

Extended Thomas-Fermi density functional for the unitary Fermi gas

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We determine the energy density $\xi(3/5)n\varepsilon_F$ and the gradient correction $\lambda\hbar^2(\nabla n)^2/(8mn)$ of the extended Thomas-Fermi (ETF) density functional, where n is the number density and ε_F is the Fermi energy, for a trapped two-component Fermi gas with infinite scattering length (unitary Fermi gas) on the basis of recent diffusion Monte Carlo (DMC) calculations [Phys. Rev. Lett. **99**, 233201 (2007)]. In particular we find that $\xi=0.455$ and $\lambda=0.13$ give the best fit of the DMC data with an even number N of particles. We also study the odd-even splitting $\gamma N^{1/9}\hbar\omega$ of the ground-state energy for the unitary gas in a harmonic trap of frequency ω determining the constant γ . Finally we investigate the effect of the gradient term in the time-dependent ETF model by introducing generalized Galilei-invariant hydrodynamics equations.

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I. INTRODUCTION

The crossover from the weakly paired Bardeen-Cooper-Schrieffer (BCS) state to the Bose-Einstein condensate (BEC) of molecular dimers with ultra cold two-hyperfine-component Fermi vapor atoms has been investigated by several experimental groups with ^{40}K atoms [1–3] and ^6Li atoms [4,5]. In the unitary limit of infinite scattering length [6] obtained by tuning an external background magnetic field near a Feshbach resonance [7], the Fermi superfluid exhibits universal properties [7–10].

It has been suggested that at zero-temperature the unitary Fermi gas can be described by the density functional theory (DFT) [11–18]. Bulgac and Yu [11] introduced a superfluid DFT (SDFT) based on a Bogoliubov–de Gennes (BdG) approach to superfluid fermions, in the same spirit as the density functional formulation for superconductors [19]. Papenbrock and Bhattacharyya [14] have instead proposed a Kohn-Sham (KS) density functional with an effective mass to take into account nonlocality effects. To treat nonuniform systems, other authors [12,13,16–18] have added a gradient term to the leading Thomas-Fermi energy, since such a term is surely necessary when surfaces are present [20,21], at least in three spatial dimensions [22]. An energy functional for fermions not written in terms of single-particle orbitals but only in terms of the density and its derivatives is usually called extended Thomas-Fermi (ETF) functional [23,24]. It may be seen as an effective field theory where the gradient correction $\lambda\hbar^2(\nabla n)^2/(8mn)$ can be interpreted as the next-to-leading term [16,18], with $n(\mathbf{r})$ the local number density and m the atomic mass.

We wish to point out that both the energy functionals proposed by Bulgac and Yu [11] and Papenbrock and Bhattacharyya [14] are functionals of the density through single particle orbitals (the BdG or KS orbitals). Therefore they can be used in actual numerical calculations only when the number of fermions is small, since they require a self-consistent calculation of single-particle states whose number increases linearly with the number of particles.

On the contrary, one encounters no limitation in the number of particles which may be treated through ETF functionals, since in this case the functional depends only on a single

function of the coordinate, i.e., the particle density. Of course one trades simplicity with accuracy: while the BdG and KS schemes are built to account for the main contribution to the kinetic energy, and treat it exactly in noninteracting systems even with a nonuniform density varying in space, the TF approach gives the exact kinetic energy only for a uniform system and even when extended with the addition of gradient and higher order derivatives of the density, the ETF functional is not able to reproduce shell effects in the density profile [23,24].

In spite of this limitation, but in the light of the great simplification introduced in numerical calculations, we believe that it is useful to analyze the ETF approximation and comment on its dynamical generalization, which amounts to introducing a quantum pressure term $-\lambda\hbar^2\nabla^2\sqrt{n}/(2m\sqrt{n})$ into the hydrodynamic equations of superfluids.

The value of the coefficient λ is debated. In the papers of Kim and Zubarev [12] and Manini and Salasnich [13] the authors set $\lambda=1$ over the full BCS-BEC crossover. More recently we have suggested $\lambda=1/4$ [17,25]. This suggestion is in good agreement with a theoretical estimate based on an epsilon expansion around $d=4-\varepsilon$ spatial dimensions in the unitary regime [18].

In this paper we comment on the ETF for a two-component Fermi gas at unitarity and determine its parameters by fitting recent Monte Carlo results [26,27] for the energy of fermions confined in a spherical harmonic trap of frequency ω in this regime.

Since the interaction potential does not introduce any new length, the universal contribution to the energy density in an ETF functional appropriate to a spin balanced Fermi liquid at unitarity may be considered, in its simplest form, as the sum of a term proportional (ξ being the constant of proportionality) to the energy density of a uniform noninteracting system with the same density and of a term containing the gradient of the density with a coefficient λ meant to take into account phenomenologically also higher order derivatives [28].

By minimizing such ETF functional for a fixed number of particles, we find that the values $\xi=0.455$ and $\lambda=0.13$ give the closest results to the Monte Carlo energies of a fully superfluid system with an even number N of fermions confined in a harmonic well at unitarity, as calculated by Ref.

[27]. When treating systems with an odd number of particles, we must correct the calculated value of the ETF ground state energies corresponding to these parameters to account for the presence of the unpaired particle. According to Son [29], for fermions confined by a harmonic potential, the correction depends on the number of particle and takes the form $\Delta E = \gamma N^{1/9}$ (in units of $\hbar\omega$). We then find that $\gamma=0.856$ provides the best fit to the DMC data [27]. In Sec. IV, we investigate the effect of the gradient term on the dynamics of the Fermi superfluid by introducing generalized hydrodynamics equations and a Galilei-invariant nonlinear Schrödinger equation of the Guerra-Pusterla type [30,31] which is fully equivalent to them.

II. EXTENDED THOMAS-FERMI FUNCTIONAL

Let us consider an interacting Fermi gas trapped by a potential $U(\mathbf{r})$. Its TF energy functional is

$$E_{TF} = \int d^3\mathbf{r} n(\mathbf{r}) [\varepsilon(n(\mathbf{r})) + U(\mathbf{r})], \quad (1)$$

where $\varepsilon(n)$ is the energy per particle of a uniform Fermi system with density n equal to the local density $n(\mathbf{r})$ of fermions. The total number of fermions is

$$N = \int d^3\mathbf{r} n(\mathbf{r}). \quad (2)$$

By minimizing E_{TF} with respect to the density $n(\mathbf{r})$, with the constraint of a fixed number of particles, one finds

$$\mu(n(\mathbf{r})) + U(\mathbf{r}) = \bar{\mu}, \quad (3)$$

where $\mu(n) = \frac{\partial(n\varepsilon(n))}{\partial n}$ is the bulk chemical potential of a uniform system of density n and $\bar{\mu}$ is the chemical potential of the nonuniform system, i.e., the Lagrange multiplier fixed by the normalization (2).

In the unitary limit, no characteristic length is set by the interatomic-potential since its s -wave scattering length a_F diverges ($a_F \rightarrow \pm\infty$). The energy per particle of a uniform two-spin components Fermi gas at unitarity must then depend only on \hbar , on the mass of fermions m , and on the only length characterizing the system, i.e., the average distance between particles $\propto n^{-1/3}$ [7]. It is usually written as

$$\varepsilon(n) = \xi \frac{3}{5} \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n^{2/3}, \quad (4)$$

where ξ is a universal parameter which can be determined from *ab initio* calculations. Notice that $(\hbar^2/2m)(3\pi^2)^{2/3}n^{2/3} = \varepsilon_F$, where ε_F is the Fermi energy of the ideal fermionic gas. Thus ξ is simply the ratio between the energy per particle of the uniform interacting system at unitarity and the corresponding energy in a noninteracting system. Monte Carlo calculations for a uniform unpolarized two-spin components Fermi gas suggest $\xi \approx 0.45$; in particular, $\xi = 0.42 \pm 0.01$ according to [9] and $\xi = 0.44 \pm 0.02$ according to [10]. The bulk chemical potential associated to Eq. (4) is

$$\mu(n) = \xi \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n^{2/3}. \quad (5)$$

If the system is confined by a spherically symmetric harmonic potential,

$$U(\mathbf{r}) = \frac{1}{2} m \omega^2 r^2, \quad (6)$$

its density profile $n(\mathbf{r})$ obtained from Eq. (3) is

$$n(\mathbf{r}) = n(0) \left(1 - \frac{r^2}{r_F^2} \right)^{3/2}, \quad (7)$$

where $n(0) = (2m\bar{\mu})^{3/2} / (3\pi^2\hbar^3\xi^{3/2})$, $r_F = \sqrt{2\bar{\mu}/(m\omega^2)}$, and $\bar{\mu} = \hbar\omega\sqrt{\xi}(3N)^{1/3}$. Obviously, the expression (7) for the TF density profile of the unitary Fermi gas in a harmonic potential coincides with that of an ideal Fermi gas [32], but its parameters are modified by the presence of ξ in the equation of state (4).

As previously stressed the TF functional must be extended to take into account other characteristic lengths related to the spatial variations of the density, besides the average particle separation. As a consequence, the energy per particle must contain additional terms, which scale as the square of the inverse of these various lengths. For this reason, as a simple approximation, we add to the energy per particle of Eq. (4) a term

$$\lambda \frac{\hbar^2}{8m} \left(\frac{\nabla n}{n} \right)^2 = \lambda \frac{\hbar^2}{2m} \left(\frac{\nabla \sqrt{n}}{\sqrt{n}} \right)^2, \quad (8)$$

which may be seen as the first term in a gradient expansion. We notice that, according to the Kirzhnits expansion of the quantum kinetic operator in powers of \hbar [21], λ must take the value $\lambda=1/9$ [33,34] for an ideal, noninteracting, Fermi gas. Historically, a term of this form, but with $\lambda=1$, was introduced in a pioneering paper [20] by von Weizsäcker to treat surface effects in nuclei.

Instead of trying to determine it from first principles, we consider λ as a phenomenological parameter accounting for the increase of kinetic energy due to the entire spatial variation of the density. We remark that this attitude is adopted in many applications of density functional theory to atomic and molecular physics where the gradient term (8) takes into account phenomenologically, through λ , all the possible corrections of a gradient expansion [28].

The new energy functional reads [21,33–35]

$$E = \int d^3\mathbf{r} n(\mathbf{r}) [\varepsilon_g(n(\mathbf{r}), \nabla n(\mathbf{r})) + U(\mathbf{r})], \quad (9)$$

where

$$\varepsilon_g(n, \nabla n) = \varepsilon(n) + \lambda \frac{\hbar^2}{8m} \frac{(\nabla n)^2}{n^2} \quad (10)$$

is a generalized energy per particle which includes the \hbar -dependent gradient correction.

We remark that in our ETF the constants ξ and λ are independent, implying that the ratios between the energies per particle corresponding to the two terms in a unitary and in a noninteracting Fermi system may be different. Equal ratios imply $\lambda = \xi/9$ [21].

By minimizing the energy functional (9) with the constraint (2) one gets the partial differential equation obeyed by the ground state density:

$$\left[\lambda \frac{\hbar^2}{2m} \nabla^2 + \mu(n(\mathbf{r})) + U(\mathbf{r}) \right] \sqrt{n(\mathbf{r})} = \bar{\mu} \sqrt{n(\mathbf{r})}. \quad (11)$$

For the study of hydrodynamics in Fermi superfluids Kim and Zubarev [12], and also Manini and Salasnich [13], used $\lambda=1$ over the full BCS-BEC crossover. More recently we have suggested $\lambda=1/4$ [17] on the basis of the correct relationship between phase and superfluid velocity [25]. This suggestion is in agreement with the theoretical estimate of Rupak and Schäfer [18], obtained from an epsilon expansion around $d=4-\epsilon$ spatial dimensions for a Fermi gas in the unitary regime. In particular, by using the expansion of Rupak and Schäfer [18] we obtain the ETF functional (9) with $\xi=0.475$ and $\lambda=0.25$.

Very recently two theoretical groups [26,27] have studied the two-component Fermi gas in the harmonic trap of Eq. (6) at unitarity by using Monte Carlo algorithms. Chang and Bertsch [26] have used a Green-function Monte Carlo method, while Blume, von Stecher, and Greene [27] have applied a fixed-node diffusion Monte Carlo (FNDMC) approach. They have obtained the ground-state energy for increasing values of the total number N of fermions.

Notice that by inserting the Thomas-Fermi profile (7) into Eq. (9) one gets the ground-state energy of N fermions in a harmonic potential with frequency ω in the form

$$\frac{E}{\hbar\omega} = \sqrt{\xi} \left(\frac{(3N)^{4/3}}{4} + \frac{9\lambda}{\xi} \frac{(3N)^{2/3}}{8} \right). \quad (12)$$

We will refer to this expression as the ‘‘beyond-TF’’ energy. The first term is the TF contribution to the ground-state energy, while the second term is the leading correction. Chang and Bertsch [26] and Blume, von Stecher, and Greene [27] have determined ξ by fitting their MC data with Eq. (12) under the hypothesis that the relation

$$\lambda = \frac{\xi}{9} \quad (13)$$

appropriate to a noninteracting system holds also in the unitary regime. They find respectively the values $\xi=0.50$ [26] and $\xi=0.465$ [27], which are compatible with previous determinations of the parameter ξ based on Monte Carlo calculations for the uniform system [9,10]. The corresponding value $\lambda=\xi/9 \approx 0.05$ for the coefficient of the gradient is instead much smaller than previous suggestions [12,13,17,18,25].

It is important to stress that the formula in Eq. (12) does not give the minimum of the ETF functional (9), since it corresponds to the density profile of Eq. (7) and not to the true ground-state density solution of Eq. (11).

In the upper panel of Fig. 1 we plot ETF density profiles (solid lines) and compare them with the TF ones (dashed lines). The ETF density profiles have been determined by solving Eq. (11) with $\xi=0.44$ and $\lambda=1/4$ with a finite-difference numerical code [36]. As expected, there are visible differences, in particular near the surface. In the lower panel

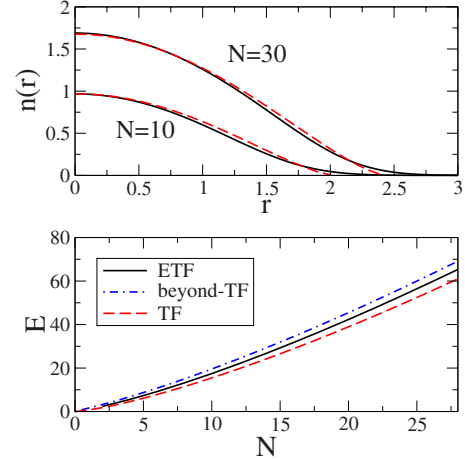


FIG. 1. (Color online) Unitary Fermi gas under harmonic confinement of frequency ω . Upper panel: Density profiles $n(r)$ for $N=10$ and $N=30$ fermions obtained with ETF (solid lines) and TF (dashed lines). Lower panel: Ground-state energy E vs N with ETF (solid line), beyond-TF formula (dotted-dashed line), and TF (dashed line). In all calculations: universal parameter $\xi=0.44$ and gradient coefficient $\lambda=1/4$. Energy in units of $\hbar\omega$ and lengths in units of $a_H = \sqrt{\hbar/(m\omega)}$.

of Fig. 1 we plot the ground-state energy E for increasing values of the number N of fermions. Here the differences between TF (dashed line), beyond-TF (dotted-dashed line), and ETF (solid line) are quite large. The figure clearly shows that the beyond-TF formula (12) is not very accurate.

We stress here once again that the values of the parameters ξ and λ in the ETF functional should be universal, i.e., independent on the confining potential $U(\mathbf{r})$ [24,28]. Moreover, we consider λ as taking into account phenomenologically all possible corrections of a gradient expansion in the unitary regime and treat ξ and λ as independent parameters. To determine them, instead of using the inaccurate Eq. (12), we look for the values of the two parameters which lead to the best fit of the FNDMC ground-state energies [27] for even N . After a systematic analysis we find $\xi=0.455$ and $\lambda=0.13$ as the best parameters in the unitary regime. It is important to observe that the value $\xi=0.455$ of our best fit coincides with that obtained by Perali, Pieri, and Strinati [38] by using the extended BCS theory with beyond-mean-field pairing fluctuations.

In Fig. 2 we plot the ground-state energy E of the Fermi gas under harmonic confinement, comparing different results: the FNDMC data for an even number N of atoms of [27] (diamonds with error bar), the best ETF results, with $\lambda=0.13$ and $\xi=0.455$ (solid line), and the ETF results obtained by using the values $\xi=0.475$ and $\lambda=0.25$ coming from the ϵ expansion [18] (dotted-dashed line).

We remark that fixing ξ to the value $\xi=0.44$ and looking for the best fitting λ we have found $\lambda=0.18$. In this case the curve of the energy will be practically superimposed to the solid one of Fig. 2.

For the sake of completeness in Table I we report the fixed node DMC energies of Blume, von Stecher, and C. H. Greene [27], our optimized ETF results with $\xi=0.575$ and $\lambda=0.13$, and also the SDFT calculations of Bulgac [37]. Re-

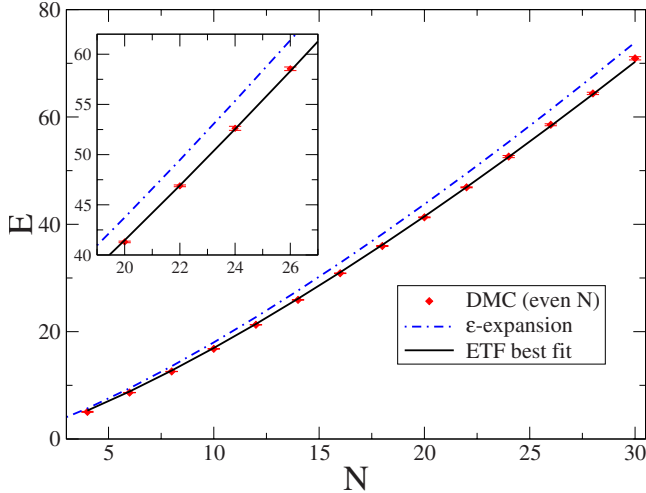


FIG. 2. (Color online) Ground-state energy E for the unitary Fermi gas of N atoms under harmonic confinement of frequency ω . Symbols: DMC data with even N [27]; solid line: ETF results with best fit ($\xi=0.455$ and $\lambda=0.13$); dotted-dashed line: ETF results obtained from ε -expansion [18] ($\xi=0.475$ and $\lambda=0.25$). Energy in units of $\hbar\omega$.

markably the ETF energies are slightly closer to the DMC values than the SDFT ones, reported in Ref. [37]. The optimized ETF energies for even number N of particles are obtained from our density functional (9), while the energies with odd number N of particles are calculated taking into account the odd-even splitting, as discussed in Sec. III.

III. ODD-EVEN SPLITTING

Up to now we have analyzed the unitary gas with an even number N of particles. The Monte Carlo calculations [26,27] show a clear odd-even effect, reminiscent of the behavior of the nuclear binding energy. In particular, denoting by E_N the ground state energy of N particles in a isotropic harmonic trap, for odd N one finds

$$E_N = \frac{1}{2}(E_{N-1} + E_{N+1}) + \Delta_N, \quad (14)$$

where the splitting Δ_N is always positive. This effect is related to pairing: given the superfluid cloud of even particles, the extra particle is localized where the energy gap is smallest, which is near the edge of the cloud [29,37]. On this basis, recently Son [29] has suggested that, for fermions at unitarity, confined by a harmonic potential with frequency ω , the odd-even splitting grows as

$$\Delta E_N = \gamma N^{1/9} \hbar\omega, \quad (15)$$

where γ is an unknown dimensionless constant. After a systematic investigation we find that $\gamma=0.856$ gives the odd-even splitting which best fit entire FNDMC data, with both even and odd particles [27]. In Fig. 3 we report the FNDMC data (diamonds) and the optimized ETF results (solid line). The figure, which displays the zigzag behavior of the energy E as a function of N , shows that the optimized ETF functional plus the odd-even correction (15) ($\xi=0.455$, $\lambda=0.13$,

TABLE I. Ground-state energy E of the unitary Fermi gas of N even atoms under harmonic confinement, in units of the harmonic energy $\hbar\omega$. Comparison among different calculations: fixed node diffusion Monte Carlo [27] (E_{DMC}), our optimized extended Thomas-Fermi with $\xi=0.455$ and $\lambda=0.13$ (E_{ETF}), and the superfluid density functional theory [37] (E_{SDFT}).

N	E_{DMC}	E_{ETF}	E_{SDFT}
2	2.002	2.17	2.33
3	4.281	4.65	4.62
4	5.051	5.19	5.52
5	7.61	7.98	7.98
6	8.64	8.71	9.07
7	11.36	11.73	11.83
8	12.58	12.61	12.94
9	15.69	15.81	16.06
10	16.80	16.83	17.15
11	20.11	20.19	20.36
12	21.28	21.32	21.63
13	24.79	24.82	24.96
14	25.92	26.04	26.32
15	29.59	29.67	29.78
16	30.88	30.99	31.21
17	34.64	34.73	34.81
18	35.96	36.13	36.27
19	39.83	39.99	40.02
20	41.30	41.46	41.51
21	45.47	45.41	45.42
22	46.89	46.96	46.92
23	51.01	51.01	
24	52.62	52.63	
25	56.85	56.76	
26	58.55	58.45	
27	63.24	62.66	
28	64.39	64.41	
29	69.13	68.70	
30	70.93	70.51	

$\gamma=0.856$) is extremely good in reproducing all FNDMC data.

IV. GENERALIZED HYDRODYNAMICS

Let us now analyze the effect of the gradient term (8) on the dynamics of the unitary Fermi gas. At zero temperature the low-energy collective dynamics of this fermionic gas can be described by the equations of generalized hydrodynamics [35,39,40], where the Hamiltonian of the classical hydrodynamics [40] is modified by including gradient corrections. In our case the generalized Hamiltonian reads

$$H = \int d^3\mathbf{r} n \left[\frac{1}{2} m v^2 + \varepsilon_g(n, \nabla n) + U(\mathbf{r}) \right], \quad (16)$$

where the local density $n(\mathbf{r}, t)$ and the local velocity $\mathbf{v}(\mathbf{r}, t)$ are the hydrodynamics variables [39,40]. By writing the

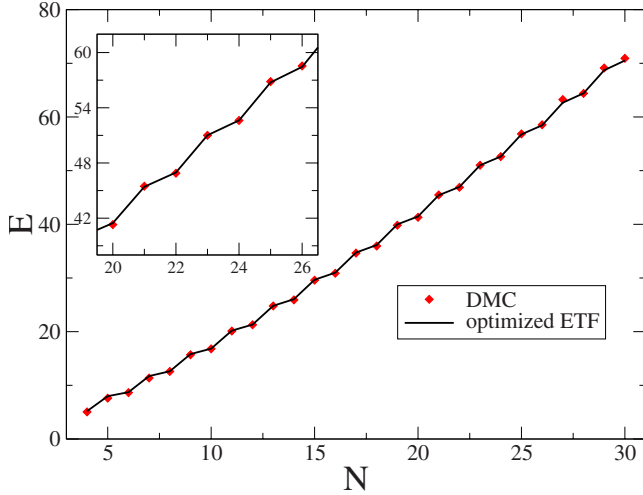


FIG. 3. (Color online) Ground-state energy E for the unitary Fermi gas of N atoms under harmonic confinement of frequency ω . Diamonds: DMC data with both even and odd N [27]; solid line: optimized ETF results ($\xi=0.455$, $\lambda=0.13$, $\gamma=0.856$). Energy in units of $\hbar\omega$.

Poisson brackets [40] of the hydrodynamics variables with the Hamiltonian (16), one gets the generalized hydrodynamics equations

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0, \quad (17)$$

$$m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \mathbf{v} + \nabla [\mu_g(n, \nabla n) + U(\mathbf{r})] = 0, \quad (18)$$

where

$$\mu_g(n, \nabla n) = \frac{\delta [n \varepsilon_g(n, \nabla n)]}{\delta n} = \mu(n) - \lambda \frac{\hbar^2 \nabla^2 \sqrt{n}}{2m \sqrt{n}}. \quad (19)$$

Equation (17) is the continuity equation, while Eq. (18) is the conservation of linear momentum. These equations are valid for the inviscid unitary Fermi gas at zero temperature. If the unitary Fermi gas is superfluid then it is not only inviscid but it is also irrotational, i.e.,

$$\nabla \times \mathbf{v} = 0. \quad (20)$$

By using this condition and the identity

$$(\mathbf{v} \cdot \nabla) \mathbf{v} = \nabla \left(\frac{1}{2} v^2 \right) - \mathbf{v} \times (\nabla \times \mathbf{v}), \quad (21)$$

Eq. (18) can be simplified into

$$m \frac{\partial \mathbf{v}}{\partial t} + \nabla \left[\frac{1}{2} m v^2 + \mu_g(n, \nabla n) + U(\mathbf{r}) \right] = 0. \quad (22)$$

The low-energy collective dynamics of the superfluid Fermi gas in the BCS-BEC crossover is usually described by the equations of classical superfluid hydrodynamics, which are the time-dependent version of the local density approximation with the Thomas-Fermi energy functional [7]. Equations (17) and (22) are a simple generalization of classical superfluid hydrodynamics which takes into account surface ef-

fects. The gradient term, i.e., the quantum correction, is necessary in a superfluid to avoid unphysical phenomena like the formation of wave front singularities in the dynamics of dispersive shock waves [41].

Combining Eqs. (17) and (22) one finds the dispersion relation of low-energy collective modes of the uniform unitary Fermi gas in the form

$$\frac{\Omega}{q} = \sqrt{\xi} c_0 \sqrt{1 + \frac{\lambda}{\xi} \left(\frac{\hbar q}{2mc_0} \right)^2}, \quad (23)$$

where Ω is the collective frequency, q is the wave number, and c_0 is the speed of sound in a uniform, noninteracting Fermi gas.

For an irrotational fluid it is possible to write down [40,42] a Lagrangian by using as dynamical variables the scalar potential $\theta(\mathbf{r}, t)$ of the velocity $\mathbf{v}(\mathbf{r}, t)$ and the local density $n(\mathbf{r}, t)$. For a fermionic superfluid one has

$$\mathbf{v}(\mathbf{r}, t) = \frac{\hbar}{2m} \nabla \theta(\mathbf{r}, t), \quad (24)$$

where $\theta(\mathbf{r}, t)$ is the phase of the condensate wave function of Cooper pairs [7]. In our case, the familiar Lagrangian of the Fermi superfluid [16,42] must be modified by including the gradient correction. The generalized Lagrangian density then reads

$$\mathcal{L} = -n \left(\frac{\hbar}{2} \dot{\theta} + \frac{\hbar^2}{8m} (\nabla \theta)^2 + U(\mathbf{r}) + \varepsilon_g(n, \nabla n) \right). \quad (25)$$

The Euler-Lagrange equations of this Lagrangian with respect of n and θ give the generalized hydrodynamics equations of superfluids (17) and (22).

We observe that the generalized hydrodynamics equations (17) and (22) can be formally written in terms of a nonlinear Schrödinger equation of the Guerra-Pusterla type [30], which is Galilei invariant [31]. In fact, by introducing the complex wave function

$$\Psi(\mathbf{r}, t) = \sqrt{n(\mathbf{r}, t)} e^{i\theta(\mathbf{r}, t)}, \quad (26)$$

which is the zero-temperature Ginzburg-Landau order parameter normalized to the total number N of superfluid atoms [17,25], and taking into account the correct phase-velocity relationship given by Eq. (24), the equation

$$i\hbar \frac{\partial}{\partial t} \Psi = \left[-\frac{\hbar^2}{4m} \nabla^2 + 2U(\mathbf{r}) + 2\mu(|\Psi|^2) + (1 - 4\lambda) \frac{\hbar^2 \nabla^2 |\Psi|}{4m |\Psi|} \right] \Psi \quad (27)$$

is strictly equivalent to Eqs. (17) and (22). Notice that in the stationary case where $\Psi(\mathbf{r}, t) = \sqrt{n(\mathbf{r})} e^{-i2\bar{\mu}t/\hbar}$, Eq. (27) becomes exactly Eq. (11). Remarkably, only if $\lambda=1/4$ the equation acquires the familiar structure of a nonlinear Schrödinger equation such as the Gross-Pitaevskii equation which describes the two-spin component Fermi system, but in the extreme BEC regime [43]. From the linearization of Eq. (27) one finds for the uniform Fermi gas the Bogoliubov excitations given precisely by Eq. (23).

Finally, we stress that Eq. (27) can be seen as the Euler-Lagrange equation of the following Galilei-invariant Lagrangian density:

$$\mathcal{L} = \Psi^* \left(i \frac{\hbar}{2} \frac{\partial}{\partial t} + \frac{\hbar^2}{8m} \nabla^2 - U(\mathbf{r}) \right) \Psi - \varepsilon_g (|\Psi|^2, \nabla(|\Psi|^2)) |\Psi|^2 + \frac{\hbar^2}{8m} (\nabla|\Psi|)^2, \quad (28)$$

that is equivalent to the generalized Lagrangian of Eq. (25).

V. CONCLUSIONS

We have obtained the value of the coefficient λ of the gradient correction $\lambda \hbar^2 (\nabla n)^2 / (8mn)$ for the extended Thomas-Fermi density functional in the unitary regime. By fitting diffusion Monte Carlo data with an even number N of particles we have found $\lambda = 0.13$. In addition, we have determined the coefficient ξ of the energy density $\xi(3/5)n\varepsilon_F$, finding $\xi = 0.455$. Fixing ξ to the value $\xi = 0.44$ proposed in [10] and looking for the best fitting λ we have found instead $\lambda = 0.18$. We stress that in our energy functional the gradient term takes into account phenomenologically all corrections of a gradient expansion. With our functional one can easily get the ground state properties (energy and density) for large as for small numbers of fermions; its main limitation is that

it cannot account for the shell effects in the density profile. Moreover, we have shown that it is possible to take into account the odd-even splitting of the ground-state energy of the unitary gas in a harmonic trap of frequency ω by considering a correction proportional to $N^{1/9} \hbar \omega$ as suggested by Son [29], where the constant of proportionality is found to be $\gamma = 0.856$. Finally, we have analyzed the effect of the gradient term in the dynamics of the unitary Fermi gas by introducing generalized hydrodynamics equations, which can be written for superfluid motion in the form of a Galilei-invariant nonlinear Schrödinger equation. As a final remark, we remind that the values of ξ and λ we have found are independent on the external potential and therefore our generalized energy functional can be used to investigate the unitary superfluid Fermi gas in various trapping configurations. Obviously in the limit of large numbers of particles the gradient term and the exact value of λ are less important since the dominant term becomes the usual Thomas-Fermi one. More extensive Monte Carlo calculations with a larger number of particles will be certainly useful to have a more accurate determination of the value of ξ .

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