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Density-functional theory for fermions close to the unitary regime

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We consider interacting Fermi systems close to the unitary regime and compute the corrections to the energy density that are due to a large scattering length and a small effective range. Our approach exploits the universality of the density functional and determines the corrections from the analyical results for the harmonically trapped two-body system. The corrections due to the finite scattering length compare well with the result of Monte Carlo simulations. We also apply our results to symmetric neutron matter.

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Ultracold fermionic atom gases have attracted a lot of interest since Fermi degeneracy was achieved by DeMarco and Jin [1]. These systems are in the metastable gas phase, as three-body recombinations are rare. Most interestingly, the effective two-body interaction itself can be controlled via external magnetic fields. This makes it possible to study the system as it evolves from a dilute Fermi gas with weak attractive interactions to a bosonic gas of diatomic molecules. This transition from a superfluid BCS state to Bose-Einstein condensation (BEC) has been the subject of many experimental [2–12] and theoretical works [13–25].

At the midpoint of this transition, the two-body system has a zero-energy bound state and the scattering length diverges. If other parameters such as the effective range of the interaction can be neglected, the interparticle spacing becomes the only relevant length scale. This defines the unitary limit. In this limit, the energy density is proportional to that of a free Fermi gas, the proportionality constant denoted by ξ. Close to the unitary limit, corrections are due to a finite, large scattering length a and a small effective range r_0 of the potential. Within the local density approximation (LDA), the energy density can be written as

$$\mathcal{E}[\rho] = \mathcal{E}_{\mathrm{FG}}\left(\xi + \frac{c_1}{a\rho^{1/3}} + c_2 r_0 \rho^{1/3}\right). \tag{1}$$

Here,

$$\mathcal{E}_{\mathrm{FG}}[\rho] = \frac{3}{10}(3\pi^2)^{2/3}\frac{\hbar^2}{m}\rho^{5/3} \tag{2}$$

is the energy density of the free Fermi gas. The first two terms of the functional have been discussed in Ref. [17]; the third term is motivated through a simple scaling argument given below. The universal constant ξ has been computed by several authors. Monte Carlo calculations by Carlson *et al.* [21], Astrakharchik *et al.* [22], and Bulgac *et al.* [23] agree well with each other and yield $\xi \approx 0.44 \pm 0.01$, $\xi \approx 0.42 \pm 0.01$, and $\xi \approx 0.42$, respectively. A calculation by Steele [26] based on effective field theory yields $\xi = 4/9$, while an application of density-functional theory (DFT) [27,28] yields $\xi \approx 0.42$ [29]. A many-body approach incorporating pairing fluctuations beyond mean field by Perali *et al.* [24] yields $\xi \approx 0.455$. Other calculations deviate considerably from these results. Heiselberg [19] obtained $\xi = 0.326$, while Baker [30] found $\xi = 0.326$ and $\xi = 0.568$ from different Padé approximations to Fermi gas expansions. Engelbrecht *et al.* [31] obtained $\xi = 0.59$ in a calculation based on BCS theory, and Bruun [25] obtained $\xi = 0.7$ by modeling an interacting system of atoms and molecules, while a very recent Monte Carlo simulation by Lee [32] yields $\xi \approx 0.25$. The experimental values are $\xi \approx 0.74 \pm 0.07$ [6], $\xi = 0.51 \pm 0.04$ [12], $\xi \approx 0.7$ [4], and $\xi = 0.27^{+0.12}_{-0.09}$ [9]. These values can, e.g., be extracted from the density profiles of the trapped gases (see, e.g., [24]) or from a test of the equation of states (see, e.g., Ref. [17]). The constant c_1 in Eq. (1) has also been determined. The Monte Carlo results by Chang *et al.* [33] and by Astrakharchik *et al.* [22] yield $c_1 \approx -0.28$ [17] and are very close to Steele's analytical result [26]. We are not aware of any estimate for the constant c_2 in Eq. (1) that concerns the correction due to a small effective range. It is the purpose of this work to fill this gap. This is particularly interesting as experiments also have control over the effective range. Note that the regime of a large effective range has recently been discussed by Schwenk and Pethick [20] and that superfluid properties in the BCS approximation have been investigated for finite range potentials by De Palo *et al.* [34]

In this work, we determine the coefficients c_1 and c_2 via density-functional theory. Recall that the density functional is supposed to be universal; i.e., it can be used to solve the N-fermion system for any particle number N and for any external potential. Unfortunately, the exact density functional is not known. However, the unitary limit poses severe constraints on the LDA of the exact density functional and this approximation is quite accurate in the unitary regime even for nonuniform densities [29]. Exploiting the universality of the density functional, the parameters c_1 and c_2 can be obtained from a fit to an analytically known solution—i.e., the harmonically trapped two-fermion system [35]. This simple approach has recently been applied [29] to determine the universal constant ξ and will be followed and extended below.

Let us briefly turn to the harmonically trapped two-fermion system. The wave function $u(r)$ in the relative coordinate $r = r_1 - r_2$ of the spin-singlet state is given in terms of

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the parabolic cylinder function $U(-\varepsilon, r/\lambda)$ [35–37]. Here, $\varepsilon\hbar\omega$ is the energy of the relative motion and $\lambda=\sqrt{\hbar/(m\omega)}$ denotes the oscillator length. We are dealing with a short-ranged two-body interaction and quantize the energy through the boundary condition at the origin,

$$\left.\frac{\partial_r u(r)}{u(r)}\right|_{r=0} = k \cot \delta, \tag{3}$$

where $\hbar^2k^2/m=\varepsilon\hbar\omega$ and δ denotes the s-wave phase shift. The evaluation of Eq. (3) for the parabolic cylinder function yields

$$\sqrt{2}\frac{\Gamma(3/4-\varepsilon/2)}{\Gamma(1/4-\varepsilon/2)} = \frac{\lambda}{a} - \frac{r_0\varepsilon}{2\lambda}. \tag{4}$$

Here, we have employed the effective range expansion of the phase shift—i.e., $k \cot \delta=-1/a+r_0k^2/2$. Note that Eq. (4) is valid for arbitrary values of the scattering length a and the effective range r_0. In what follows, we employ density-functional theory within the LDA. Our approach is based on the scaling law

$$\rho \propto \lambda^{-3}, \tag{5}$$

which relates the density to the oscillator length.

As an introductory example, we consider the case of a dilute Fermi gas with a small value of the (positive) scattering length $a \ll \lambda$ and zero range. We expand Eq. (4) around the energy of the noninteracting system as $\varepsilon=3/2+\Delta\varepsilon$. The energy correction fulfills $\Delta\varepsilon \ll 1$, and we find

$$\Delta\varepsilon = \sqrt{\frac{2}{\pi}}\frac{a}{\lambda}. \tag{6}$$

Thus, Eqs. (6) and (5) suggest that the energy density of the weakly interacting system is that of the noninteracting system plus the term

$$\Delta\mathcal{E}[\rho] = c(a\rho^{1/3})\frac{\hbar^2}{m}\rho^{5/3}, \tag{7}$$

which is due to the scattering length. We want to determine the coefficient c in Eq. (7). Recall that Kohn-Sham DFT is variational and that we are dealing with a small perturbation $a\rho^{1/3} \ll 1$. Thus, we can insert the density of the noninteracting system $\rho(r)=2\pi^{-3/2}\lambda^{-3}e^{-r^2/\lambda^2}$ into Eq. (7) and integrate over all space. Equating the result with the energy correction given by Eq. (6) yields $c=\pi$, which is in full agreement with many-body perturbation theory [38–40]. This result is not really surprising. The interaction is a contact interaction, and the energy correction given by Eq. (7) is the Hartree-Fock approximation of this interaction. Nevertheless, it is encouraging that the simple DFT approach via the two-body system yields a result in agreement with many-body theory.

Let us turn to the vicinity of the unitary regime. Consider the case of a large scattering length $a \gg \lambda$ and zero range. We expand Eq. (4) around the energy corresponding to the unitary regime as $\varepsilon=1/2+\Delta\varepsilon$ and find

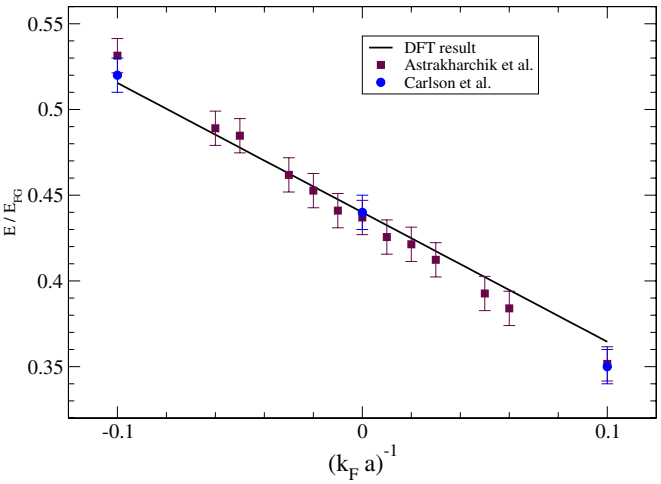

FIG. 1. (Color online) Energy per particle (in units of the free Fermi gas) as a function of $(k_Fa)^{-1}$ in the vicinity of the unitary regime. Solid line: slope estimated in this work. Data points: Monte Carlo results from Ref. [21] (dots) and from Ref. [22] (squares), respectively.

$$\Delta\varepsilon = -\sqrt{\frac{2}{\pi}}\frac{\lambda}{a}. \tag{8}$$

This expression and the scaling law (5) indicate that the correction to the energy density $\xi\mathcal{E}_{\mathrm{FG}}$ in the unitary limit is of the form

$$\Delta\mathcal{E}_1[\rho] = \frac{c_1}{a\rho^{1/3}}\mathcal{E}_{\mathrm{FG}}[\rho], \tag{9}$$

in agreement with Eq. (1). We insert the exact density at the unitary regime,

$$\rho(r) = \frac{4e^{-2(r/\lambda)^2}}{\pi^{3/2}\lambda^2 r}\int_0^{r/\lambda} dx e^{x^2} = \frac{2e^{-2r^2/\lambda^2}}{\pi\lambda^2 r}\mathrm{Erfi}(r/\lambda), \tag{10}$$

into the correction given by Eq. (9) and integrate. Equating the result with the exact result (8) yields $c_1=-0.244$. Monte Carlo calculations predict $c_1 \approx -0.28$. Our result deviates only 13% from the results of the Monte Carlo calculations (see Fig. 1). The deviation is due to the fact that the simple functional in Eq. (9) is the LDA of the (unknown) exact density functional. Given the simplicity of our approach, the estimate is remarkably accurate.

Let us consider the corrections due to a nonzero effective range $r_0 \ll \lambda$. Again, we expand Eq. (4) around the energy of the unitary regime as $\varepsilon=1/2+\Delta\varepsilon$ and find

$$\Delta\varepsilon = \frac{1}{\sqrt{8\pi}}\frac{r_0}{\lambda}. \tag{11}$$

The form of this energy correction and the scaling law (5) imply that the term

$$\Delta\mathcal{E}_2[\rho] = c_2 r_0 \rho^{1/3}\mathcal{E}_{\mathrm{FG}}[\rho] \tag{12}$$

has to be added to the energy density $\xi\mathcal{E}_{\mathrm{FG}}$ [see Eq. (1)]. For a determination of the coefficient c_2, we insert the density given by Eq. (10) into Eq. (12) and integrate. Comparison of

the result with the exact result (11) yields $c_2=0.142$. This is one of the main results of this work. We estimate that the systematic error of this coefficient (due to the LDA) is about 5%–15%, as this is the deviation by which the DFT estimates for ξ [29] and c_1 deviate from the Monte Carlo predictions [21,22]. The estimate for c_2 enables us to discuss a small systematic correction of the universal constant obtained from Monte Carlo calculations. Recall that the Monte Carlo calculations [21,22] are based on potentials with a small effective range of about $r_0\rho^{1/3}\approx 0.05$ and $r_0\rho^{1/3}=0.01$, respectively. This suggests that their predictions for the universal constant ξ involve the effect of a very small finite range and are therefore overestimated by $c_2 r_0\rho^{1/3}\approx 0.007$ and $c_2 r_0\rho^{1/3}\approx 0.001$, respectively. These small corrections are within the statistical error of these simulations.

We also tried to improve the accuracy of our estimates for c_1 and c_2 by going beyond the LDA through the inclusion of gradient terms. The main idea consists of adding gradient terms to the energy functional and to use Kohn-Sham DFT. The systematic inclusion of the nonlocal kinetic energy density in the energy functional can lead to improvements in the density and energy spectrum [41,42]. Here, we follow a phenomenological approach. We replace the functional in Eq. (1) by the functional [29]

$$\mathcal{E}[\rho]=\xi\mathcal{E}_\xi[\rho]+\frac{c_1}{a\rho^{1/3}}\mathcal{E}_a[\rho]+c_2(r_0\rho^{1/3})\mathcal{E}_{r_0}[\rho]. \tag{13}$$

Here

$$\mathcal{E}_\xi[\rho]=\frac{\hbar^2}{m}\left(\frac{f_\xi}{2}\sum_{j=1}^{N}|\nabla\phi_j|^2+(1-f_\xi)\frac{3}{10}(3\pi^2)^{2/3}\rho^{5/3}\right), \tag{14}$$

and similar expressions with parameters f_a and f_{r_0} are employed for the terms involving the scattering length and the effective range, respectively. Note that the functional (1) is the Thomas-Fermi approximation of the functional (13) and that both functionals are identical for $f_\xi=f_a=f_{r_0}=0$. Note also that the density-dependent term in Eq. (14) is the Thomas-Fermi approximation of the corresponding gradient term. Thus, the functional (13) differs from the LDA (1) by explicit gradient terms while keeping the Thomas-Fermi limit unchanged. In Ref. [29], the universal constant ξ was determined by a density functional of this form. In particular, the universal constant ξ was very insensitive to variations of the parameter f_ξ. This robustness can be traced back to the approximate equality of the integrals $\int d^3r\Sigma_{j=1}^{N}\frac{1}{2}|\nabla\phi_j|^2$ and $\int d^3r\frac{3}{10}(3\pi^2)^{2/3}\rho^{5/3}$ when evaluated for the density (10). This is very different for the parameter pairs (c_1,f_a) and (c_2,f_{r_0}), as the corresponding integrals energy differ by a factor of 2.1 and 0.7, respectively, from each other. This finding indicates that the functionals $\mathcal{E}_a[\rho]$ and $\mathcal{E}_{r_0}[\rho]$ exhibit considerable finite-size corrections (as the gradient terms differ from their respective Thomas-Fermi limits for the two-body system). For this reason, we do not use phenomenological gradient corrections for a more accurate determination of the constants c_1 and c_2.

Let us also investigate the deep bound-state limit ($\varepsilon\to -\infty$) of the two-body system corresponding to a positive scattering length $a\ll\lambda$ and zero range. Taking this limit in Eq. (4) and noting that $\Gamma(x+1/2)/\Gamma(x)\to\sqrt{x}$ for $x\to\infty$, we find that the binding energy is $\varepsilon\hbar\omega=-\hbar^2/(ma^2)$. Thus, one can trivially write down the density functional for the system in this limit as

$$\mathcal{E}_B[\rho]=-\frac{\hbar^2}{2ma^2}\rho \tag{15}$$

and the energy per particle is $-\frac{\hbar^2}{2ma^2}$. Interestingly, this value coincides exactly with the $1/a^2$ correction that Bulgac and Bertsch [17] obtained from a fit to Monte Carlo results close to the unitary regime, and it is about 20% larger than the analytical result that can be inferred from Steele's work [26].

Finally, we apply Eq. (1) to neutron matter, for which $a=-18.3$ fm and $r_0=2.7$ fm. We drop the $r_0\rho^{1/3}$ term in Eq. (1), as this correction is only small for very small densities. In Fig. 2 we compare our results to the equation of state (EOS) obtained by Friedman and Pandharipande [43]. Their calculation is based on a variational approach and employs a realistic Hamiltonian, which includes higher partial waves and three-body interactions. Recall that our approach is limited to s waves and a two-body interaction. The inset of Fig. 2 shows the comparison for very small densities; here, the correction due to the effective range is included and the restriction to s waves is justified. We note that the inclusion of the effective range correction for values of $r_0\rho^{1/3}$ less than 0.6 improves the DFT result.

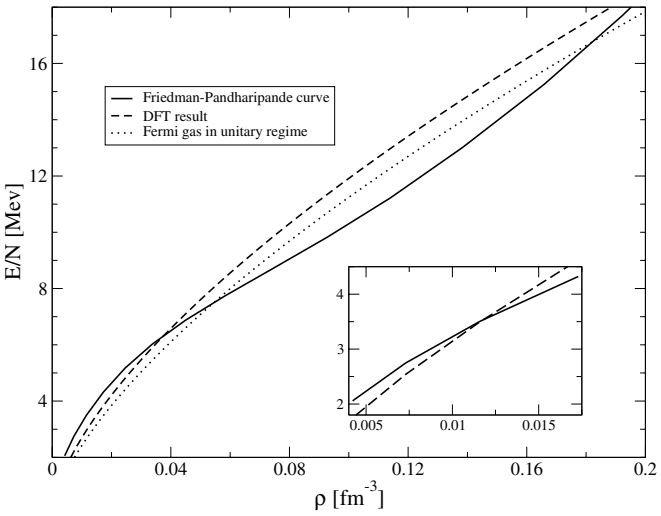

FIG. 2. Energy per particle for symmetric neutron matter as a function of the density. Solid line: equation of state by Friedman and Pandharipande [43]. Dashed line: result from density-functional theory (DFT). Dotted curve: Fermi gas in unitary regime. The inset shows the DFT result and includes finite-range corrections.

To summarize, we have considered interacting dilute Fermi systems near the unitary regime and computed the corrections to its energy density due to a large scattering length and a finite effective range of the two-body interaction. Our calculations are based on the universality of the density functional, and we determine its local density approximation through comparison with exact results for the

harmonically trapped two-fermion system. The correction due to the large scattering length agrees well with results from Monte Carlo calculations and effective field theory, while the correction due to the finite range implies a small systematic correction of order 0.01 to the universal constant extracted from Monte Carlo results. The phenomenological inclusion of gradient terms is difficult due to finite-size corrections. We also applied our results to neutron matter.

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