Self-interaction errors in nuclear energy density functionals

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Abstract

When applied to a single nucleon, nuclear energy density functionals may yield a non-vanishing internal energy thus implying that the nucleon is interacting with itself. It is shown how to avoid this unphysical feature for semi-local phenomenological functionals containing all possible bilinear combinations of local densities and currents up to second order in the derivatives. The method outlined in this Rapid Communication could be easily extended to functionals containing higher order terms, and could serve as a guide for constraining the time-odd part of the functional.

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I. INTRODUCTION

The density functional theory (DFT) [1] has been very successfully employed in a wide variety of fields, from chemistry [2] to condensed matter physics [3–5]. A somehow similar approach called the nuclear energy density functional (EDF) theory, has been developed in nuclear physics [6]. Even though the EDF theory is very often referred to as nuclear DFT, it is conceptually different due to the breaking of various symmetries in its current formulations (see e.g. [7–9]). The EDF theory is a method of choice for describing the structure and the dynamics of medium-mass and heavy nuclei. Phenomenological nuclear functionals are now able to fit essentially all experimental nuclear mass data with rms deviations falling below 0.6 MeV [10]. Moreover the EDF theory is particularly well-suited for studying the dense inhomogeneous nuclear matter found in neutron stars and supernova cores.

Nevertheless it has been known for a long time in condensed matter physics that the internal energy of a single electron as calculated by the DFT may be non-zero owing to a spurious interaction of the electron with itself (for a recent review, see for instance Section I.B of Ref. [11] and references therein). This problem is not inherent to the DFT, but is induced by the use of approximate expressions for the electron exchange-correlation part which violate the Pauli exclusion principle. The presence of self-interaction causes various errors and is currently one of the main deficiencies of existing density functionals. For instance, this leads to an artificial spreading of the electron density owing to an incorrect asymptotic behavior of the Kohn-Sham potential. This spurious effect spoils the calculations of chemical properties. In particular, functionals contaminated by self-interactions fail to correctly describe the dissociation behavior of some homonuclear and heteronuclear diatomic radicals. The removal of self-interactions in the DFT has lead to the development of orbital-dependent density functionals [11, 12].

This self-interaction problem was also recognized a long time ago in nuclear physics [13, 14], but it has been barely discussed in the literature until recently [6, 9, 15–19]. Nuclear functionals have been traditionally derived from effective interactions using the Hartree-Fock approximation [15, 20] which guarantees that in the one-particle limit, the internal energy correctly vanishes due to the exact cancellation between direct and exchange terms. On the other hand, the development of nuclear functionals which are not directly constructed from effective forces [21–23] calls for a closer examination of their internal consistency.
In this Rapid Communication, it will be shown how to eliminate self-interaction errors in the one-nucleon limit in semi-local nuclear energy density functionals containing all possible bilinear combinations of local densities, currents and their derivatives up to second order.

II. SKYRME FORCE VERSUS NUCLEAR ENERGY DENSITY FUNCTIONAL

Throughout this paper, pure nucleon states will be assumed. The more general formalism involving neutron-proton mixing has been developed in Ref. [24]. The nuclear energy density functionals that we consider here are of the form

\[ E = E_{\text{kin}} + E_{\text{Coul}} + E_{\text{Sky}}, \]

where \( E_{\text{kin}} \) is the kinetic energy, \( E_{\text{Coul}} \) is the Coulomb energy and \( E_{\text{Sky}} = \int d^3r \mathcal{E}_{\text{Sky}}(r) \) is the nuclear energy. The latter is a functional of the density matrix in coordinate space assumed to be purely diagonal in isospin space with elements \( \rho_q(r, \sigma; r', \sigma') \) with \( q = n, p \) for neutron and proton respectively (denoting the spin states by \( \sigma, \sigma' = 1, -1 \) for spin up and spin down respectively). In particular, \( \mathcal{E}_{\text{Sky}}(r) \) can be expressed in terms of the following local densities and currents (\( \hat{\sigma} \) is used to indicate the Pauli spin matrices and \( \mu, \nu, \kappa \) are indices of Cartesian tensors):

(i) the density

\[ \rho_q(r) = \sum_{\sigma = \pm 1} \rho_q(r, \sigma; r, \sigma), \]

(ii) the kinetic density

\[ \tau_q(r) = \sum_{\sigma = \pm 1} \int d^3r' \delta(r - r') \nabla \cdot \nabla' \rho_q(r, \sigma; r', \sigma), \]

(iii) the current-vector density

\[ j_q(r) = -\frac{i}{2} \sum_{\sigma = \pm 1} \int d^3r' \delta(r - r') (\nabla - \nabla') \rho_q(r, \sigma; r', \sigma), \]

(iv) the spin pseudovector density

\[ s_q(r) = \sum_{\sigma, \sigma' = \pm 1} \rho_q(r, \sigma; r, \sigma') \langle \sigma' | \hat{\sigma} | \sigma \rangle, \]
(v) the spin pseudovector kinetic density

\[ T_{q\mu}(r) = \sum_{\sigma,\sigma'=\pm 1} \int d^3r' \delta(r-r') \nabla' \cdot \nabla' \rho_q(r, \sigma; r', \sigma') \langle \sigma' | \hat{\sigma}_\mu | \sigma \rangle \]  

(vi) the spin current pseudotensor density

\[ J_{q\mu}(r) = -\frac{i}{2} \sum_{\sigma,\sigma'=\pm 1} \int d^3r' \delta(r-r') (\nabla_{\mu} - \nabla'_{\mu}) \rho_q(r, \sigma; r', \sigma') \langle \sigma' | \hat{\sigma}_\nu | \sigma \rangle \]  

and (vii) the tensor-kinetic pseudovector density

\[ F_{q\mu} = \frac{1}{2} \sum_{\sigma,\sigma'=\pm 1} \sum_{\nu} \int d^3r' \delta(r-r') (\nabla_{\mu} \nabla'_{\nu} + \nabla'_{\mu} \nabla_{\nu}) \rho_q(r, \sigma; r', \sigma') \langle \sigma' | \hat{\sigma}_\nu | \sigma \rangle \]  

It is convenient to introduce the isospin index \( t = 0, 1 \) for isoscalar and isovector quantities respectively. Isoscalar quantities (also written without any subscript) are sums over neutrons and protons (e.g. \( \rho_0 = \rho = \rho_n + \rho_p \)) while isovector quantities are differences between neutrons and protons (e.g. \( \rho_1 = \rho_n - \rho_p \)). The energy density \( E_{\text{Sky}} \) constructed from all possible bilinear terms up to second order in the derivatives that are invariant under time reversal, space inversions and rotations, is given by

\[ E_{\text{Sky}} = \sum_{t=0,1} (E_t^{\text{even}} + E_t^{\text{odd}}) \]  

\[ E_t^{\text{even}} = C_t^0 \rho_t^2 + C_t^\Delta \rho_t \Delta \rho_t + C_t^\nabla J \rho_t \nabla \cdot J_t + C_t^J \sum_{\mu,\nu} J_{t,\mu\nu} J_{t,\nu\mu} \] 

\[ + \frac{1}{2} C_t^{TrJ} \left( \sum_{\mu} J_{t,\mu\mu} \right)^2 + \frac{1}{2} C_t^{J^2} \sum_{\mu,\nu} J_{t,\mu\nu} J_{t,\nu\mu} \]  

\[ E_t^{\text{odd}} = C_t^s \rho_t^2 + C_t^{\Delta s} \Delta \rho_t \cdot \Delta s_t + C_t^T s_t \cdot T_t + C_t^J j_t^2 + C_t^{\nabla j} s_t \cdot \nabla \times j_t + C_t^{\nabla^2} (\nabla \cdot s_t)^2 \] 

\[ + C_t^F s_t \cdot F_t \]  

The “time-even” part \( E_t^{\text{even}} \) (“time-odd” part \( E_t^{\text{odd}} \)) contains only even (odd) densities and currents with respect to time reversal. In situations for which the time-reversal symmetry is preserved, the time-odd densities \( j_q(r), s_q(r), T_q(r) \) and \( F_q(r) \) must vanish. The coupling “constants” \( C_t^0 \) and \( C_t^\sigma \) generally depend on the isoscalar density \( \rho = \rho_n + \rho_p \) as follows

\[ C_t^\sigma = a_t^\sigma + b_t^\sigma \rho^\alpha \]  

(10)
The spin-current vector density $J_q(r)$ appearing in Eq. (9b) is defined by

$$J_q(r) = \sum_{\mu} \epsilon_{\mu \nu \kappa} J_{q \nu \kappa}$$

where $\epsilon_{\mu \nu \kappa}$ is the Levi-Civita tensor. Gauge (including Galilean) invariance imposes the following relations [25, 26]

$$C_i^j = -C_i^r, \quad C_i^j = -C_i^T, \quad C_i^{\Sigma j} = C_i^{\Sigma J}, \quad C_i^{TrJ} = -C_i^{F} = C_i^{J^z}.$$  \hspace{1cm} (13)

Historically the type of functionals given by Eqs. (1) and (9a)-(9c) was obtained from the Hartree-Fock approximation using effective zero-range interactions of the Skyrme type [15, 20, 24, 27]

$$v_{i,j} = t_0(1 + x_0 P_\sigma)\delta(r_{ij}) + \frac{1}{2} t_1(1 + x_1 P_\sigma) \frac{1}{\hbar^2} [p_{ij}^2 \delta(r_{ij}) + \delta(r_{ij}) p_{ij}^2]$$

$$+ t_2(1 + x_2 P_\sigma) \frac{1}{\hbar^2} [p_{ij} \cdot \delta(r_{ij}) p_{ij} + \frac{1}{6} t_3(1 + x_3 P_\sigma) \rho(r)^A \delta(r_{ij})$$

$$+ \frac{i}{\hbar^2} W_0(\hat{\sigma}_i + \hat{\sigma}_j) \cdot p_{ij} \times \delta(r_{ij}) p_{ij}$$

$$+ \frac{1}{2} t_c \left[ 3(\hat{\sigma}_i \cdot p_{ij}) (\hat{\sigma}_j \cdot p_{ij}) - (\hat{\sigma}_i \cdot \hat{\sigma}_j) p_{ij}^2 \right] \delta(r_{ij}) + \delta(r_{ij}) \left[ 3(\hat{\sigma}_i \cdot p_{ij}) (\hat{\sigma}_j \cdot p_{ij}) - (\hat{\sigma}_i \cdot \hat{\sigma}_j) p_{ij}^2 \right]$$

$$+ t_a \left[ 3(\hat{\sigma}_i \cdot p_{ij}) \delta(r_{ij}) (\hat{\sigma}_j \cdot p_{ij}) - (\hat{\sigma}_i \cdot \hat{\sigma}_j) p_{ij} \cdot \delta(r_{ij}) p_{ij} \right],$$ \hspace{1cm} (14)

where $r_{ij} = r_i - r_j$, $r = (r_i + r_j)/2$, $p_{ij} = -i\hbar(\nabla_i - \nabla_j)/2$ is the relative momentum and $P_\sigma$ is the two-body spin-exchange operator. The relations between the coupling constants in Eqs. (9b) and (9c) and the parameters of the effective force in Eq. (14), can be found for instance in Table I of Ref. [24]. The parameters of the force are generally fitted to a selected set of nuclear data, mainly involving the time-even part of the functional. The coupling constants of the time-odd terms are then obtained from those of the time-even terms making use of the aforementioned correlations (see e.g. Tables IV and VI in Ref. [26]). However, since time-odd terms are not directly fitted to experimental data it is rather unlikely that nuclear properties involving those terms will be correctly described in this way. In particular, one of the main deficiencies of Skyrme forces is that they predict the occurrence of spurious transitions to spin-ordered phases in the dense matter found in neutron stars and supernova cores [28, 30]. It has been recently found that finite-size instabilities could arise at even lower densities thus spoiling self-consistent calculations in finite nuclei [31, 32].
Over the past decades, the conventional wisdom has been to regard the nuclear energy density functional as being more fundamental than effective forces and the development of microscopic functionals using many-body techniques with realistic nucleon-nucleon interactions has triggered a burst of activity. Unfortunately such kinds of ab initio nuclear energy density functionals able to reproduce existing experimental nuclear data with the same degree of accuracy as effective interactions are not yet available. In the meantime semi-microscopic functionals have been constructed by first fitting the bulk part of the functional to realistic calculations of uniform infinite nuclear matter, and second adding a phenomenological surface part whose parameters are adjusted to reproduce properties of finite nuclei. A complementary approach guided by effective field theories consists in constructing semi-local phenomenological functionals from combinations of local densities and currents up to a given order in the derivatives that are invariant under time reversal, space inversion, spatial rotations and gauge transformations. The expansion in terms of higher-order derivatives has been shown to converge rapidly. The coupling constants associated with each term are then directly fitted to a selected set of nuclear data. However, such kinds of unrestricted fits could lead to formal inconsistencies. In particular the resulting functional may allow a nucleon to interact with itself. As will be discussed in the next section, this unphysical feature can be avoided by imposing suitable constraints on the coupling constants of the functional.

III. REMOVAL OF SELF-INTERACTION ERRORS

The cancellation of spurious self-interactions in nuclear energy density functionals was studied in Ref. [14]. The main assumption was that the nuclear functional can be calculated from the expectation value of some general Hamiltonian with a Slater determinant. However it remains to be proved that the exact functional can be obtained in this way. Moreover the nuclear functional was supposed to be purely local and depend on the densities and the spin densities only. In the following, the self-interaction problem will be reconsidered for any semi-local functionals given by Eqs. (1) and (9a)–(9c).

In the one-particle limit, the density matrix is simply given by \( \rho_q(r, \sigma; r', \sigma') = \varphi^{(q)}(r' \sigma')^* \varphi^{(q)}(r \sigma) \) where \( \varphi^{(q)}(r \sigma) \) is the single-nucleon wavefunction and the asterisk indicates complex conjugation. Inserting this expression into Eqs. (2)–(8), substituting in
Eqs. (9a)–(9c) and making use of the gauge invariance Eq. (13) yield

\[ \mathcal{E}_t^{\text{even}} + \mathcal{E}_t^{\text{odd}} = (C'_0 + C'_1) \varphi^\dagger \varphi + \left[ \frac{1}{4} (C'_1 - C'_T) - (C'_0 + C'_s) \right] \left[ \varphi^\dagger \nabla \varphi + (\nabla \varphi^\dagger) \varphi \right]^2 \]

\[ + (C'_T - 2C'T - 4C'_s - C'_F) \left[ (\varphi^\dagger \varphi)(\nabla \varphi^\dagger) \cdot \nabla \varphi - \varphi^\dagger (\nabla \varphi) \cdot (\nabla \varphi^\dagger) \right] \]

\[ + \left( \frac{1}{4} C'_F + C'_s \right) \left[ \sum_{\mu} \varphi^\dagger \sigma^\mu \nabla_{\mu} \varphi + (\nabla_{\mu} \varphi^\dagger) \sigma^\mu \varphi \right]^2 \]

(15)

where \( \varphi \) denotes the two-component spinor wavefunction and the superscript \( \dagger \) indicates the adjoint operation. Now the functional should be devoid of self-interactions whether the nucleon is free or is embedded in an external potential, i.e. for any single-nucleon wavefunction. The requirement that the nuclear energy \( E_{\text{Sky}} \) vanishes thus leads to the four identities

\[ C'_0 + C'_1 + C'_s + C'_s = 0 \quad , \]

(16)

\[ C'_0 + C'_1 + C'_T + C'_T = 4(C'_0 + C'_0 + C'_0 + C'_1) \quad , \]

(17)

\[ 4(C'_0 + C'_s) + C'_F + C'_F = 0 \quad , \]

(18)

\[ C'_0 + C'_1 - 2(C'_0 + C'_T) - (C'_0 + C'_T) + 4(C'_0 + C'_1) = 0 \quad . \]

(19)

If the coefficients \( C'_0 \) and \( C'_1 \) are allowed to depend on density according to Eqs. (10) and (11), following the same analysis entails that Eq. (16) would have to be replaced by

\[ a'_0 + a'_1 + a'_s + a'_s = 0 \quad , \]

(20a)

\[ b'_0 + b'_1 + b'_0 + b'_1 = 0 \quad . \]

(20b)

Note that these two conditions lead to Eq. (16), but the reverse is not necessarily true. Equation (16), was already noticed in Ref. [36], even though its origin was not discussed.

Equations (16)–(19) can be automatically satisfied by first fitting the parameters of a Skyrme force given by Eq. (14) and then calculating the corresponding coupling constants. But this usual fitting protocol imposes a lot more relations on the different terms of the
functional than what is required by the cancellation of self-interactions (see e.g. Tables IV and VI in Ref. [26]). Actually these relations are generally not strictly enforced so that the functional may be contaminated by self-interactions. For example, the coupling constant $C^J_t$ (hence also $C^T_t$ due to gauge invariance) is set to zero in most Skyrme parametrizations [30]. It has been suggested to also drop the isoscalar terms associated with $C^s_0$ and $C^s_0$ in the time-odd part of the functional [20, 37].

Self-interaction errors in the one-particle limit can contaminate systems consisting of many particles. Let us consider for instance cold fully polarized neutron matter. Assuming that all spins are aligned along the $z$-axis and neglecting the anisotropies induced by the polarization, Eqs. (9a)–(9c) lead to the following expression for the energy density of polarized neutron matter

$$E_{\text{pol NeuM}}^\tau = \left[ \frac{\hbar^2}{2M_n} + \left( C^\tau_0 + C^\tau_1 + C^T_0 + C^T_1 + \frac{1}{3}(C^F_0 + C^F_1) \right) \rho \right] \tau_{\text{pol n}}^\tau + \left( C^\rho_0 + C^\rho_1 + C^s_0 + C^s_1 \right) \rho^2 ,$$

(21)

with the kinetic density

$$\tau_{\text{pol n}}^\tau = \frac{3}{5}(6\pi^2)^{2/3} \rho^{5/3} .$$

(22)

It can thus be seen from Eqs. (16) and (21) that the error caused by self-interactions is given by

$$\delta E_{\text{NeuM}}^\text{pol} = \left( C^\rho_0 + C^\rho_1 + C^s_0 + C^s_1 \right) \rho^2 .$$

(23)

As expected the magnitude of this spurious term grows with increasing density and could thus lead to large deviations when such functionals are applied to the high-density matter found in neutron stars. In particular if $\delta E_{\text{NeuM}}^\text{pol} < 0$, self-interaction errors will drive a ferromagnetic collapse of neutron matter with the energy (21) decreasing asymptotically with increasing density. Such a pathological behavior is obviously contradicted by neutron-star observations.

**IV. CONCLUSIONS**

Phenomenological nuclear functionals based on Skyrme forces have been very successful in describing various nuclear systems, from finite nuclei to neutron stars and supernova
cores. Nevertheless the use of effective forces introduces tight correlations between different terms of the functional which hamper further improvements. For instance, adding density- and momentum-dependent terms in $t_1$ and $t_2$ contributes to the eight coupling constants $C^r_t$, $C^T_t$, $C_t^{\Delta \rho}$ and $C_t^{\Delta s}$, and also generates many new terms [28]. Improving one part of the functional may therefore deteriorate other parts.

A different approach to improve Skyrme functionals systematically consists in constructing semi-local functionals from all possible combinations of local densities and currents up to a given order in the derivatives, that are invariant under time reversal, space inversion, spatial rotations and gauge transformations [23]. The coupling constants appearing in the functional are treated as free adjustable parameters and are directly fitted to a selected set of nuclear data. Unfortunately such functionals inspired by effective field theories may allow a single nucleon to interact with itself thus indicating a violation of the Pauli exclusion principle. This unphysical feature can be avoided by imposing suitable restrictions on the coupling constants. These constraints have been derived for semi-local functionals up to second order in the derivatives and are given by Eqs. (16)–(19). The method outlined in this Rapid Communication can be easily extended to functionals of higher order.

Self-interaction errors in the one-particle limit can also contaminate systems consisting of many particles. For instance, it has been shown that in some cases these errors can lead to a catastrophic ferromagnetic collapse of neutron matter in contradiction with neutron-star observations. More generally, because a single nucleon breaks time-reversal symmetry, preventing a nucleon from interacting with itself necessarily requires the presence of time-odd densities and currents in the functional. The cancellation of self-interactions could thus serve as a guide for constraining the time-odd part of the functional, which still remains poorly known.

Even though Eqs. (16)–(19) ensure the vanishing of the internal energy in the limit of a single nucleon, other kinds of self-interactions and self-pairing could still arise in many-body calculations [17]. Nuclear energy density functionals obtained from the Hartree-Fock method with effective forces may also be spoiled by such many-body self-interactions. In particular, it is well-known that the density-dependent $t_3$ term in the Skyrme force (13) is formally inconsistent from the many-body theory point of view. Whereas its contribution to the ground-state energy vanishes in the one-nucleon limit, this term contains spurious many-body self-interactions which can become manifest when dealing with more than one particle.
Correcting for these many-body self-interactions would provide additional constraints on nuclear energy density functionals.

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