Density-functional theory for resonantly interacting fermions with effective range and neutron matter

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A density-functional theory is proposed for strongly interacting fermions with arbitrary large negative scattering length. The functional has only two parameters that are directly fixed to reproduce the universal properties of unitary gas: the so-called Bertsch parameter ξ_0 and a parameter η_e related to the possible influence of the effective range r_e at infinite scattering length a. Using most recent quantum Monte Carlo (QMC) estimates of these two parameters, it is shown that the functional properly reproduces the experimental measurements of interacting Fermi systems not only at unitarity but also away from this limit over a wide range of $(ak_F)^{-1}$ values. The functional is applied to obtain an expression of Tan's contact parameter including the effect of r_e. Application is finally made to neutron matter. It is shown that most recent QMC results are well reproduced.

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During the last ten years, important progress has been made to manipulate Fermi gas by tuning the interaction between particles [1,2]. Special attention has been paid close to the unitarity regime when the s-wave scattering length becomes infinite in dilute systems. In this case, the interacting system properties become universal. The energy of the system is directly proportional to the free Fermi gas energy, and the ratio between these two energies is a universal parameter $\xi_0 \simeq 0.37$ [3–6], the so-called Bertsch parameter [7]. The experimental advances in atomic Fermi systems have motivated tremendous theoretical efforts to understand systems at unitarity as well as the transition from BCS to Bose-Einstein condensate (BEC) regimes (see, for instance, the collection of review articles in Ref. [8]). Due to the universal behavior of the energy for unitary gases, it was shown that simple local density functionals directly adjusted on QMC approaches can accurately describe various static or dynamical properties of these systems [9–12]. These functionals, however, strictly apply to $|a| \to \pm\infty$ in the low-density regime and cannot describe unitary gases with a possibly nonzero effective range r_e. The description of Fermi gas with nonzero effective range and anomalously large a is motivated by (i) the possibility to uncover new effects in a wider class of unitary systems and (ii) neutron systems that enter into such a class of interacting fermions.

A first step to including effective range influence is made in Refs. [13,14] showing nontrivial effects due to r_e. In that work, a minimal generalization of the previously proposed density-functional theory (DFT) is made by allowing explicitly the parameters of the functional to vary with r_e. Alternatively, finite-range effects can be investigated at low density using effective field theory (EFT) and systematic expansion in the Fermi momentum (see, for instance, [15,16]). One success of EFT is the improvement of the universal Lee-Yang (LY) formula [17,18], including r_e effects for low-density Fermi systems. The EFT approach, however, cannot be directly applied to unitary gases unless specific resummations of infinite-order in-medium loops are made. This has led to the description of systems at or close to unitary with varying success [19–21]. Here, inspired by the EFT approach with resummation, a DFT for Fermi systems is proposed that is optimized at unitarity and smoothly behaves away from unitarity.

I consider here spin-degenerated Fermionic systems with an s-wave interaction characterized by a negative scattering length a and an effective range r_e. These two quantities are defined as usual as the leading and next-to-leading order of the expansion of the s-wave phase-shift δ in terms of relative momentum k of the interacting particles:

$$k \cot\delta = -\frac{1}{a} + \frac{1}{2} r_e k^2 + O(k^4). \quad (1)$$

The functional proposed below is strongly guided by the resummation technique used in EFT to tackle the problem of unitary gas. In this case, simplified resummed formula has been obtained in Refs. [19–21]. Here, I introduce a resummed formula that accounts for nonzero r_e and write the energy as a functional of the Fermi momentum k_F as follows:

$$\frac{E}{N} = \frac{\hbar^2 k_F^2}{2m}\left\{\frac{3}{5} + \frac{(ak_F)A_0}{1 - A_0^{-1}[A_1 + (r_e k_F)A_2]ak_F}\right\}. \quad (2)$$

(A_0, A_1, A_2) are three constants to be determined. One possibility that has been explored in Refs. [21,22], neglecting possible r_e effects, is to constrain the functional by matching the low-density limit with the universal Lee-Yang expansion of the energy [17,18]. This gives $A_0 = 2/(3\pi)$,

$$A_1 = \frac{4}{35\pi^2}(11 - 2\ln 2), \quad \text{and} \quad A_2 = \frac{1}{10\pi}.$$

The advantages of formula (2) are that (i) it can be reinterpreted as a density-functional theory through the relation $k_F = (3\pi^2 n)^{1/3}$ where n is the density, (ii) it can be expanded in powers of (ak_F), $(ak_F)^{-1}$ or $(r_e k_F)$, and (iii) it has a definite limit as $a \to +\infty$. Taking this specific limit, we obtain $E = \xi(r_e k_F)E_{FG}$ where E_{FG} is the free Fermi gas energy, $E_{FG}/N = [3\hbar^2 k_F^2/(10m)]$, and

$$\xi(r_e k_F) = \left\{1 - \frac{5}{3}\frac{A_0^2}{[A_1 + (r_e k_F)A_2]}\right\}. \quad (3)$$

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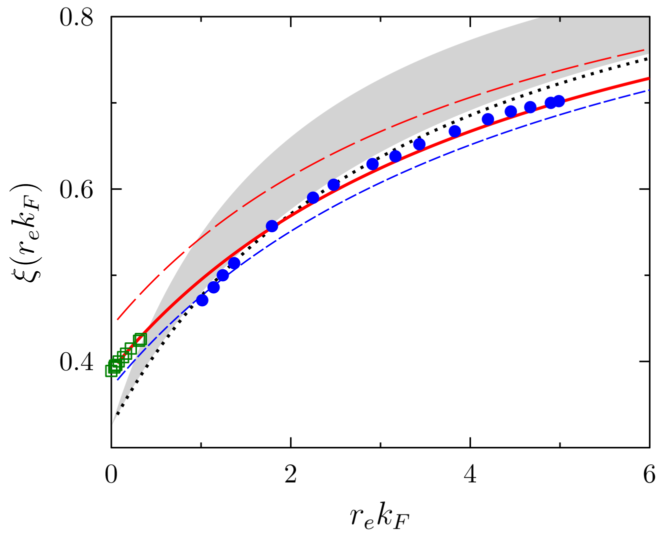

FIG. 1. Illustration of formula (3) (black dotted curve) giving the effective range dependence of the ξ parameter for unitary gas. The results are compared with the ones of Ref. [23] (blue points) and with the low-density results of [13,14] (green open squares). Note that in Ref. [23], results are given for the Hartree-Fock energy only. The red solid line is obtained using Eq. (6) with the values given in Refs. [13,14]: $\xi_0 = 0.3897$ and $\eta_e = 0.127$. The short-dashed blue line and long-dashed red line correspond to $\xi_0 = 0.37$ and $\xi_0 = 0.44$, respectively, both with $\eta_e = 0.127$. These values are compatible with those reported in Ref. [3]. The grey area corresponds to the results given in Ref. [21] and reflects the renormalization scale dependence in EFT calculations. The latter case includes resummation of correlation effects.

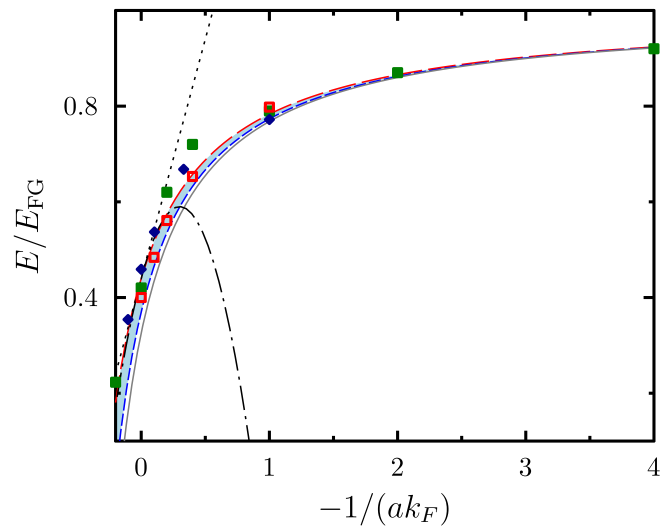

FIG. 2. Energy of a Fermi gas with zero effective range obtained with the Monte Carlo calculations [26] (dark blue diamond), [27] (green square), and the more recent result of Ref. [28] (red open square). The results of formula (5) with $\xi(r_e k_F) = \xi_0$ are shown for $\xi_0 = 0.37$ (blue short dashed line) and $\xi_0 = 0.44$ (red long dashed line). The blue area illustrates the uncertainty on ξ_0. For comparison, the first- and second-order expansions in $(ak_F)^{-1}$, Eq. (7), using $\zeta = \nu = 1$ (see discussion in Ref. [29]) are displayed, respectively, with black dotted and black dot-dashed lines. Results obtained using directly the functional constrained with the Lee-Yang expansion ($\xi_0 = 0.326$) together with Eq. (5) are also displayed with the grey solid line.

For unitary gas, with small but nonzero effective range, this expression can be expanded as

$$\xi(r_e k_F) \simeq \left(1 - \frac{5}{3}\frac{A_0^2}{A_1}\right) + \frac{5}{3}\frac{A_0^2 A_2}{A_1^2}(r_e k_F) - \frac{5}{3}\frac{A_0^2 A_2^2}{A_1^3}(r_e k_F)^2$$
$$\equiv \xi_0 + (r_e k_F)\eta_e + (r_e k_F)^2 \delta_e. \quad (4)$$

With the values of $\{A_i\}$ parameters deduced from the low-density constraint, one gets $\xi_0 = 0.326$, $\eta_e = 0.19$, and $\delta_e = -0.055$. The two former values have been obtained using a phase-space average in Ref. [21]. Not only is ξ_0 close to the expected value for unitary gas, i.e., $\xi_0 \simeq 0.37$, but also, the effective range dependence is not too far from the result obtained with the fixed-node QMC calculations of Refs. [13,14]. More generally the $(r_e k_F)$ dependence deduced from Eq. (3), while not perfect, is globally consistent with elaborated T-matrix estimates [21,23] (see Fig. 1). The Lee-Yang formula contains solely mean-field and second-order perturbation terms. The fact that a constraint on LY is close to the observed properties at unitarity indicates that strong cancellations of higher-order effects occur. Attempts have been made to further improve the expression of the energy by resumming higher-order effects [19–21], leading to various results for ξ_0. However, the values obtained strongly depend on the strategy used to select loops in the expansion.

As an intermediate summary, functional (2) has many interesting features. However, starting from the low-density expansion, it only provides a very rough description of Fermi gas at and around unitarity.

For this reason, here I follow a more pragmatic strategy and directly constrain functional (2) assuming that its Taylor expansion matches Eq. (4) up to first order in $(r_e k_F)$. Then, the functional will depend only on the two parameters ξ_0 and η_e. Since Eq. (2) has three parameters and the Taylor expansion around unitarity only leads to two constraints, I again assume that $A_0 = 2/(3\pi)$ so that the LY formula is also reproduced up to k_F^3 in dilute systems. The resulting energy then reads

$$\frac{E}{N} = \frac{\hbar^2 k_F^2}{2m}\left\{\frac{3}{5} + \frac{2}{3\pi}\frac{ak_F}{1 - \frac{10}{9\pi}(ak_F)/[1 - \xi(r_e k_F)]}\right\}, \quad (5)$$

with

$$\xi(r_e k_F) = \left\{1 - \frac{(1-\xi_0)^2}{(1-\xi_0) + (r_e k_F)\eta_e}\right\}. \quad (6)$$

These two formulas are the main results of the present paper. In the following, I explore the range of applicability of the proposed functional as well as possible applications. Note that ξ_0 and η_e are not free parameters in the sense that they are fixed by recent measurements or QMC calculations in unitary gas. Note that an equation similar to (5) was also considered for a Fermi gas with vanishing effective range in Refs. [24,25].

In Fig. 2, an illustration of the energy obtained as a function of $(ak_F)^{-1}$ for different ξ_0 (and $r_e = 0$) are shown and compared to experiments. It is interesting to mention that the result obtained using directly the Lee-Yang expansion as a constraint, i.e., using Eq. (5) with $\xi_0 = 0.326$, gives already a good approximation especially for $-(ak_F)^{-1} > 1$. However, around unitarity, the energy is underestimated. With constraints imposed at unitarity, the energy is reasonably reproduced both as $1/(ak_F) \to 0$ and for large values of $(ak_F)^{-1}$.

It is worth noticing that for $r_e = 0$, close to unitarity, we deduce from Eq. (5)

$$\frac{E}{N} \simeq \frac{3}{5}\frac{\hbar^2 k_F^2}{2m}\left\{\xi_0 - \frac{\zeta}{ak_F} - \frac{5}{3}\frac{\nu}{(ak_F)^2} + \cdots\right\}, \tag{7}$$

with

$$\zeta = \frac{9\pi}{10}(1-\xi_0)^2, \quad \nu = \frac{3}{5}\frac{\zeta^2}{(1-\xi_0)}. \tag{8}$$

For $\xi_0 = 0.37$, this gives $\zeta = 1.12$ and $\nu = 1.19$, while for $\xi_0 = 0.44$, we obtain $\zeta = 0.89$ and $\nu = 0.84$. These values are rather close to those reported in QMC ($\zeta = 0.9$) [26,27] or fixed node diffusion Monte Carlo ($\zeta = 0.95$) [30]. In Ref. [29], a direct fit to QMC leads also to $\zeta \simeq \nu \simeq 1$. The range of validity of the expansion (7) is illustrated by the dotted and dot-dashed lines in Fig. 2. We clearly see that it applies only for $1/|ak_F| \ll 1$ while the new functional applies on a wider range of density. Using directly ξ_0 and η_e to constrain the functional also leads to a better description of the possible effective range dependence. In Fig. 1, I present the quantity $\xi(r_e k_F)$, given by Eq. (6) using the values $\xi_0 = 0.3897$ and $\eta_e = 0.127$ [13,14]. The QMC results with nonzero effective range are perfectly described while keeping a description at larger $(r_e k_F)$ consistent with the many-body calculations of Refs. [21,23].

I now illustrate how the functional can be used, first to reproduce some observables measured in unitary gas and second to predict their possible effective range dependence. A typical example, which has been the subject of intensive experimental and theoretical works [31], is the Tan contact parameter [32–34]. Here, I follow closely [31]. In the present case of an infinite spin saturated system, the contact parameter C can be related to the contact density $\mathcal{C}$ through $C/(Nk_F) = (3\pi^2)\mathcal{C}/k_F^4$ which is itself related to the energy density $\mathcal{E}$ through $\mathcal{C} = 4\pi m a^2 (d\mathcal{E}/da)/\hbar^2$. The energy density is given by $\mathcal{E} = k_F^3 E/(3\pi^2 N)$. Using expression (5), we deduce that the contact parameter expresses as

$$\frac{C}{Nk_F} = \frac{4}{3}\frac{(ak_F)^2}{\left\{1 - \frac{10}{9\pi}(ak_F)/[1-\xi(r_e k_F)]\right\}^2}. \tag{9}$$

The resulting contact parameter is shown as a function of $(ak_F)^{-1}$ in Fig. 3 for the specific case $r_e = 0$. C deduced from the new functional is in good agreement with the experimental observations and within the error bars of most recent theoretical estimates. We also show for comparison the result of the functional obtained using parameters deduced from the low-density Lee-Yang expansion. It is interesting to note that these results are very close to the one obtained by setting the constraint at unitarity. In particular, different curves cannot be distinguished for $(ak_F)^{-1} < -1$. However, around unitarity, differences are noticeable. It should also be mentioned that the comparison between Eq. (9) and experiments is given here only as an illustration since this formula applies to uniform systems while experimental data are performed with finite-size nonuniform atomic clouds. A consistent comparison would require performing calculations accounting for finite-size effects using, for example, a local-density approximation. This development will be considered in the near future.

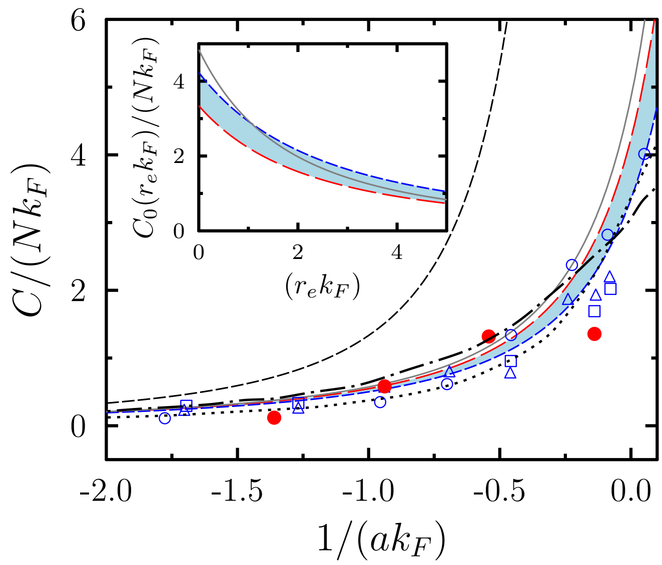

FIG. 3. Contact parameter as a function of $(ak_F)^{-1}$ obtained with Eq. (9) assuming $r_e = 0$. The light blue area is the region between the two results obtained either with $\xi_0 = 0.37$ or $\xi_0 = 0.44$. The black dashed line is the BCS result given by $4(ak_F)^2/3$. The black dotted and dot-dashed lines are the theoretical results of Refs. [35,36], respectively. The blue open circles, triangles, and squares are the moment, PES, and rf measurements of [37]. The red filled circles are the measures of Ref. [38]. In the inset, the dependence of the contact parameter for unitarity gas with nonzero effective range r_e is shown (for ξ_0 from 0.37 to 0.44) using a value $\eta_e = 0.127$ in Eq. (10). In the figure and in the inset, the gray solid line corresponds to the contact parameter obtained using the values $\xi_0 = 0.326$ and $\eta_e = 0.19$ (constraint with the low-density LY expansion).

Focusing now on the unitarity limit, I denote by C_0 the contact parameter as $a \to +\infty$. We then have

$$\frac{C_0}{Nk_F} = \frac{27}{25}\pi^2[1-\xi(r_e k_F)]^2, \tag{10}$$

which includes possible effective range dependence. This dependence is illustrated in the inset of Fig. 3. It is predicted that a reduction of C_0 should occur for unitary gas with nonzero effective range. The experimental observation of such reduction would be a stringent test of the present functional theory. In addition, since the contact parameter in the unitary limit has direct connection with many properties [31], number of closed channel, shear viscosity, and tail of the momentum distribution, I also anticipate that these properties will be modified as r_e increases while keeping the scattering length infinite. Note, however, that most connections with the Tan parameter have been obtained using the zero-range model and a more careful study for nonzero r_e is desirable. It is finally interesting to mention that the present functional can be directly combined with the technique proposed in Ref. [35] to obtain the contact

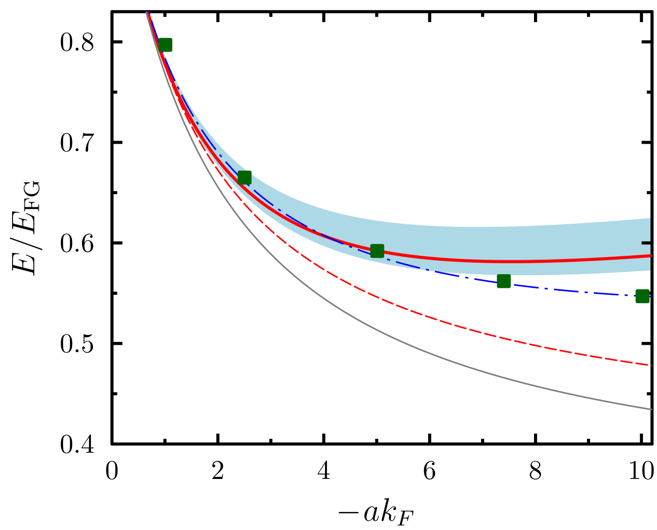

FIG. 4. Energy obtained with Quantum Monte-Carlo approach in neutron matter assuming a finite range s-wave interaction (green square) [39]. The red curves are the result obtained with formula (5) together with (6) assuming $\xi_0 = 0.3897$, $\eta_e = 0.127$ (thick solid line) [13,14] or $\eta_e = 0$ (dashed line). The blue area indicates the variation of the result when ξ_0 varies from 0.37 to 0.44 keeping η_e fixed. For comparison, I also show the result obtained using $\xi_0 = 0.44$ and $\eta_e = 0.03$ that perfectly match the QMC approach (blue dot-dashed line). In all cases presented here, I took $a = -18.9$ fm and $r_e = 2.7$ fm. For comparison, I also show the result obtained (thin solid gray line) using the Lee-Yang expansion as a constraint ($\xi_0 = 0.326$ and $\eta_e = 0.19$).

parameter for finite systems in a trap by reinterpreting the energy as a functional of the local density $n(\mathbf{r})$.

A realistic example of a system that has a large but finite negative scattering length and nonzero effective range is the case of neutron matter. In this case, the neutron-neutron scattering length is $a \simeq -18.9$ fm and $r_e \simeq 2.7$ fm. In particular, the ratio $|r_e/a| \simeq 0.14$ is much larger than the one generally obtained in cold atoms (see for instance the discussion in Ref. [21]). Consequently, a density functional based on EFT techniques together with low-density expansion only applies in a very narrow range of densities verifying that $|ak_F| \ll 1$ and the effective range effect should be included [15,16]. In Fig. 4, the results of the new functional are compared with QMC calculations [39–41]. For the comparison, I did not adjust the ξ_0 and η_e parameters but directly took the values reported in Refs. [13,14]. The blue area indicates the possible dependence of the result with the ξ_0 value. The proposed functional (red solid line) reproduces remarkably well the exact QMC results even if (ak_F) is much greater than unity. Some deviations are observed for $|ak_F| > 5$. This deviation might come from the fact that Eq. (6) is constrained to reproduce the QMC only up to second order in $(r_e k_F)$ and higher-order corrections might be needed. It is worth mentioning that these deviations can also be reduced either by keeping $\xi_0 = 0.3897$ and reducing η_e slightly to 0.08 or by varying both parameters. An example is given in Fig. 4 with the dot-dashed line. The effect of r_e is clearly pointed out by comparing the full results with the result obtained by keeping the same value of ξ_0 and setting artificially η_e to 0. Important differences are observed uncovering the non-negligible effect of the effective range. I note that the result obtained empirically in Ref. [19] is also close to the QMC. However, this result were obtained neglecting the effect of r_e and the agreement is most probably accidental. In Ref. [22], an alternative functional has been proposed and shown to match the equation of state of neutron matter from very low to higher density. In this case, the parameters were adjusted to directly reproduce a set of *ab initio* calculations. Restricting the range of density considered, it is shown that the functional proposed here can reproduce exact QMC results by having as unique parameters the universal parameters deduced independently at unitarity. This clearly opens new perspectives to less empirical nuclear density-functional theories.

Another important conclusion is that the results obtained using parameters deduced only from low-density constraints (gray thin solid line) fail to describe the neutron matter in the density range considered here. This indicates that for nuclear systems with very large scattering lengths in the s-wave channel and nonzero effective range, the unitary regime seems to be a better starting point than the low-density expansion. Interestingly enough this strategy has been recently explored in Ref. [42] where calculations are made for small nuclei setting the unitary limit as the leading order.

In the present work, inspired by the resummed expression obtained in EFT, I propose a new functional for strongly interacting Fermi systems. The functional parameters are directly constrained to reproduce the universal behavior of Fermi gas at unitarity including the possible effective range influence. The resulting functional has only two parameters, the so-called Bertsch parameter ξ_0 and the effective range parameter η_e that can be taken from previous studies on unitary gas. The proposed functional further has the advantage to naturally extend functionals [9–12] proposed for unitary gas at low density while being able to (i) describe systems with finite scattering length, (ii) include possible effective range effects, and (iii) applies to a wider range of density, even if $|ak_F| \gg 1$. I apply the functional to estimate the energy of Fermi gas on a wide range of (ak_F) values showing good reproduction of experimental results as well as QMC calculations. I use the functional to obtain an expression of the Tan contact parameter at and away from unitarity. The possible effects of nonzero effective range at unitarity are also discussed. It is finally shown that the functional can reproduce well recent QMC results obtained for symmetric neutron matter.

The present work promotes the idea that the unitary regime can be a proper starting point for describing systems with large s-wave scattering length and eventually nonzero effective range. Here, I concentrated on infinite uniform systems. To apply the functional to finite systems like atomic clouds and/or nuclei a number of issues should be clarified. The most natural way to extend a functional designed for infinite systems to finite systems is to use a local-density approximation. Then, the energy becomes functional of the local density. It is anticipated, however, that such a rough approximation will improperly describe nonuniform systems. For instance, the effective mass of nuclear or atomic systems are known to differ from the bare mass. A proper treatment of the effective mass would require one to introduce an explicit gradient correction in the functional.

A second important aspect is superfluidity, which is crucial in both nuclei and atomic clouds. The energy provided by the functional (5) is describing the total energy of interacting fermionic systems and therefore contains implicitly the effect of superfluidity. For finite system, however, it is well known that effects like odd-even staggering require the explicit introduction of the anomalous density. The treatment of the pairing field with the proposed functional needs also to be clarified in the near future to extend the present work to finite systems.

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