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Density-functional theory for fermions in the unitary regime

T. Papenbrock
Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA
and Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA
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In the unitary regime, fermions interact strongly via two-body potentials that exhibit a zero range and a (negative) infinite scattering length. The energy density is proportional to the energy density of the free Fermi gas with a proportionality constant ξ. The author uses a simple density functional parametrized by an effective mass and the universal constant ξ, and employs Kohn-Sham density-functional theory to obtain the parameters from fit to one exactly solvable two-body problem. This yields $\xi=0.42$ and a rather large effective mass. The form of the density functional is checked by similar Kohn-Sham calculations for the exactly solvable Calogero model.

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Ultracold atomic Fermi gases have received considerable experimental and theoretical interest since the achievement of Fermi degeneracy by DeMarco and Jin [1]. One of the most interesting features is the ability to tune the interparticle interaction itself via a Feshbach resonance, and to study the system as it evolves from the BCS regime with weakly attractive interaction toward the point where the interaction is strong enough to form diatomic molecules, and the system may undergo Bose-Einstein condensation (BEC). Very recently, the BEC-BCS crossover has been the subject of numerous experimental [2] and theoretical studies [3,4].

The dividing point of this BCS-BEC crossover defines the unitary regime and is of particular interest [5–8]. Here, the two-body system exhibits a bound state at zero energy, and the two-body scattering length diverges. For dilute systems, the interparticle distance is much larger than the range of the interaction and much smaller than the scattering length. Thus, the interparticle distance is the only relevant length scale, and the energy must be proportional to that of a free Fermi gas,

$$E(N) = \xi E_{\mathrm{TF}}(N), \tag{1}$$

the dimensionless proportionality constant being denoted as ξ. Here, $E(N)$ is the energy of the fully paired N-fermion system while $E_{\mathrm{TF}}(N)$ is the Thomas-Fermi energy of N noninteracting spin-$\frac{1}{2}$ fermions. The constant ξ is universal, as it describes the physics of any dilute Fermi gas in the unitary regime. Approximately, it also describes systems close to the unitary regime, and can also be applied to dilute neutron gases as the two-neutron system also exhibits a scattering length that is much larger than the range of the nucleon-nucleon interaction. The exact determination of the universal constant ξ is thus an important task.

Recently, this constant was reliably determined through Monte Carlo simulations as $\xi\approx 0.44\pm 0.01$ by Carlson *et al.* [6] and as $\xi=0.42\pm 0.01$ by Astrakharchik *et al.* [7]. So far, simpler approaches have failed to agree on the value of ξ, and they deviate considerably from the Monte Carlo results. Heiselberg [8] obtained $\xi=0.326$, while Baker [9] found $\xi=0.326$ and $\xi=0.568$ from different Padé approximations to Fermi gas expansions. Engelbrecht *et al.* [10] obtained $\xi=0.59$ in a calculation based on BCS theory.

It is the purpose of this paper to present a simple calculation that determines the universal constant ξ. It is based on Kohn-Sham density-functional theory (DFT) with a two-parameter density functional that is fit to one analytically known result. The resulting value $\xi\approx 0.42$ is close to recent Monte Carlo results. This paper is organized as follows. Its first part deals with DFT for the Fermi systems in the unitary regime. The density functional has a particularly simple and constrained form in the unitary regime. The second part tests and validates the density functional through calculations for the exactly solvable Calogero model.

Carlson *et al.* [6] performed quantum Monte Carlo simulations for systems of N fermions in the unitary regime, with the number of fermions N ranging from $N=10$ to approximately $N\approx 40$. They found in particular that the relation (1) holds with very good accuracy for all even-number systems. This is a remarkable finding, since exact quantum-mechanical energies usually differ from the corresponding Thomas-Fermi energies due to finite-size effects and shell effects, both of which are apparently very small for fermions in the unitary regime. This suggests that the density functional from Thomas-Fermi theory

$$\mathcal{E}_{\mathrm{TF}}[\rho] = \xi(\hbar^2/m)c\rho^{5/3} \tag{2}$$

with $c=\frac{3}{10}(3\pi^2)^{2/3}$ is a good approximation of the exact density functional, and that corrections might easily be accounted for via full-fledged Kohn-Sham DFT.

As a starting point, we thus consider Thomas-Fermi theory of harmonically trapped fermions in the unitary regime. The density functional is

$$\mathcal{E}^{\mathrm{HO}}_{\mathrm{TF}}[\rho] = \mathcal{E}_{\mathrm{TF}}[\rho] + (m/2)\omega^2 r^2 \rho. \tag{3}$$

This functional is minimized under the condition that the density is normalized to N particles. This yields the Thomas-Fermi density

$$\rho_{\mathrm{TF}}(r) = (3\pi^2)^{-1}(2/\xi l^2)^{3/2}[(3N)^{1/3}\xi^{1/2} - (r/2l)^2]^{3/2}, \quad (4)$$

where $l=(\hbar/m\omega)^{1/2}$ is the oscillator length of the harmonic trap. For the Thomas-Fermi energy, one inserts the density (4) into the functional (3) and integrates over space. This yields

$$E_{\mathrm{TF}} = 4^{-1}(3N)^{4/3}\xi^{1/2}\hbar\omega. \quad (5)$$

For the two-fermion system, the exact quantum-mechanical result for the energy is [11]

$$E_{\mathrm{ex}} = 2\hbar\omega. \quad (6)$$

Let us assume that the relation (1) also holds for harmonically trapped systems. Thus, we might equate Eq. (6) with Eq. (5) for $N=2$, and solve for the universal constant ξ. This yields $\xi=64/6^{8/3}\approx 0.54$. Note that this simple result deviates only about 20% from the Monte Carlo results [6,7]. This is quite encouraging and motivates us to compute a more accurate estimate for ξ via Kohn-Sham DFT.

In Kohn-Sham DFT [12], the ground-state density and energy of an interacting N-fermion system is obtained from varying the (generally nonlocal and unknown) density functional. Unfortunately, there is no simple recipe that permits one to construct the density functional. For dilute systems with sufficiently small range and positive scattering length, a systematic and constructive approach has been given by Puglia *et al.* [13]. For electronic systems, one usually follows an empirical approach and parametrizes the density functional in terms of local densities and their gradients, and fits the considerable number of parameters to experimental data and theoretical results for infinite systems. This elaborate and cumbersome approach has been successfully implemented in recent decades in quantum chemistry (see, e.g., Ref. [14] and references therein), and a similar approach is also pursued in nuclear structure [15]. Note that DFT has also been successfully applied to study the BCS-BEC crossover. In their study, Kim and Zubarev [4] employed a density functional that was fit to known results in the regime of very small scattering length and to the Monte Carlo results for the unitary regime, and employed a Padé approximation for intermediate values of the scattering length.

Fortunately, the empirical approach is much simpler for the unitary regime. In what follows, we consider small even-number systems with an equal number of fermions in the two spin states. As the interaction does not introduce any new length scale into the system, a local density functional can only contain density terms proportional to $\rho^{5/3}\hbar^2/m$ and gradients of the form $\rho^{-(2k-2)/3}(\partial^{2k}\rho)\hbar^2/m$, with integer $k>0$. Here, we allow only for the density-dependent term and incorporate gradient terms through an effective mass. The ansatz for the density functional thus becomes

$$\mathcal{E}[\rho] = \frac{\hbar^2}{m}\left[\frac{m}{2m_{\mathrm{eff}}}\sum_{j=1}^{N}|\nabla\phi_j(\vec{r})|^2 + \left(\xi - \frac{m}{m_{\mathrm{eff}}}\right)c\rho^{5/3}\right]. \quad (7)$$

The density is given as $\rho=\Sigma_{j=1}^{N}|\phi_j(\vec{r})|^2$. The universal constant ξ and the effective mass m_{eff} are parameters that will be determined below. The effective mass is, in principle, N-dependent, but we suppress this dependency here. Note that this density functional has two important properties: First, its Thomas-Fermi limit is given in Eq. (2) and is thus proportional to the density functional of the free Fermi gas. Second, nonlocalities of the density are introduced through the effective mass. Note that more elaborate approaches for superfluid systems also introduce pairing densities [16] in the density functional in order to approximate the (unknown) nonlocal functional for superfluid systems. The quality of the results presented below, however, suggests that this is not necessary for the purpose of this study.

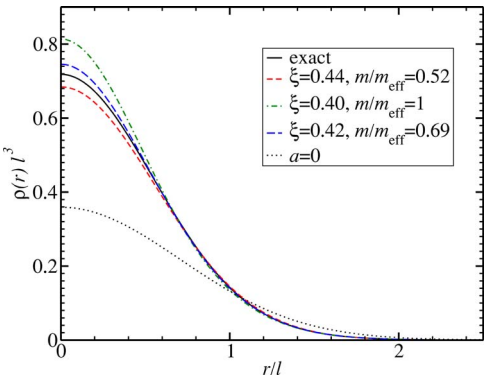

FIG. 1. (Color online) Density of the harmonically trapped two-fermion system. Exact result (full line) compared to Kohn-Sham results from three different density functionals (dashed lines and dashed-dotted line), and the noninteracting system (dotted line).

For a determination of the parameters ξ and m_{eff}, we consider the problem of two spin-$\frac{1}{2}$ fermions inside a harmonic trap that interact via a zero-range interaction with infinite scattering length. The ground state of the two-fermion system is a spin singlet, and the relative coordinate wave function has been given by Busch *et al.* [11],

$$\psi_{\mathrm{ex}}(r) = (2\pi\lambda^3)^{-1/2}(\lambda/r)e^{-(r/\lambda)^2/2}. \quad (8)$$

Here, $\lambda=\sqrt{2}l$ is given in terms of the oscillator length l. The wave function diverges like $1/r$ for small distances due to the infinite scattering length; in practice, this divergence could be cut off by any nonzero range of the interaction potential (see, e.g., the discussion in Ref. [6]), and it does not cause any problems in the normalization of the wave function. Recall that the ground-state energy (6) of the two-fermion system is considerably lower than for noninteracting fermions. Employing the relative wave function (8) and the Gaussian ground state for the center-of-mass coordinate, one arrives at the density

$$\rho_{\mathrm{ex}}(r) = \frac{4}{\pi^{3/2}l^3}\frac{l}{r}e^{-2(r/l)^2}\int_0^r dx e^{x^2}. \quad (9)$$

A plot of this density is shown in Fig. 1 as a full line, and can be compared to the noninteracting case (dotted line).

One adds the term $(m/2)\omega^2r^2\rho(\vec{r})$ of the harmonic confinement to the density functional (7) and employs Kohn-Sham theory to compute the density for given sets of parameters ξ and m_{eff}. The best agreement with the exact density (9) and exact energy (6) is obtained for $\xi=0.42$ and $m/m_{\mathrm{eff}}=0.69$. The resulting density is plotted as the long-dashed

line in Fig. 1 and exhibits only small deviations from the exact density. The energy deviates about 0.1% from its exact value (6). Note that the DFT value of the universal constant is very close to the Monte Carlo results [6,7].

Let us estimate the robustness and stability of the DFT results. For this purpose, we consider the following two cases. First, the value of the universal constant is fixed to the Monte Carlo result $\xi=0.44$ by Carlson *et al.* [6]. One obtains the effective mass $m/m_{\text{eff}}=0.52$ from the best fit to the exact density and energy. The resulting density is shown as the short-dashed line in Fig. 1, and the energy deviates less than 1% from the exact result. Second, the effective mass is set to $m/m_{\text{eff}}=1$, and one obtains $\xi=0.40$ from the fit of the density functional. The resulting density is depicted as the dashed-dotted line in Fig. 1, while the energy again deviates less than 1% from the exact result. These results show that DFT yields quite robust results for the universal constant ξ, and systematically improves upon the naive Thomas-Fermi result. This suggests that the good agreement of the best value $\xi=0.42$ with the Monte Carlo results is not merely accidental but due to the quality of the density functional. Note that the approach [9] also predicts a relatively large effective mass.

One might even take this approach a step further and obtain a simple analytical estimate for the universal constant ξ. Due to the relatively large value of the effective mass, the prefactor of the density-dependent term in the density functional (7) becomes rather small, and one might neglect it by simply setting $m/m_{\text{eff}}=\xi$. In the presence of the confining harmonic potential, the Kohn-Sham equation is then identical to the Schrödinger equation of a three-dimensional harmonic oscillator where the kinetic energy is modified by a factor ξ. The analytical result for the ground-state energy of the two-fermion system is then $E=3\hbar\omega\xi^{1/2}$, and comparison with the exact result (6) yields $\xi=\frac{4}{9}$. Note that the resulting density is very close to the short-dashed line in Fig. 1 (labeled as $\xi=0.44$, $m/m_{\text{eff}}=0.52$).

In the unitary regime, the rather simple density functional (7) does yield much improved and reliable results compared to Thomas-Fermi theory. To further test the form of this density functional, we consider another interacting N-body system whose density functional is also proportional to that of a free Fermi gas. The Calogero model [17] with Hamiltonian

$$H=\frac{\hbar^2}{m}\sum_{j=1}^{N}\left(-\frac{1}{2}\frac{\partial^2}{\partial x_j^2}+\sum_{j<i}\frac{\frac{\beta}{2}\left(\frac{\beta}{2}-1\right)}{(x_i-x_j)^2}+\frac{1}{2}\frac{m^2\omega^2}{\hbar^2}x_j^2\right)$$

is exactly solvable in one dimension. Here, $\beta\geqslant 1$ is a dimensionless coupling constant. The exact ground-state energy of this Hamiltonian is

$$E_{\text{ex}}=\hbar\omega[N/2+\beta N(N-1)/4]. \tag{10}$$

Let us focus on the two-body interaction. The inverse square potential does not introduce any new length scale into the Hamiltonian as it scales as the kinetic energy. Thus, the interparticle distance is the only length scale, and the density-dependent energy must be proportional to the one-dimensional Fermi gas, the proportionality constant being denoted as η^2. Thus, $\mathcal{E}_{\text{TF}}[\rho]=\eta^2(\pi^2/6)(\hbar^2/m)\rho^3$. In this respect, the Calogero model is similar to the Fermi gas in the unitary regime. This approach leads directly to the Thomas-Fermi theory for the Calogero model [18].

The constant η^2 can be determined from Thomas-Fermi theory once we add the confining harmonic potential and thereby make contact with exactly known results. Thus, the density functional becomes

$$\mathcal{E}[\rho]=\mathcal{E}_{\text{TF}}[\rho]+(m/2)\omega^2x^2\rho, \tag{11}$$

and it is minimized by the normalized density

$$\rho_{\text{TF}}=(\pi\eta l)^{-1}[2N\eta-(r/l)^2]^{1/2}. \tag{12}$$

Here, $l=(\hbar/m\omega)^{1/2}$ again denotes the oscillator length. The Thomas-Fermi density (12) is Wigner's semicircle, and agrees with the standard approach [19].

One inserts the density (12) into the functional (11) and integrates. The resulting Thomas-Fermi energy is

$$E_{\text{TF}}=\eta\hbar\omega N^2/2, \tag{13}$$

and comparison with the exact result (10) fixes $\eta=\beta/2$. Note that the Thomas-Fermi energy (13) differs from the exact result (10) by considerable finite-size corrections, and this is a difference from the Fermi gas in the unitary regime.

Let us apply Kohn-Sham DFT to the Calogero model. The ansatz for the density functional is in full analogy to the one for the Fermi gas in the unitary regime,

$$\mathcal{E}[\rho]=\frac{\hbar^2}{m}\left[\frac{m}{2m_{\text{eff}}}\sum_{j=1}^{N}|\partial_x\phi_j(x)|^2+\frac{\pi^2}{6}\left(\eta^2-\frac{m}{m_{\text{eff}}}\right)\rho^3\right]+(m/2)\omega^2x^2\rho(x). \tag{14}$$

Here the effective mass m_{eff} is the only fit parameter, and the term due to the harmonic confinement is already included.

One determines the effective mass by solving the Kohn-Sham equation for the density functional (14) and compares the resulting density with exact results. Note that the exact density of the Calogero model is only known for a few values of the coupling constant β, though the many-body ground state of this model is known for decades. For $\beta=1$, $\beta=2$, and $\beta=4$, the density is related to the eigenvalue dis-

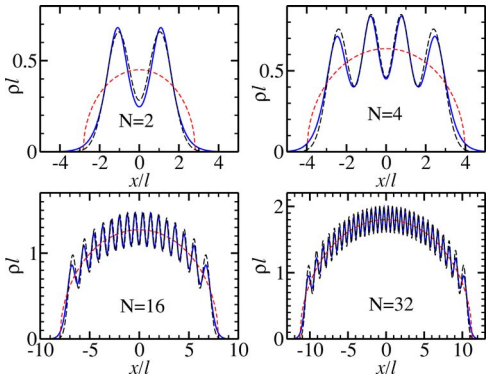

FIG. 2. (Color online) Densities of the Calogero model for $\beta=4$ for different numbers of particles N. Full line: density-functional theory; long-dashed line: long-dashed line: exact density; short-dashed line: Thomas-Fermi theory.

tribution of the orthogonal, unitary, and symplectic Gaussian random matrix ensemble, respectively. Analytical expressions are given in Ref. [20]. We focus on the case $\beta=4$, and determine the effective mass by fit. From calculations for particle numbers $N=2$, 4, 16, and 32, one obtains approximately $m/m_{\mathrm{eff}} \approx 6.3+8.0/N^2$. Thus, the effective mass is considerably smaller than the mass. Figure 2 shows that the Kohn-Sham densities are close to the exact results. The Thomas-Fermi result is also shown for comparison. Note that only a relatively small effective mass reproduces the density oscillations. Note also that the deviation of the DFT energies from the exact result is about half as large as the error of the corresponding Thomas-Fermi energies. This shows that the simple density functional (14) yields significantly improved energies and densities.

In summary, this paper used density-functional theory to compute the universal constant of the Fermi gas in the unitary regime. This approach is based on the observation that the Thomas-Fermi energy is a reasonable first-order approximation to the quantum-mechanical results, and on the constraints that the unitary regime imposes on the form of the density functional. The estimate $\xi=0.42$ results from a best fit to the density and energy of the harmonically trapped two-fermion system, and is in good agreement with much more elaborate Monte Carlo studies. The result is stable with respect to variations of the density functional, and favors a sufficiently large effective mass. The particular form of the density functional could also be tested in applications to the Calogero model.

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