Effective 3-Body Interaction for Mean-Field and Density-Functional Theory

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Density functionals for nuclei usually include an effective 3-body interaction that depends on a fractional power of the density. Using insights from the many-body theory of the low-density two-component Fermi gas, we consider a new, nonlocal, form for the energy functional that is consistent with the Fock space representation of interaction operators. In particular, there is a unique spatially nonlocal generalization of the contact form of the interaction that preserves the $\rho^{7/3}$ density dependence required by the many-body theory. We calculate the ground state energies for particles in a harmonic trap using the nonlocal induced 3-body interaction, and compare them to numerically accurate Green’s Function Monte Carlo calculations. Using no free parameters, we find that a nonlocality in the space domain provides a better description of the weak-coupling regime than the local-density approximation.

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Self-consistent mean-field theory is the only practical tool to calculate properties of heavy nuclei without region-specific parametrizations. Two of the leading implementations, namely those following Skyrme or Gogny, rely on interactions that depend on density, and even on fractional powers of density, making them density-functional theories rather than Hamiltonian theories. We would like to go beyond the density-functional theory as currently formulated, and possibly back to effective Hamiltonian theories, for several reasons. Correlation energies associated with angular momentum or particle number conservation are significant and need to be treated outside of the mean-field approximation. Restoration of good particle number can be carried out in many different ways in a Hamiltonian theory, but density-functional theory can lead to inconsistencies if the parameterization makes use of nonintegral powers of density \cite{1,2}. Empirical evidence on nuclear compressional dynamics favors precisely such non-integral powers \cite{3,4}, although there have been attempts to keep only integral powers \cite{4,7}. Also, it is far from clear that further accuracy can be achieved without dropping some of the assumptions made, such as the Local Density Approximation (LDA). These are our motivations for this Letter, to explore nonlocal alternatives to the commonly used LDA energy functional. This is not the first time the question has been raised; in a 2005 workshop\textsuperscript{8} the problem was formulated:

**Problem 2.** How can one replace in a nuclear density functional: (i) dependence on momentum by dependence on density, or (ii) dependence on density by dependence on momentum? The fact of life that nuclei are finite systems composed of protons and neutrons must not be ignored, forgotten, disregarded, neglected, or otherwise assumed irrelevant. The consequences of the proposed replacements must be considered in the context of (i) constructing functionals from first principles (e.g., how to replace the Fermi momentum for the density), (ii) conserving symmetries (e.g., how to construct an isospin-invariant density functional from microscopic results for asymmetric matter), and (iii) restoring broken symmetries.

Equation of state results for pure infinite neutron matter at densities $\rho \geq 0.04$ fm$^{-3}$ have been commonly used to constrain Skyrme and other density-functional approaches to large nuclei \cite{9,10}. It has recently become possible to use the density dependence of the $1S_0$ gap in low-density neutron matter \cite{11} to constrain Skyrme-Hartree-Fock-Bogoliubov treatments and especially their description of neutron-rich nuclei \cite{12}. At low densities it is possible to express the ground-state energy as an analytically known function of $(k_Fa)$, the product of the Fermi momentum and the $s$-wave scattering length. Thus, finite systems of low density offer a good model for testing candidate effective 3-body interactions and comparing with density-functional theory in the local density approximation.

As shown by Lee and Yang \cite{13}, the ground-state energy of a low-density Fermi gas with short-range interactions can be expanded as a power series in the scattering length $a$. The first 3 terms are:

$$E/N = \frac{\hbar^2 k_F^2}{2m} \left( \frac{3}{5} + \frac{2}{3\pi}ak_F + \frac{4}{35\pi^2} (11 - 2\ln 2) (ak_F)^2 \right),$$

(1)

where $E/N$ is the energy per particle and $k_F$ is the Fermi momentum.

The corresponding energy density $\mathcal{E}$ expressed as a function of ordinary density $\rho = (k_F/3\pi^2)$ is

$$\mathcal{E} = \frac{3\hbar^2}{10m} (3\pi^2)^{2/3} \rho^{5/3} + \frac{\hbar^2 \pi a}{m} \rho^2 + \frac{2\hbar^2 a^2 3\pi^2}{35m} (11 - 2\ln 2) \rho^{7/3}.$$

(2)

The first and second terms are just the kinetic and two-particle interaction energies of mean-field theory, using the scattering-length approximation to the effective interaction. The third term, which we call an effective 3-
body interaction, expresses an energy density functional that is proportional to $\rho^{7/3}$.

The origin of that term and its fractional density dependence may be understood from the graphs in Fig. 1. The low-density expansion makes use of the scattering length, which is calculated by a ladder sum in the two-particle channel. One of the terms in that sum is shown in Fig. 1a. However, in the many-body context, shown in Fig. 1b, that contribution should be excluded if either $k_3$ or $k_4$ is below the Fermi momentum. The third term in the Lee-Yang expansion is simply subtracting out graphs of the form Fig. 1b, where the cross on the particle line indicates that its momentum is below $k_F$ (and thus it is not a proper Goldstone many-body graph). In standard formulations of many-body theory [14–17], the graph Fig. 1b is calculated as the integral

$$I_{LY} = V \int \frac{d^3k_1}{(2\pi)^3} \frac{d^3k_2}{(2\pi)^3} \frac{d^3k_3}{(2\pi)^3} \frac{n_{k_1}n_{k_2}n_{k_3}}{k_1^2 + k_2^2 - k_3^2 - k_3^2}$$  \hspace{1cm} \quad (3)$$

where $n_k = \theta(k_F - k)$ is the occupation number of the orbital $k$.

If we take the second-order perturbative expression for the energy, but without assuming Fermi gas wave functions, and an interaction of contact form the formula is:

$$I = \sum_{1,2,3} \sum_{4} \int d^3r d^3r' \frac{\phi_r^* \phi_{r'}^* \phi_{r''}^* \phi_{r'''}}{E_1 + E_2 - E_3 - E_4}$$  \hspace{1cm} \quad (4)$$

where $\phi_r$ is the orbital function of the $i$-th particle at position $r$, and occ signifies the fact that the states are occupied.

The minimal generalization of a 3-body contact interaction is one that is a function of two positions, $r$ and $r'$. Such an assumption leads naturally to a precisely defined effective 3-body interaction that overcomes the problems associated with the $\rho^{7/3}$ density functional but still reproduces the Lee-Yang functional dependence.

The Fock-space representation of this operator is

$$\hat{H}_3 = f(r, r') \sum_\sigma \psi_{\sigma r}^\dagger \psi_{\sigma r'}^\dagger \psi_{\sigma r} \psi_{\sigma r'} \psi_{\sigma r} \psi_{\sigma r'}$$  \hspace{1cm} \quad (5)$$

The two coordinates $r$ and $r'$ represent the two interaction points in Fig. 1b. The prescription to calculate expectation values with this operator is to take the contractions in the Hartree-Fock ground state that correspond to Fig. 1b, where the following triply contracted terms are the only ones to survive:

$$\langle \hat{H}_3 \rangle = \int d^3r d^3r' f(r, r') \sum_\sigma \langle \psi_{\sigma r}^\dagger \psi_{\sigma r'} \psi_{\sigma r} \psi_{\sigma r'} \rangle$$  \hspace{1cm} \quad (6)$$

Note that since the orbital $k_3$ is occupied, the graph is forbidden (does not occur in a Goldstone expansion) and is marked with an $x$. Its contribution to the effective two-body interaction must be subtracted as part of the effective 3-particle interaction.

The function $f(r, r')$ should be translationally and rotationally invariant, i.e. it can only depend on $|r - r'|$. Moreover, we want the functional that follows from the new operator to have the same dependence on the density as the last term in Eq. (2) (i.e. $\rho^{7/3}$) and we demand that it contain $\hbar^2 a^2/m$ so as to correspond to that term. Finally, we see from Eq. (6) that $f(r, r')$ should have dimensions of $EL^3$. The only way to satisfy all the above constraints is with an $f(r, r')$ of the form:

$$f(r, r') = \frac{\hbar^2 a^2}{m} \frac{C}{|r - r'|}$$  \hspace{1cm} \quad (7)$$

To obtain the dimensionless coefficient $C$, we demand that Eqs. (6) & (7) reduce to the Lee-Yang energy functional in the limit of uniform matter. In that limit, we can express the density matrices as

$$\langle \psi_{\sigma r}^\dagger \psi_{\sigma r'} \rangle = \int \frac{d^3k}{(2\pi)^3} \frac{e^{ik\cdot(r-r')}}{\epsilon_k + \Delta_{\sigma,\sigma'}} n_k \delta_{\sigma,\sigma'}$$  \hspace{1cm} \quad (8)$$

where $n_k$ is the Fermi gas occupation factor. Carrying out the spatial integrals in Eq. (6), we have

$$\langle \hat{H}_3 \rangle = 8\pi L^3 C \frac{\hbar^2 a^2}{m} \int \frac{d^3k_1}{(2\pi)^3} \frac{d^3k_2}{(2\pi)^3} \frac{d^3k_3}{(2\pi)^3} \frac{n_{k_1}n_{k_2}n_{k_3}}{k_1 - k_1 - k_2}$$  \hspace{1cm} \quad (9)$$

We match the result of this integral to the second-order Lee-Yang coefficient. This allows us to go back to Eq. (5) and express the 3-body operator as a function of the two coordinates $r$ and $r'$, with an operator structure that is guided by the terms in Eq. (6):

$$\hat{H}_3(r, r') = \frac{\hbar^2 a^2}{m} \frac{C}{|r - r'|} \sum_\sigma \psi_{\sigma r}^\dagger \psi_{\sigma r} \psi_{\sigma r}^\dagger \psi_{\sigma r}$$  \hspace{1cm} \quad (10)$$
where

\[ C = \frac{64\pi(11 - 2\ln 2)}{3(92 - 27\ln 3)} \approx 10.336 \]  

(11)

Since we are dealing with a system of two fermionic species, in Eq. (10) we have chosen to call them spin-up (↑) and spin-down (↓). The two middle terms are free to take on either value of the spin.

A finite range 3-body effective interaction like the one we propose in Eq. (10) is much softer than usually assumed. This fact could have important consequences on the density profile of different systems. The price to be paid for the conceptual clarity and microscopic derivation of our 3-body effective interaction is the emergence of challenging computational issues. If \( N \) is the number of particles under study and \( N_r \) is the number of amplitudes in the numerical vector representing an orbital, then for the usual way of doing Skyrme calculations, where the interaction depends only on the one-particle diagonal density, the latter is of order \( N N_r \). In contrast, the form of Eq. (10) is of order \( N^3 N_r^2 \).

With a view to testing the effective interaction of Eq. (10) we consider the model problem of dilute fermions in a harmonic trap, as in Ref. [18]. We calculate the ground-state energies in density-functional theory with the LDA functional, and with Eq. (10) replacing the Lee-Yang term in the functional. For our purposes, we may take the orbitals to be of the harmonic oscillator form \( \psi(r) = P(r) e^{-\alpha r^2/2} \) where \( P(r) \) is a polynomial and \( \alpha \) is a variational parameter. We write down the variational energy of the system using the density as follows:

\[ E_\nu = T[\rho] + V_{\text{ext}}[\rho] + \int d^3 r \mathcal{E}_I[\rho] + E_{II} . \]  

(12)

In this expression, the kinetic energy is:

\[ T[\rho] = \sum_{i=1}^N \int d^3 r \frac{\hbar^2}{2m} \nabla^2 \phi_i(r) \]  

(13)

and the trap potential energy is:

\[ V_{\text{ext}}[\rho] = \int d^3 r \frac{1}{2} m \omega^2 r^2 \rho(r) . \]  

(14)

The \( \mathcal{E}_I \) is the second term in the Lee-Yang expansion Eq. (2) and is simply:

\[ \mathcal{E}_I[\rho] = \frac{\hbar^2 \pi a}{m} \rho^2 . \]  

(15)

For the last term, \( E_{II} \), we choose two different forms: a) one following from the Lee-Yang expansion Eq. (2) and b) one that corresponds to the new 3-body effective interaction given in Eq. (10). These are:

\[ E_{II}^{LY} = \int d^3 r \mathcal{E}_{II}^{LY} = \frac{2\hbar^2 a^2 3\pi^2}{35m} (11 - 2\ln 2) \int d^3 r \rho^2 . \]  

(16)

and

\[ E_{II}^{LY} = \frac{\hbar^2 a^2}{m} \sum_i \sum_j \sum_k I_{ijk} \]  

(17)

with

\[ I_{ijk} = \int d^3 r d^3 r' \frac{C}{|r - r'|} \rho_i(r) \rho_j(r') \rho_k(r) . \]  

(18)

The equation for \( E_{II}^{LY} \) contains products of one-body density matrices. The sum is taken in such a way that there are no repeated terms other than those allowed by the restriction (clear by inspecting Eq. (10)) that only the ↑↑↓ and ↑↓↓ configurations are allowed.

We examine a system of 8 particles (4 spin-up and 4 spin-down). We choose 8 particles since this is the smallest non-trivial closed shell system: we find 128 terms in total (64 for ↑↓↓ and 64 for ↓↑↑). In Table I we show the results of variational minimizations of the functionals given in Eq. (12) varying levels of sophistication. Shown are the energies of the system at the minima. We list the results when we keep a) only the kinetic energy and the external potential terms in Eq. (12), b) the same two terms plus the next one (\( \mathcal{E}_I \)), which is proportional to the scattering length \( a \), c) the above three terms plus the Lee-Yang highest order term (\( \mathcal{E}_I^{LY} \)), proportional to \( a^2 \), and d) similarly to the previous case but with \( \mathcal{E}_I^{LY} \) replaced by \( \mathcal{E}_{II}^{LY} \).

To test the accuracy of the different approaches, we have performed Green’s Function Monte Carlo simulations, which have already been proved to be dependable in describing the electron gas, light nuclei, and cold atoms [19–23]. As before, we study 8 trapped fermions, assuming a Hamiltonian of the form:

\[ \mathcal{H} = \sum_{k=1}^N (-\frac{\hbar^2}{2m} \nabla^2_k + \frac{1}{2} m \omega^2 r_k^2) + \sum_{i<j} v(r_{ij}) . \]  

(19)

where \( N \) is the total number of particles and \( \omega \) is the trap frequency. The interaction between the particles is

TABLE I: Results for the ground-state energy (in units of \( \hbar \omega \)) of a harmonically trapped system of 8 pairwise repulsively interacting particles. The interaction is at the dilute limit, \( a \approx 0.2082 \sqrt{\hbar/m\omega} \).

| Method | Energy \( E \) [\( \hbar \omega \)] |
|--------|---------------------------------|
| Kinetic + External Energy | 18.0 |
| DFT (LY LO) | 19.197 |
| DFT (LY LO + NLO) | 19.436 |
| DFT (LY LO + H\(_3\) NLO) | 19.465 |
| GFMC | 19.485(1) |
taken to be of the modified Pöschl-Teller type:

\[ v(r) = v_0 \frac{\hbar^2 \mu^2}{m_r \cosh^2(\mu r)}, \]  

(20)

where \( \mu \) is a parameter that is related to the inverse of the effective range and \( v_0 \) is a parameter we can use to tune the s-wave scattering length. The scattering length for Table II is \( a = 0.2082 \sqrt{\hbar/m_\omega}. \) For that case, the numerical calculations were performed taking \( v_0 = 10.28 \) and \( \mu^{-1} = 0.1 \) in units of the oscillator length \( \sqrt{\hbar/m_\omega}. \) Since the effective range is much smaller than the oscillator length, this interaction is appropriate to describe a low-density system. Also, we have taken the interaction to be repulsive to avoid problems with superfluidity. We believe that the errors associated with the fixed-node approximation are inconsequential at the level of accuracy we are considering here.

We are now in a position to compare the various energies from Table II to the microscopic results. The Green’s Function Monte Carlo result is close to the density-functional theory calculation which includes all the terms in the Lee-Yang expansion, but even closer to the results following from our new term \( H_3. \) We have also extended these calculations to different couplings, and gather our results in Fig. 2. At weak coupling, the new operator leads to results that are identical with the Lee-Yang \( a^2 \) dependence, while as the coupling gets stronger the \( H_3 \) contributions are more repulsive than in Lee-Yang (though they have the same power-law behavior), and thus provide a more accurate description of the microscopic simulation. Importantly, our approach contains no free parameters: Eq. (10) contains the parameter \( C, \) but that is matched to the appropriate Lee-Yang coefficient for uniform matter, while our subsequent calculation was performed for a finite particle number in a harmonic trap.

In summary, we have attempted to combine an awareness of the theory of the weakly interacting 2-component Fermi gas with the desired behavior of density functionals, and have proposed a new form of the effective 3-body interaction that has a finite range. By including a new term of the form of Eq. (10), we are providing realistic density functionals with a way to match the analytically known behavior at very weak coupling. We want to stress that to implement the proposed 3-body operator and functional what is required is only the one-body density matrix. This is computationally more challenging than nuclear physics functionals based on the local density, but it is still much simpler than approaches (such as coupled-cluster theory or the MBPT approximation of quantum chemistry) that deal with correlations explicitly.

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