma}_{\tau''\tau'}^{\sigma''\sigma'''}(r') \). To this end, we use the property of the Biedenharn-Rose phase convention employed in Refs. 16, 22, by which all scalars are always real. Note that for the spherical representation of Pauli matrices, the Biedenharn-Rose phase convention implies the transposition of spin indices, that is,
\[
\left( \sigma_{\psi \mu}^{\sigma'\sigma} \right)^{*} = (-1)^{v+\mu} \sigma_{\psi,\mu}^{\sigma'\sigma}. \tag{40}
\]
where \( \mu = 0 \) for \( v = 0 \) and \( \mu = -1, 0, 1 \) for \( v = 1 \) denote tensor components of scalar and vector Pauli matrices, respectively.

Finally, in Eqs. 36 and 37, the complex conjugation only affects coefficients \( \chi^{\beta;\delta}_{\alpha,\sigma,\gamma} \) which gives,
\[
\hat{\Gamma}_{\tau''\tau'}^{\sigma''\sigma'''}(r') = \hat{\Gamma}_{\tau''\tau'}^{\sigma''\sigma'''}(r'), \tag{41}
\]
for
\[
\hat{\Gamma}_{\tau''\tau'}^{\sigma''\sigma'''}(r') = \sum_{\gamma,t} \left[ \left( U_{\gamma}^{t}(r') D_{\gamma,\gamma} \right)_{v_{\gamma},v_{\gamma}} \sigma_{v_{\gamma}v_{\gamma}}^{\sigma''\sigma'''} \right]_{0}^{\tau''\tau'} 0. \tag{42}
\]
and
\[
U^{t}_{\gamma}(r') = \sum_{\alpha\beta}\sum_{\delta} (-1)^{n_{\gamma}+m_{\gamma}+m_{d}} C^{\beta,t}_{\alpha\gamma} \chi^{\beta;\delta}_{\alpha,\sigma,\gamma} D^{\delta}_{\beta}(r') J_{\gamma}. \tag{43}
\]
It means that in all further derivations we must use the second set of potentials \( U^{t}_{\gamma}(r') \) with signs of terms modified according to the phase \((-1)^{n_{\gamma}+m_{\gamma}+m_{d}} \). It is now obvious that the CEs will hold independently of the spin-isospin coordinates if, and only if, the pseudopotentials fulfill the condition
\[
\sum_{\sigma''\tau''} \left( \hat{\Gamma}_{\tau''\tau'}^{\sigma''\sigma'''}(r) \rho(r,\sigma''\tau'', \sigma',\tau') - \hat{\Gamma}_{\tau''\tau'}^{\sigma''\sigma'''}(r') \rho(r,\sigma,\tau, \sigma''\tau'', t) \right)_{r'=r} = 0. \tag{44}
\]

We are now in a position to separate the four spin-isospin channels in Eq. (39). We do so by multiplying both sides of the equation with \( \sigma_{\psi \mu}^{\sigma''\sigma'''}(r) \) and summing over \( \sigma,\tau, \sigma',\tau' \). From Eq. (44) it is then obvious that, in close analogy to Sec. 11A, after setting \( r' = r \), we obtain the CEs (28) in the four spin-isospin channels, provided terms coming from one-body pseudopotentials do not contribute, as in Eq. (44). When evaluating this condition for the four spin-isospin channels, we use the expression for the trace of three Pauli matrices in spherical representation, which reads [32],
\[
\text{Tr} \left[ \sigma_{\psi \mu}^{\sigma} \sigma_{\psi \mu'}^{\sigma'} \sigma_{\psi \mu'}^{\sigma''} \right] = A(v + v' + v'')(1)^{-\mu} C_{\psi \mu \psi \mu'}^{\sigma \sigma'}, \tag{45}
\]
where we introduced \( A(v + v' + v'') \) as a shorthand symbol for numerical coefficients coming from the computation of the trace. In the calculation, we only need values of \( A(0) = 2, A(2) = 2\sqrt{3}, A(3) = 2\sqrt{7} i \). After a trivial but lengthy calculation, we obtain the final result:
For our practical implementation of the CE condition \([\text{Ref.} \, 10]\), we proceed by transforming the two differential operators, \(D_{n\gamma L\gamma}\) and \(D_{nL'}\), which act on two different variables \(r\) and \(r'\), respectively, with the recoupling methods developed in Ref. \([\text{Ref.} \, 22]\), and we obtain,

\[
D_{n\gamma L\gamma} = \sum_{nL'n'\gamma} K^{nL'nL'}_{nL'nL'}(i)^{n-n'} [D_{n'L''}\, L_{nL'}]_{L\gamma}, \quad (47)
\]

\[
D'_{n\gamma L\gamma} = \sum_{nL'n'\gamma} K^{nL'nL'}_{nL'nL'}(-i)^{n-n'} [D_{n'L''}\, L_{nL'}]_{L\gamma}, \quad (48)
\]

On the right-hand sides, operators \(K_{nL}\) are the higher-order spherical tensor derivatives \([18]\) built of the relative momenta, \(k = (\mathbf{v} - \mathbf{v}')/2t\), and operators \(D_{n'L'}\) act on variable \(r\) after one sets \(r' = r\). The 91 numerical coefficients \(K^{nL'nL'}_{nL'nL'}\), which are needed up to \(N^3\)LO, have been derived in Ref. \([22]\). By using Eqs. \((47)\) and \((48)\), one can express the last line of the Eq. \((49)\) as a linear combination of products of pairs of secondary densities coupled in the spin and isospin spaces to ranks \(v\) and \(t\), respectively. This final form, which for brevity is not shown here explicitly, is used in obtaining the results of Sec. \[\text{III}\]

### III. CONTINUITY EQUATIONS IN THE FOUR SPIN-ISOSPIN CHANNELS

Condition \([\text{Ref.} \, 10]\) sets constraints on the coupling constants \(C_{i,j}^{L,T}\) of the EDF. In our study, these explicit constraints were obtained, with the aid of the symbolic programming, as solutions of a linear system of equations, where each equation is found by considering the coefficients standing at a given product of pairs of secondary densities. Indices \((i,j)\) correspond to the choice of the channel under examination: \((0,0)\) for the CE in the scalar-isoscalar channel, \((0,1)\) for the CE in the scalar-isovector channel, \((1,0)\) for the CE in the vector-isoscalar channel, and \((1,1)\) for the CE in the vector-isovector channel.

As a result of this analysis, for each spin-isospin channel we can classify the coupling constants in four categories defined in Ref. \([10]\), namely, unrestricted, vanishing, independent, and dependent. The unrestricted coupling constants are not affected by condition \((49)\) and vanishing ones are forced by this condition to be equal to zero. The remaining coupling constants obey sets of linear conditions, whereby one can express the dependent ones through independent ones. Obviously, for a given set of linear conditions, this can be done in very many different ways; below we present in each case only one choice thereof. We also use the name of a free coupling constant to denote either the unrestricted or independent one.

The structure of this section is as follows. First, in Table \(\text{III}\) we present for the four spin-isospin channels an overview of results by showing the number of unrestricted (U), vanishing (V), independent (I), and dependent (D) coupling constants of the EDF. The sum of the unrestricted and independent coupling constants gives the number of the free ones. Second, in Sec. \[\text{III A}\] we discuss the simplest case of the zero-order terms, where one-body pseudopotentials reduce to simple potential functions, and we can link our results to those presented in the introductory Sec. \[\text{II A}\]. Next, in Sec. \[\text{III C}\] we briefly describe the results obtained for the standard CE in the scalar-isoscalar channel. For the CEs in the three other spin-isospin channels, we present our results in Secs. \[\text{III B}\] and \[\text{III E}\], where, for clarity, only the second-order terms and general rules are discussed, while the results for fourth and sixth orders are collected in Appendices \[\text{A}\] and \[\text{C}\].

### A. Constraints for zero-order terms

For zero-order terms, condition \([\text{Ref.} \, 10]\) gives no constraints on the coupling constants, apart from those in the vector-isovector channel, where we have,

\[
C_{00,0000}^{0000,1} = \frac{1}{\sqrt{3}} C_{00,0000}^{0001,1}, \quad (49a)
\]

\[
C_{00,0010}^{0000,1} = \frac{1}{\sqrt{3}} C_{00,0000}^{0011,1}\quad (49b)
\]

whereas the coupling constant \(C_{00,0000}^{0000,0}\) is unrestricted.

It is interesting to discuss these results in connection with the derivation of the CE for a spin-\(\frac{1}{2}\) particle moving in a local potential, which we gave in Sec. \[\text{II A}\]. There, we pointed out that the CE in the vector channel is valid when the vector potential is parallel to the spin density. Exactly this situation occurs for the zero-order EDF, where in each spin-isospin channel the potential functions are simply proportional to densities.

In fact, the simple algebraic rule of the vector product in Eq. \((1)\) is equivalent to the coupling of pairs of identical commuting rank 1 tensors to rank 1, which is...
TABLE I: Number of unrestricted (U), vanishing (V), independent (I), and dependent (D) coupling constants of different orders in the EDF up to N^3LO, shown for the four spin-isospin channels.

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

Identically null. This is just the case for the coupling to rank v = 1 (t = 1) in the spin (isospin) space for the vector-isoscalar (scalar-isovector) channel of the CE, in which the identically null tensors formed by the pairs of densities at zero order leave the corresponding coupling constants unrestricted. However, when the coupling to a rank-1 tensor is simultaneously performed in both spin and isospin space (v = 1 and t = 1), as is the case in the vector-isovector channel of the CE, the two negative signs in the commutation of the pair of densities give an overall positive sign, and the above selection rule does not apply. This explains why, at zero order of the vector-isovector channel, condition (46) does induce constraints on coupling constants – those given in Eqs. (49a) and (49b).

**B. Constraints for the scalar-isoscalar channel**

For the standard CE in the scalar-isoscalar channel, Eq. (25), the constraints that we found from Eq. (46) are exactly the same as those defining the gauge-invariant functional up to N^3LO. This constitutes an explicit verification of the general result presented in Sec. II B 1. As in Ref. 10, we obtained two sets of independent constraints, one for the isoscalar coupling constants C_{a,0}^{β,0} and one for the isovector coupling constants C_{a,α}^{β,1}. Within each isospin channel, the linear conditions for the scalar coupling constants, C_{aαLαJα}^{n,0}J_{β}^{0,t}, are disconnected from the linear conditions for the vector coupling constants, C_{aαLαJα}^{n,0}J_{β}^{1,t}, C_{aαLαJα}^{n,0}J_{β}^{1,t}, and C_{aαLαJα}^{n,0}J_{β}^{1,t}.

**C. Constraints for the scalar-isovector channel**

Validity of the CE for the scalar-isovector density, Eq. (28) for v = 0 and t = 1, imposes through Eq. (46) certain specific constraints on the coupling constants of the functional. At second order we obtain,

\[ C_{0000,t}^{00,2000} = -\frac{3}{\sqrt{3}} C_{0011,t}^{00,1101,1-t}, \]

(50a)

\[ C_{1110,t}^{00,1110} = -\frac{3}{\sqrt{3}} C_{0011,t}^{00,1201} - \frac{3}{\sqrt{3}} \sqrt{C_{0011,t}^{00,2211}}, \]

(50b)

\[ C_{1111,t}^{00,1111} = \frac{3}{\sqrt{3}} C_{0011,t}^{00,1201} + \frac{3}{\sqrt{3}} \sqrt{C_{0011,t}^{00,2211}}, \]

(50c)

\[ C_{1112,t}^{00,1112} = -\frac{3}{\sqrt{3}} C_{0011,t}^{00,1201} - \frac{3}{\sqrt{3}} \sqrt{C_{0011,t}^{00,2211}}, \]

(50d)

\[ C_{0000,t}^{1101,t} = C_{0000,t}^{1101,t}, \]

(50e)

\[ C_{20,0000}^{0011,1200,0011} = C_{20,0000}^{0011,1200,0011} = 0. \]

(50f)

Constraints in Eqs. (50a)–(50f) connect the isoscalar and isovector coupling constants. The numerical coefficients of the corresponding linear combinations are the same as those for the scalar-isoscalar CE, see Eqs. (C1)–(C4) of Ref. 16, apart from factors of \(\sqrt{3}\) explained before Eq. (34). However, conditions for the scalar-isoscalar CE keep the coupling constants in the two isospin channels disconnected. Moreover, in the scalar-isovector channel the spin-orbit coupling constants must vanish, Eq. (50c), along with the isovector surface coupling constants, Eq. (50f). On the other hand, the corresponding isoscalar surface coupling constants, C_{20,0000}^{0011,0}, C_{20,0011}^{0011,0}, and C_{22,0011}^{0011,0}, are left unrestricted.

For the fourth and sixth orders, analogous constraints are presented in Appendix A.

**D. Constraints for the vector-isoscalar channel**

Validity of the CE for the vector-isoscalar density, Eq. (28) for v = 1 and t = 0, imposes through Eq. (46) at second order the following constraints on the coupling

...
constants of the functional,

\begin{align}
C_{00,1110}^{1101, t} &= -\frac{1}{\sqrt{3}} C_{00,2011}^{0011, t}, \\
C_{00,1111}^{1110, t} &= -\frac{1}{\sqrt{3}} C_{00,2000}^{0000, t}, \\
C_{00,1111}^{1111, t} &= -C_{00,2000}^{1100, t}, \\
C_{00,1112}^{1112, t} &= -\sqrt{\frac{5}{3}} C_{00,2000}^{0000, t}, \\
C_{00,2211}^{0011, t} &= -C_{22,0011}^{1101, t}, \\
C_{20,2211}^{0011, t} &= 0,
\end{align}

(51a)

(51b)

(51c)

(51d)

(51e)

(51f)

(51g)

whereas the two coupling constants \(C_{00,0000}^{0000, t}\) are left unrestricted. We note here that the constraints now connect scalar and vector coupling constants. Altogether, at second order, for the vector-isoscalar channel of the CE we have 6 free and 8 dependent coupling constants. Apart from that, 10 second-order coupling constants must vanish, which includes the surface ones in Eq. (51c), spin-orbit ones of the Eq. (51d), and tensor ones in Eq. (51e).

For the fourth and sixth orders, analogous constraints are presented in Appendix B.

E. Constraints for the vector-isovector channel

Validity of the CE for the vector-isovector density, Eq. (48) for \(v = 1\) and \(t = 1\), imposes through Eq. (46) constraints on the coupling constants that relate them in both spin and isospin spaces. At all the orders, we can express all dependent coupling constants through only one vector coupling constant, which can be chosen either in the set of the vector-isoscalar or vector-isovector ones. At second order, these constraints read,

\begin{align}
C_{00,2000}^{0000, t} &= -\sqrt{3}(\sqrt{3}) C_{00,1110}^{1101, t}, \\
C_{00,1111}^{1110, t} &= \sqrt{3}(\sqrt{3}) C_{00,1100}^{1110, t}, \\
C_{00,1111}^{1111, t} &= \sqrt{3}(\sqrt{3}) C_{00,1110}^{1111, t}, \\
C_{00,1112}^{1112, t} &= \sqrt{3}(\sqrt{3}) C_{00,1100}^{1112, t}, \\
C_{20,0011}^{0011, t} &= -3(\sqrt{3}) C_{00,1100}^{1110, t}, \\
C_{20,0011}^{0011, t} &= C_{22,0011}^{1101, t} = 0, \\
C_{20,0000}^{0000, t} &= 0, \\
C_{20,0000}^{0000, t} &= 0, \\
C_{11,0011}^{1111, t} &= C_{11,0011}^{1111, t} = 0,
\end{align}

(52a)

(52b)

(52c)

(52d)

(52e)

(52f)

(52g)

(52h)

(52i)

(52j)

and only coupling constant \(C_{20,0000}^{0000, t}\) is unrestricted. Altogether, at second order for the vector-isovector channel of the CE we have 2 free coupling constants and 11 coupling constants that are dependent. All the remaining 11 second-order coupling constants, which includes the surface ones in Eqs. (52a), (52h), the tensor ones in Eq. (52i), and spin-orbit ones in Eq. (52j), are forced to be equal to zero.

For the fourth and sixth orders, analogous constraints are presented in Appendix B.

IV. CONCLUSIONS

In the present work, we have derived sets of constraints on the coupling constants of the N\(^3\)LO energy density functional that guarantee the validity of the continuity equation in the four spin-isospin channels. In the scalar-isoscalar channel, these constraints are identical to those induced by the standard local gauge invariance conditions. We extended this connection to vector and isovector channels, where the validity of the continuity equations is equivalent to the local gauge invariance with respect to spin and isospin rotations, respectively.

We note here that in our analysis we implicitly assumed that all densities that build the N\(^3\)LO energy density functional are nonzero. Of course, there can be many specific situations when some densities vanish, and thus the coupling constants related to them become unrestricted. This occurs, for instance, when densities are restricted by some symmetry conditions. Obviously, the methods developed in the present work can then be applied to derive new (weaker) sets of constraints that correspond to each one particular case. For example, when the proton-neutron symmetry is conserved, see, e.g., Refs. [31, 32], the ±1 components of all isovector densities (\(v = 1\)) vanish, and the energy density is invariant with respect to a one-dimensional U(1) gauge rotation in the isospin space, that is, with respect to \(U = \exp(i\gamma_{10}\tau^{10})\). Then, the continuity equations for neutrons and protons decouple from one another and become independently valid, provided the isoscalar and isovector coupling constants independently obey the standard gauge-invariance conditions.

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Appendix A: Constraints for the scalar-isovector channel (fourth and sixth orders)

At fourth order we found that the isoscalar and isovector coupling constants are connected or not depending on the parity of quantum numbers \(n\). Moreover, similarly as for the scalar-isoscalar channel of the CE, the
scalar and vector coupling constants are kept apart. The constraints among the scalar coupling constants read,

\[ C_{00,00}^{0000.t} = \frac{3C_{202,t}^{2222}}{2\sqrt{5}}, \quad C_{00,00}^{2000.t} = \frac{1}{2}\sqrt{5}C_{00,2222}^{202.t}, \quad C_{00,00}^{1101.t} = -2\sqrt{\frac{3}{5}}C_{00,2222}^{2222}, \quad C_{00,00}^{3101.t} = -2\sqrt{\frac{3}{5}}C_{00,2222}^{2222}, \]

and those among the vector coupling constants read,

\[ C_{00,3110}^{1110.t} = -2\sqrt{\frac{3}{5}}C_{00,2222}^{2222} - \frac{7}{\sqrt{15}}3^{t}C_{00,4211}^{0011}, \quad C_{00,3111}^{1111.t} = -2(3^{t})\sqrt{\frac{3}{5}}C_{00,2222}^{2222}, \quad C_{00,3112}^{1112.t} = -2(3^{t})C_{00,2222}^{2222} - \frac{14}{3^{t}}\sqrt{\frac{5}{3}}C_{00,4211}^{0011}, \quad C_{00,3312}^{1112.t} = -2\sqrt{\frac{3}{5}}C_{00,2222}^{2222} - \frac{7}{\sqrt{15}}C_{00,4211}^{0011}, \]

We also found that the fourth-order surface isovector coupling constants must vanish,

\[ C_{00,00}^{0000,1} = C_{00,00}^{0011,1} = C_{00,4201}^{0011,1} = 0, \]

whereas the corresponding isoscalar coupling constants are unrestricted. Apart from the coupling constants discussed above, all the remaining 54 fourth-order coupling constants are forced to be equal to zero.

In the same way, at sixth order we found the following constraints for the scalar,

\[ C_{00,00}^{0000,1} = 3C_{00,3303}^{202,1-t} - 3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \quad C_{00,00}^{1110,1} = -3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \quad C_{00,00}^{1111,1} = -3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \quad C_{00,00}^{1112,1} = -3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \quad C_{00,00}^{1113,1} = -3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \quad C_{00,00}^{1114,1} = -3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \]

and vector coupling constants,

\[ C_{00,00}^{0000,1} = 3C_{00,3303}^{202,1-t} - 3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \quad C_{00,00}^{1110,1} = -3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \quad C_{00,00}^{1111,1} = -3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \quad C_{00,00}^{1112,1} = -3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \quad C_{00,00}^{1113,1} = -3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \quad C_{00,00}^{1114,1} = -3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \]

We also found that the sixth-order surface isovector coupling constants must vanish,

\[ C_{00,00}^{0000,1} = 3C_{00,3303}^{202,1-t} - 3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \quad C_{00,00}^{1110,1} = -3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \quad C_{00,00}^{1111,1} = -3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \quad C_{00,00}^{1112,1} = -3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \quad C_{00,00}^{1113,1} = -3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \quad C_{00,00}^{1114,1} = -3^{t}\sqrt{\frac{3}{5}}C_{00,4211}^{0011,1-t}, \]

whereas the corresponding isoscalar coupling constants are unrestricted. Apart from the coupling constants discussed above, all the remaining 200 sixth-order coupling constants are forced to be equal to zero.

We have seen that for the scalar-isovector channel, the coupling constants are diagonal or nondiagonal in the isospin quantum number \( t \). We can understand this point considering the fact that in order to separate the scalar-isovector channel of the CE and obtain condition
that all the remaining fourth-order coupling constants are
Apart from these 6 free and 20 dependent coupling con-
can be produced by two terms of the functional that are
isospin space.

Appendix B: Constraints for the vector-isoscalar
channel (fourth and sixth orders)

At fourth order, we again found two identical sets of linear combinations of the isoscalar and isovector coupling constants, in which the scalar and vector coupling constants are in same case connected to one another, that is,

\[
C_{00,4000} = \frac{3C_{2202,t}}{2\sqrt{5}}, \quad (B1)
\]
\[
C_{00,2000} = \frac{1}{2}\sqrt{5}C_{00,2202} \quad (B2)
\]
\[
C_{00,3101} = \frac{6C_{2212,t}}{\sqrt{5}} \quad (B3)
\]
\[
C_{00,3110} = -2\sqrt{\frac{3}{5}}C_{00,2202} \quad (B4)
\]
\[
C_{00,3111} = \frac{6C_{2202}}{\sqrt{5}} \quad (B5)
\]
\[
C_{00,3112} = -2\sqrt{\frac{3}{5}}C_{00,2202} \quad (B6)
\]
\[
C_{00,4011} = \frac{3}{2}\sqrt{\frac{3}{5}}C_{2212,t} \quad (B7)
\]
\[
C_{00,2011} = \frac{1}{2}\sqrt{15}C_{00,2212} \quad (B8)
\]
\[
C_{00,2211} = \sqrt{\frac{3}{5}}C_{2212,t} \quad (B9)
\]
\[
C_{00,2213} = \frac{3}{5}C_{2212,t} \quad (B10)
\]
\[
C_{00,2211} = C_{1112,t,00,3312} = C_{0011,t,00,4212} = 0, \quad (B11)
\]

with the two coupling constants $C_{00,4000}$ left unrestricted.

Apart from these 6 free and 20 dependent coupling constants, the vector-isoscalar channel of the CE requires that all the remaining fourth-order coupling constants are forced to be equal to zero. In particular in the Eq. (B11) we showed the vanishing coupling constants, belonging to the set of ones with indices $m = 0$ and $I = 0$, which were found to be non-vanishing in the scalar-isoscalar channel.

At sixth order the pattern of the results is the same, and we have,

\[
C_{00,3303} = \frac{1}{3}\sqrt{\frac{7}{15}}C_{2212,t,00,4212} \quad (B12)
\]
\[
C_{00,00,6000} = \frac{1}{2\sqrt{15}}C_{1112,t,00,5112} \quad (B13)
\]
\[
C_{00,00,4000} = \frac{7C_{1112,t,00,5112}}{2\sqrt{15}} \quad (B14)
\]
\[
C_{2202,t,00,4202} = -\frac{2C_{1112,t,00,5112}}{\sqrt{3}} \quad (B15)
\]
\[
C_{00,5101} = \frac{3C_{2212,t,00,4212}}{2\sqrt{5}} \quad (B16)
\]
\[
C_{00,3101} = \frac{21C_{2212,t,00,4212}}{10\sqrt{5}} \quad (B17)
\]
\[
C_{00,5110} = \frac{3C_{1112,t,00,5112}}{\sqrt{5}} \quad (B18)
\]
\[
C_{00,5111} = \frac{\sqrt{7}}{5}C_{1112,t,00,5112} \quad (B19)
\]
\[
C_{00,3110} = \frac{7C_{1112,t,00,5112}}{5\sqrt{5}} \quad (B20)
\]
\[
C_{00,3111} = \frac{7C_{1112,t,00,5112}}{5\sqrt{5}} \quad (B21)
\]
\[
C_{00,3112} = \frac{2}{9C_{1112,t,00,5112}} \quad (B22)
\]
\[
C_{00,3113} = \frac{2}{9\sqrt{5}}C_{1112,t,00,5112} \quad (B23)
\]
\[
C_{00,3114} = \frac{2}{9\sqrt{5}}C_{1112,t,00,5112} \quad (B24)
\]
\[
C_{00,4011} = \frac{3}{4}\sqrt{\frac{3}{5}}C_{2212,t,00,4212} \quad (B25)
\]
\[
C_{00,4011} = \frac{1}{4}\sqrt{\frac{3}{5}}C_{2212,t,00,4212} \quad (B26)
\]
\[
C_{00,4011} = \frac{7}{5}\sqrt{\frac{3}{5}}C_{2212,t,00,4212} \quad (B27)
\]
\[
C_{00,4211} = \sqrt{\frac{3}{5}}C_{2212,t,00,4212} \quad (B28)
\]
\[
C_{00,4213} = \sqrt{\frac{3}{5}}C_{2212,t,00,4212} \quad (B29)
\]
\[
C_{00,4211} = \sqrt{\frac{3}{5}}C_{2212,t,00,4212} \quad (B30)
\]
\[
C_{00,3312} = \frac{3}{5}C_{1112,t,00,5312} = C_{0011,t,00,6211} = 0, \quad (B31)
\]

with the two coupling constants $C_{00,00,6000}$ left unrestricted.

Apart from these 6 free and 36 dependent coupling constants, the vector-isoscalar channel of the CE requires that all the remaining sixth-order coupling constants are forced to be equal to zero. As before, we listed explicitly the vanishing coupling constants (see Eqs. (B30)–(B31)), which were found to be non-vanishing in the scalar-isoscalar channel.
The general rule that we have specified at the end of the Appendix A can be applied now to explain the results of this section, where at all the orders we found constraints that are nondiagonal in the spin space. Here, the reason is the possibility of having pairs of secondary densities that are coupled to rank \( v = 1 \). These pairs can appear at both scalar and vector coupling constants, which results in relating them to one another.

Appendix C: Constraints for the vector-isovector channel (fourth and sixth orders)

At fourth order we found the following constraints,

\[
\begin{align*}
C_{0000,t}^{00,0000} &= (\sqrt{3})^2 \frac{C_{0011,0}^{00,0011}}{\sqrt{3}}, \\
C_{2000,t}^{00,0000} &= (\sqrt{3})^5 C_{0011,0}^{00,0011}, \\
C_{1101,t}^{00,0011} &= (\sqrt{3})^4 C_{0011,0}^{00,0011}, \\
C_{2202,t}^{00,0000} &= (\sqrt{3})^6 \frac{C_{0011,0}^{00,0011}}{\sqrt{3}}, \\
C_{1110,t}^{00,0011} &= (\sqrt{3})^4 C_{0011,0}^{00,0011}, \\
C_{1111,t}^{00,0011} &= (\sqrt{3})^4 C_{0011,0}^{00,0011}, \\
C_{1112,t}^{00,0011} &= (\sqrt{3})^4 C_{0011,0}^{00,0011}, \\
C_{0011,0}^{00,0011} &= (\sqrt{3})^6 C_{0011,0}^{00,0011}, \\
C_{2211,t}^{00,0011} &= (\sqrt{3})^4 C_{0011,0}^{00,0011}, \\
C_{2212,t}^{00,0011} &= (\sqrt{3})^4 C_{0011,0}^{00,0011}, \\
C_{2213,t}^{00,0011} &= (\sqrt{3})^4 C_{0011,0}^{00,0011}, \\
C_{2011,t}^{00,0011} &= C_{1112,t}^{00,00312} = C_{0011,0}^{00,004211} = 0, \\
\end{align*}
\]

and only coupling constant \( C_{0000,0000}^{00,0000} \) is unrestricted. Apart from these 2 free and 23 dependent coupling constants, the vector-isovector channel of the CE requires that all the remaining fourth-order coupling constants are forced to be equal to zero. In particular in the Eq. \[ \text{C13} \] we showed the vanishing coupling constants, which were found to be non-vanishing in the scalar-isoscalar channel.

At sixth order we have,

\[
\begin{align*}
C_{0000,t}^{00,0000} &= -(\sqrt{3})^7 C_{0011,0}^{00,0011}, \\
C_{2000,t}^{00,0000} &= -(\sqrt{3})^3 \frac{C_{1112,0}^{00,0011}}{2\sqrt{15}}, \\
C_{2202,t}^{00,0000} &= -(\sqrt{3})^3 \frac{C_{1112,0}^{00,0011}}{2\sqrt{15}}, \\
C_{1101,t}^{00,0011} &= (\sqrt{3})^3 \frac{C_{1112,0}^{00,0011}}{\sqrt{3}}, \\
C_{1111,t}^{00,0011} &= (\sqrt{3})^3 \frac{C_{1112,0}^{00,0011}}{\sqrt{3}}, \\
C_{1112,t}^{00,0011} &= (\sqrt{3})^3 \frac{C_{1112,0}^{00,0011}}{\sqrt{3}}, \\
C_{1113,t}^{00,0011} &= (\sqrt{3})^3 \frac{C_{1112,0}^{00,0011}}{\sqrt{3}}, \\
C_{1114,t}^{00,0011} &= (\sqrt{3})^3 \frac{C_{1112,0}^{00,0011}}{\sqrt{3}}, \\
C_{1115,t}^{00,0011} &= (\sqrt{3})^3 \frac{C_{1112,0}^{00,0011}}{\sqrt{3}}, \\
C_{1116,t}^{00,0011} &= (\sqrt{3})^3 \frac{C_{1112,0}^{00,0011}}{\sqrt{3}}, \\
\end{align*}
\]

and only coupling constant \( C_{0000,0000}^{00,0000} \) is unrestricted. Apart from 2 free and 39 dependent coupling constants, the vector-isovector channel of the CE requires that all the remaining sixth-order coupling constants are forced to be equal to zero.
to be equal to zero. In particular, in the Eqs. (C34)–(C35) we showed the vanishing coupling constants that were found to be non-vanishing in the scalar-isoscalar channel.

The results presented in this section show simultaneously both features we saw respectively in Appendices A and B. At all orders, one can express all coupling constants through only one independent coupling constant, in such a way that the constraints are nondiagonal in both spin and isospin space. Again, this fact is due to the rank of $v=1$ and $t=1$ in the pairs of densities in the final form of condition [46], which allows the coupling constants at different spins and isospins to enter into the same constraints.