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Semicontact three-body interaction for nuclear density functional theory

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To solve difficulties related to the use of nuclear density functional theory applied in its beyond-mean-field version, we introduce a semicontact three-body effective interaction. We show that this interaction is a good candidate to replace the widely used density-dependent effective interaction. The resulting new functionals are able to describe symmetric, neutron, polarized, and neutron polarized nuclear matter as well as the effective mass properties simultaneously.

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Strongly interacting fermions can exhibit peculiar behavior in the infinite system limit from very dilute to very dense matter. In such systems, the zero-temperature equation of state (EOS), or energy per particle E/A , can be displayed in terms of the densities of various constituents. Rather commonly, specific medium effects take place and lead to an energy that is a functional that depends on noninteger powers of the density. This stems from the fact that a natural expansion parameter for a homogenous infinite system is the Fermi momentum k_F , which is proportional to $\rho^{1/3}$, where ρ is the matter density. A seminal example is the Lee-Yang formula for E/A , which holds for any diluted Fermi systems with short-range interaction [1,2] and contains a term proportional to $\rho^{4/3}$. A more recent example is the universal class of Fermi systems at unitarity, where a $\rho^{2/3}$ dependence [3] is supported by *ab initio* calculations. Cold atoms or neutron matter at a low density can enter into this class of systems [4,5]. In phenomenological approaches, as in the nuclear density functional theory (DFT) [6], this density dependence of the functional has to be mimicked in one way or another. Indeed, in nuclear systems, indirect evidence of the necessity of having a term that behaves like $\rho^{1+\alpha}$ with $1/6 \leq \alpha \leq 1/3$ in the energy is the difficulty of reproducing both the compression modulus of nuclear matter and the quasiparticle effective mass at saturation with integer powers of the density only [6].

A clear view of the density dependence of the energy is crucial for the design of an accurate DFT for the considered many-body problem. In finite systems, it might be necessary to go beyond the mean-field approximation by accounting for quantum fluctuations in collective space and restoring some symmetries that were broken to include correlations in a compact functional. An example is the treatment of superfluidity in small superconductors or nuclei that can be

included by breaking the U(1) symmetry [7,8]. It was shown recently that symmetry restoration within DFT requires a functional that is strictly derived from an N -body Hamiltonian to avoid pathologies in the energy of the symmetry restored states (see, for instance, [9–11]). It is, for instance, not possible to use a functional that depends on noninteger powers of the density [12], due to the necessity of extending the functional theory to the complex plane. The aforementioned pathologies are rooted in the violation of the Pauli principle and the occurrence of self-interaction. This has renewed the interest in deriving a DFT from a pseudopotential approach. In this case, the Hartree-Fock expression obtained from an effective Hamiltonian is used to provide the functional, whose parameters have to be fitted—at the mean-field level or beyond—to the data.

Recently, efforts have been made to extend functionals based on zero-range interactions of increasing complexity to overcome the difficulties arising from beyond-mean-field calculations [13,14]. While very useful to get a local density approximation (LDA) for the functional, it is not yet clear if contact interactions can be used to provide a convenient solution to the problem. For this reason, DFT based on finite-range pseudopotentials might appear to be an alternative solution [15–17]. A first step in that direction was made in Ref. [18], where a three-body force was proposed to describe fermions in the low-density limit.

Here, we explore the possibility of using a density-independent three-body interaction to get a functional that mimics noninteger power dependences. By imposing the translational invariance, a three-body interaction can only depend on the Jacobi coordinates $\mathbf{r}_{ij} = (\mathbf{r}_i - \mathbf{r}_j)$, $\mathbf{R}_{ij}^k = \mathbf{r}_k - (\mathbf{r}_i + \mathbf{r}_j)/2$, where $(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k)$ are the coordinates of three particles (i, j, k) in an arbitrary frame. A general three-body interaction can *a priori* have a finite range for both these coordinates. Below, we consider the case where the interaction is a contact interaction in $\mathbf{R}_{ij}^k$ and call it a three-body semicontact interaction. It has the advantage of being more flexible than a three-body contact interaction. To characterize it further, we consider three particles with spin (and isospin) degrees of freedom that interact through $\bar{v}_{ijk} =$

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TABLE I. Correspondence between the coefficients (c_1, c_2) and the interaction strengths. Coefficients $y_{k\alpha}$ defined as $c_k = \sum_k y_{k\alpha} v_\alpha$ are reported.

	c_1^{SM}	c_2^{SM}	c_1^{NM}	c_2^{NM}	c_1^{PM}	c_2^{PM}	c_1^{PNM}	c_2^{PNM}
v_0	1	-1/4	1	-1/2	1	-1/2	1	-1
v_σ	1/2	-1/2	+1/2	-1	1	-1/2	1	-1
v_τ	1/2	-1/2	1	-1/2	1/2	-1	1	-1
$v_{\sigma\tau}$	1/4	-1	+1/2	-1	1/2	-1	1	-1

$(v_{ijk} + v_{ikj} + v_{kij})/3$, with

$$v_{ijk} = \{V_0(r) + V_\sigma(r)P_\sigma + V_\tau(r)P_\tau + V_{\sigma\tau}(r)P_\sigma P_\tau\} \times \delta\left(\mathbf{r}_k - \left[\frac{\mathbf{r}_i + \mathbf{r}_j}{2}\right]\right), \quad (1)$$

where the short-hand notation $r = |\mathbf{r}_i - \mathbf{r}_j|$ is used, while P_σ (P_τ) exchanges the projections of spin (isospin) of particles i and j . Note that the interaction can be used without isospin exchange operators in the case where it is applied to fermions with spin degrees of freedom only by omitting the two terms with P_τ in Eq. (1). The functions $V_\alpha(r)$ with $\alpha = 0, \sigma, \tau$, and $\sigma\tau$ correspond to the two-body interaction acting in different channels. For simplicity, we assume that they can be written in terms of a smooth normalized function g as $V_\alpha(r) = v_\alpha g(r)$, where v_0, v_σ, v_τ , and $v_{\sigma\tau}$ are independent strength parameters.

The functional associated with the semicontact three-body interaction is directly obtained from its Hartree-Fock expression for the energy. We focus here on infinite systems and introduce the Fermi momentum k_F and the density of the Fermi gas $\rho = d k_F^3 / (6\pi^2)$, where d is the degeneracy, which depends on the specific situation. We consider the following four cases: symmetric nuclear matter (SM) with $d = 4$, neutron matter (NM) and spin polarized matter (PM) with $d = 2$, and spin polarized neutron matter (PNM) with $d = 1$. A lengthy but straightforward calculation shows that the energy per particle can be written

$$\frac{E^{\rho\rho\rho}}{A} = c_1 \frac{\rho^2}{6} \int d^3r g(r) [1 - c_3 f(k_F r / 2)^2] + c_2 \frac{\rho^2}{6} \int d^3r g(r) [f(k_F r)^2 - c_3 f(k_F r) f(k_F r / 2)^2], \quad (2)$$

where the function f is expressed in terms of the first spherical Bessel function as $f(x) = 3j_1(x)/x$. The coefficients c_1, c_2 , and c_3 depend on the specific channel. One has $c_3 = 1/2$ for SM, 1 for both NM and PM, and 2 for PNM. The correspondences between the coefficients c_1 and c_2 and the parameters v_α are listed in Table I. Equation (2) can serve, given a specific function g associated with the range a , to get expansions in powers of $(k_F a)$ and obtain the low-density behavior. Note that if a two-body interaction is used with the same finite-range part as in Eq. (1), the energy is identical to Eq. (2) with $c_3 = 0$ and $\rho^2/6 \rightarrow \rho/2$. In this case, the functional is denoted $E^{\rho\rho}$. In SM, the limit for zero-range two-body and three-body interactions is obtained by setting

$g(r) = \delta(\mathbf{r})$ and gives

$$\frac{E_{\text{zero}}^{\rho\rho\rho}}{A} = \frac{3}{8} t_3 \rho, \quad \frac{E_{\text{zero}}^{\rho\rho\rho}}{A} = \frac{t_3}{8} (1 - c_3) \rho^2, \quad (3)$$

with $t_3 = 4(c_1 + c_2)/3$. Note that for NM, PM, and PNM, $E_{\text{zero}}^{\rho\rho\rho}$ cancels out as expected.

In the present work, we are interested in the intermediate-density region (around the equilibrium configuration) where deviation from the limits, (3), is anticipated for finite-range interactions. To progress further, we assume that g is a normalized Gaussian function $g(r) = e^{-(r^2/a^2)} / (a\sqrt{\pi})^3$. In this case, using the same technique as in Ref. [16], integrals in Eq. (2) become analytical functions of $x = (ak_F)$, leading to

$$\begin{aligned} \frac{E^{\rho\rho\rho}}{A} &= \frac{\rho^2}{6} \{c_1 [1 - c_3 F_1(x)] + c_2 [F_1(x/2) - c_3 F_2(x)]\} \\ &\equiv \frac{\rho^2}{6} \mathcal{F}_3(ak_F), \end{aligned} \quad (4)$$

with

$$F_1(x) = \frac{12}{x^6} (1 - e^{-x^2}) - \frac{6}{x^4} (3 - e^{-x^2}) + \frac{6\sqrt{\pi}}{x^3} \text{Erf}(x)$$

and

$$\begin{aligned} F_2(x) &= \frac{288}{x^8} (-e^{-x^2/4} - e^{-x^2}) - \frac{24}{x^6} (12 + e^{-x^2} - 7e^{-x^2/4}) \\ &+ \frac{12}{x^4} (4e^{-x^2/4} - 7e^{-x^2}) + \frac{6\sqrt{\pi}}{x^3} \left[8 \text{Erf}(x) - 7 \text{Erf}\left(\frac{x}{2}\right) \right] \\ &+ \frac{36\sqrt{\pi}}{x^7} \left(\frac{4}{x^2} - 9 \right) \left[\text{Erf}(x) - 2 \text{Erf}\left(\frac{x}{2}\right) \right]. \end{aligned}$$

Therefore, a density dependence $\rho^{1+\alpha}$ for the energy per particle (as given by the commonly used density-dependent Skyrme or Gogny interactions) can be locally obtained if $\mathcal{F}_3(ak_F) \propto (ak_F)^{3(\alpha-1)} \propto \rho^{\alpha-1}$. Adjusting the parameters c_1 and c_2 , our semicontact three-body interaction can thus approximate the desired density dependence in a given range of densities. This is illustrated in Fig. 1, for $\alpha = 1/3$ and $\alpha = 2/3$. The functional associated with the three-body force can fairly well reproduce the effect of a density-dependent interaction with a noninteger power of the density. Systematic analyses have shown that the present interaction is suitable for the density dependence $\rho^{1+\alpha}$ of the energy per particle with $0 \leq \alpha \leq 1$. However, for very small α , i.e., $\alpha \leq 1/6$, the fit starts to deteriorate.

One of the recurrent difficulties of nuclear DFT based on zero-range interactions is the impossibility to conjointly get the proper EOSs in infinite matter and reasonable behavior of the effective mass [19,20]. The use of a finite-range three-body interaction automatically induces a contribution to the effective mass given by

$$\frac{\hbar^2}{2m^*} = \frac{\rho_0^2 a^2}{4} \left[\frac{c_1^{\text{SM}}}{24} M_1\left(\frac{x}{2}\right) - \frac{c_2^{\text{SM}}}{3} M_1(x) + \frac{c_2^{\text{SM}}}{8} M_2(x) \right]$$

in SM, with

$$M_1(x) = \frac{12}{x^6} (e^{-x^2} - 1) + \frac{6}{x^4} (e^{-x^2} + 1)$$

FIG. 1. (Color online) $\mathcal{F}_3(ak_F)$ as a function of (ak_F) obtained by adjusting the c_1^{SM} and c_2^{SM} to get a dependence similar to $1/(ak_F)$ ($\alpha = 2/3$) [solid (red) line] or $1/(ak_F)^2$ ($\alpha = 1/3$) [dashed (blue) line]. The reference curves $1/(ak_F)$ [filled (red) circles] and $1/(ak_F)^2$ [filled (blue) diamonds] are also shown. The dotted horizontal line indicates the zero-range three-body interaction limit ($\alpha = 1$). The fit was made for $(ak_F) \in [1.25, 1.75]$; note that in nuclear physics $(ak_F) \simeq 1.5$ at saturation.

and

$$M_2(x) = \frac{576}{x^8} (e^{-x^2} - e^{-\frac{x^2}{4}}) + \frac{288}{x^6} + \frac{144\sqrt{\pi}}{x^7} \left(\frac{2}{x^2} - 3 \right) \left[2 \text{Erf} \left(\frac{x}{2} \right) - \text{Erf} x \right].$$

As can be done for the energy, the three-body interaction parameters can be adjusted to reproduce specific behavior of the effective mass as a function of the density. For instance, it might be used to get the proper $\rho^{2/3}$ dependence predicted by the Galitskii formula (see Eq. (11.62) in Ref. [2] and see Ref. [21] for a recent discussion). An alternative situation is presented below, where we show that the three-body semicontact interaction conjointly used with a two-body density-independent interaction can appropriately describe the Skyrme prescription, i.e., $(m^*/m) \propto (1 + \theta\rho)^{-1}$, where the expression of the parameter θ can be found in Ref. [22].

In the nuclear context, it has recently become evident that the LDA-DFT with noninteger powers of the density leads to severe problems in describing fluctuations along collective coordinates or restoring broken symmetries [12]. Here, we show that the semicontact three-body interaction can replace the density-dependent term used with standard functionals. For this to be considered as a practical tool, we should be able to find a set of parameters that (i) provides a reasonable description of all spin/isospin channels simultaneously and (ii) conjointly describes the expected density dependence of the effective mass. In the past, requirements (i) and (ii) have been successfully fulfilled using a density-dependent term. More recently, a zero-range density-independent interaction that could meet these criteria was introduced [14] using three-body velocity-dependent terms. While possibly more difficult to implement, the semicontact three-body interaction limits the need for velocity-dependent terms, with the advantage

FIG. 2. (Color online) (a) Scalar-isoscalar effective mass and (b) equations of state for SM (red), NM (blue), PM (green), and PNM (black) as a function of the density obtained with the SLy5 functional (symbols) and with the Skyrme (two-body) + three-body functional (lines), called SLy5^{3b}. Inset: Contribution of the three-body functional to the energy per particle in symmetric matter. A simple function proportional to $\rho^{1+\alpha}$ has been adjusted on it with $\alpha \simeq 1/3$ for an optimal fit in the vicinity of the saturation density.

that it might give better control of unwanted finite-range instabilities [23].

To illustrate that the new interaction can be employed successfully in the nuclear DFT context, we have considered two commonly used functionals based on density-dependent interactions, namely, a Skyrme (zero-range) [22,24,25] and a Gogny (finite-range) [26,27] functional. More precisely, we considered the SLy5 [28] and D1M [29] sets of parameters, respectively. These two functionals are known to provide a meaningful description of the EOSs in different spin-isospin channels as well as the reasonable effective mass (see Figs. 2 and 3) and serve below as reference EOSs.

We consider the original functionals and replace the density-dependent term with the functional deduced from the three-body semicontact interaction. Doing this means that the energy density functional (EDF) can then be truly considered as the Hartree-Fock functional derived from a many-body Hamiltonian. Then a global fit is made using the new functionals, which are labeled SLy5^{3b} and D1M^{3b}, respectively, below. The parameters have been adjusted to reproduce the four EOSs (SM, NM, PM, and PNM) and the (scalar-isoscalar) effective masses simultaneously. The details of the fitting protocol are given in the Appendix. The range $a = 1.2$ fm, which is optimal for the fit to the D1M results, was chosen for the range of the semicontact term. Note that all parameters have been used for the fit except the ranges of the two-body part, which have been kept equal to the original D1M case. Altogether, the fit was made using 10 and 12 parameters for the SLy5^{3b} and D1M^{3b}, respectively. Optimal parameter

FIG. 3. (Color online) Same as Fig. 2, except that the Gogny D1M (symbols) and D1M^{3b} (lines) are shown. Inset: Again, $\alpha \simeq 1/3$ is found to be optimal.

values are listed in Table II. As shown in both Fig. 2 and Fig. 3, an accurate reproduction of the original EOSs is obtained, along with the proper density dependence of the effective mass. In particular, the SM properties, which are difficult to grasp if a strict zero-range interaction is used, are well accounted for. We see that the properties that characterize the saturation point in SM, i.e., the saturation density ρ_{sat} , binding energy per particle B , effective mass m^*/m , and compression modulus K_∞ , are reproduced with deviations between targeted and obtained values that are typical for nuclear EDFs. The values of these quantities obtained from SLy5 and D1M are compared with those computed from the new functionals in Table III.

The new functionals, SLy5^{3b} and D1M^{3b}, where the density-dependent term is replaced with the semicontact three-body interaction, provides a very good reproduction of the saturation properties of the reference functionals, SLy5 and D1M, for all considered cases. In particular, the compression modulus, which was one of the motivations for the introduction of the ρ^α term in the Skyrme and Gogny interactions, has a reasonable value.

In the present work, a simplified three-body interaction is used to construct a DFT. It is shown that this new interaction can mimic the behavior of density-dependent interactions used in the nuclear context. This interaction solves two important difficulties encountered in the applicability of nuclear DFT. First, it provides a correct description of the saturation properties and a reasonable description of the infinite matter EOSs in various spin-isospin channels as well as the effective mass density dependence for a wide range of densities. Second, as we have replaced the pathological term ρ^α in the functional with a density-independent interaction, the new functionals can be used in a DFT multireference framework, for instance, to restore symmetries or to account for configuration mixing beyond the independent particle picture.

TABLE II. Parameters of the SLy5^{3b} and D1M^{3b}. We use here standards for the two-body interaction parameters (see Refs. [28] and [29]). In both cases, the range is fixed to $a = 1.2$ fm. In the Gogny force case, the finite ranges of the two-body interaction have been kept equal to their original D1M values, $\mu_1 = 0.5$ fm and $\mu_2 = 1.0$ fm. Uncertainties in parameter values (indicated as percentages) were obtained using standard covariance analysis.

SLy5 ^{3b}	
t_0 (GeV fm ³)	-1.283 (0.05%)
t_1 (GeV fm ⁵)	0.874 (0.18%)
t_2 (GeV fm ⁵)	-0.808 (0.69%)
x_0	0.29 (1.8%)
x_1	0.51 (1.8%)
x_2	-1.08 (0.03%)
v_0 (GeV)	-15.03 (0.56%)
v_σ (GeV)	24.13 (0.82%)
v_τ (GeV)	24.99 (0.65%)
$v_{\sigma\tau}$ (GeV)	-42.12 (0.25%)
D1M ^{3b}	
W_1 (GeV)	7.60 (1.3%)
B_1 (GeV)	2.54 (5.4%)
H_1 (GeV)	2.18 (5.8%)
M_1 (GeV)	-1.47 (8.0%)
W_2 (MeV)	-1047.97 (0.80%)
B_2 (MeV)	-86.54 (10%)
H_2 (MeV)	-681.06 (1.3%)
M_2 (MeV)	47.07 (10%)
v_0 (GeV)	-14.65 (1.1%)
v_σ (GeV)	30.06 (0.82%)
v_τ (GeV)	19.02 (0.96%)
$v_{\sigma\tau}$ (GeV)	-42.71 (0.49%)

It is clear that the use of a finite-range interaction and the use of a true Hamiltonian as a starting point to construct an EDF offers less flexibility than the conventional strategy based on a density-dependent interaction, eventually differing in the mean field and pairing channel. In particular, the present interaction should overcome the following two difficulties. First, the three-body interaction supplemented with a two-body interaction should also be validated in finite nuclei. In particular, its surface properties are not constrained by uniquely fitting the EOS in infinite systems. The use of a finite-range interaction is anticipated to be much more demanding numerically compared to the LDA-EDF and specific techniques should be used. Work along this line is in progress. Second, an aspect

TABLE III. Values of the saturation density ρ_{sat} , binding energy E/A , compression modulus K_∞ , and isoscalar effective mass m^*/m for functionals considered in this work.

	SLy5	SLy5 ^{3b}	D1M	D1M ^{3b}
ρ_{sat} (fm ⁻³)	0.160	0.161	0.165	0.165
B/A (MeV)	-15.98	-15.42	-16.02	-15.82
K_∞ (MeV)	229.92	236.59	224.98	228.58
m^*/m	0.697	0.691	0.746	0.744

that is not specific to the present work is related to the use of the same interaction in both particle-hole and particle-particle channels. In particular, an interaction that is suited for the mean field should also lead to a pairing that is not too strong. In the present work, we have shown that keeping the same range of the three-body interaction in all channels is already enough to treat the mean-field energy. Therefore, we used a simplified form of the interaction. To get reasonable pairing, one might eventually consider more flexible situations where the range is optimized for each spin-isospin channel.

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APPENDIX: FITTING PROTOCOL AND RESULTS

The parameters (10 parameters for a two-body Skyrme interaction with a semicontact three-body interaction and 12 parameters for a two-body Gogny interaction with a semicontact three-body interaction) are determined by minimizing a penalty function based on pseudodata calculated with the Skyrme SLy5 or Gogny D1M interaction. This function is

$$\chi^2 = \chi_{\text{sat}}^2 + \chi_{\text{SM}}^2 + \chi_{\text{NM}}^2 + \chi_{\text{PM}}^2 + \chi_{\text{PNM}}^2 + \chi_{\text{eff}}^2. \quad (\text{A1})$$

The last term, i.e., χ_{eff}^2 , is only considered for the fit of D1M^{3b}, which has two more parameters than SLy5^{3b} and, thereby, more flexibility to adjust the effective mass. The total number of constraints is $N_c = 84$ for SLy5^{3b} and $N_c = 104$ for D1M^{3b}. Among these constraints, four are imposed directly on the nuclear matter saturation properties:

$$\chi_{\text{sat}}^2 = \left(\frac{P}{\Delta P} \right)^2 + \left(\frac{E/A - (E/A)^0}{\Delta E/A} \right)^2 + \left(\frac{K_\infty - K_\infty^0}{\Delta K_\infty} \right)^2 + \left(\frac{\hbar^2/2m^* - (\hbar^2/2m^*)^0}{\Delta \hbar^2/2m^*} \right)^2, \quad (\text{A2})$$

where P is the pressure, E/A the energy per particle, K_∞ the compression modulus, and $\hbar^2/2m^*$ the (inverse) effective mass, all calculated at the saturation density in symmetric matter. These four quantities (and the saturation density) are calculated with the parameters of the interaction we want to fit, while the corresponding quantities with a 0 exponent are calculated with the original Skyrme (SLy5) or Gogny (D1M) interaction. The tolerances are 0.1% for E/A , K_∞ , and $\hbar^2/2m^*$ and 10^{-3} MeV for the pressure.

Then the penalty function contains four terms to constrain the EOS in different states of matter,

$$\chi_X^2 = \sum_{i=1}^{20} \left(\frac{E_i/A - (E_i/A)^0}{\Delta E_i/A} \right)^2, \quad (\text{A3})$$

where $X = \text{SM, NM, PM, or PNM}$, and E_i/A is the energy per particle calculated for 20 values of $\rho_{0,i} = i \times \delta\rho_0$, with $\delta\rho_0 = 0.025 \text{ fm}^{-3}$ (i.e., from 0.025 to 0.5 fm^{-3}). The tolerances $\Delta E_i/A$ are 0.2 MeV in SM and NM and 0.5 MeV in PM and PNM.

The last term, used only for D1M^{3b}, constrains the effective mass in symmetric matter at densities $\rho_{0,i} = i \times \delta\rho_0$,

$$\chi_{\text{eff}}^2 = \sum_{i=1}^{20} \left(\frac{\hbar^2/2m_i^* - (\hbar^2/2m_i^*)^0}{\Delta \hbar^2/2m_i^*} \right)^2, \quad (\text{A4})$$

with $\Delta \hbar^2/2m_i^* = 0.1 \text{ MeV}$.

This merit function contains constraints in order to reproduce correctly (on average) the different EOSs for the entire density range and gives an additional focus on the saturation point. In the case of the fit to D1M it also constrains the effective mass to have the desired density dependence over the entire considered interval of densities.

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