Generalized superfluid hydrodynamics for the unitary Fermi gas

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Summary

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Unitary Fermi gas

Let us consider a gas of fermions with two spin components ($\sigma = \uparrow, \downarrow$).

The system is <u>dilute</u> if the effective radius r_0 of the inter-atomic potential is much smaller than the average interparticle separation $d = n^{-1/3}$, namely

$$n \, r_0^3 \ll 1 \,, \tag{1}$$

where $n = n_\uparrow + n_\downarrow$ is the total number density of the Fermi gas.

The <u>unitarity regime</u> of this dilute Fermi gas is the situation in which the s-wave scattering length a of the inter-atomic potential greatly exceeds the average interparticle separation $d = n^{-1/3}$, thus

$$n \, |a|^3 \gg 1 \,. \tag{2}$$

In few words, the unitarity regime of a dilute Fermi gas is characterized by

$$r_0 \ll n^{-1/3} \ll |a| \,. \tag{3}$$

The many-body Hamiltonian of a two-component Fermi system is given by

$$\hat{H} = \sum_{i=1}^{N_\uparrow} \left(\frac{\hat{p}_i^2}{2m} + U(\mathbf{r}_i) \right) + \sum_{j=1}^{N_\downarrow} \left(\frac{\hat{p}_j^2}{2m} + U(\mathbf{r}_j) \right) + \sum_{i,j} V(\mathbf{r}_i - \mathbf{r}_j), \qquad (4)$$

where $U(\mathbf{r})$ is the external confining potential and $V(\mathbf{r})$ is the inter-atomic potential. Here we consider $N_\uparrow = N_\downarrow$.

The inter-atomic potential of a dilute Fermi gas can be modelled by an attractive square well potential:

$$V(r) = \begin{cases} -V_0 & r < r_0 \\ 0 & r > r_0 \end{cases} \qquad (5)$$

By varying the depth V_0 of the potential one can change the value of the s-wave scattering length a, which for this potential is given by

$$a = r_0 \left(1 - \frac{tan(r_0\sqrt{mV_0}/\hbar)}{r_0\sqrt{mV_0}/\hbar} \right). \qquad (6)$$

For $r_0\sqrt{mV_0}/\hbar < \pi/2$ the potential does not support bound state and $a < 0$. For $r_0\sqrt{mV_0}/\hbar > \pi/2$ appears a bound state of binding energy ϵ_B and $a > 0$. At $r_0\sqrt{mV_0}/\hbar = \pi/2$ one has $\epsilon_B = 0$ and $a = \pm\infty$.

The unitarity limit corresponds to

$$a = \pm\infty . \tag{7}$$

Under this condition the Fermi gas is called unitary Fermi gas.

The crossover from a BCS superfluid ($a < 0$) to a BEC of molecular pairs ($a > 0$) has been investigated experimentally*, and it has been shown that the unitary Fermi gas ($|a| = \infty$) exists and is (meta)stable.

The detection of quantized vortices under rotation† has clarified that the unitary Fermi gas is superfluid.

The only length characterizing the uniform unitary Fermi gas is the average distance between particles $d = n^{-1/3}$. In this case the energy per particle must be

$$\varepsilon(n;\xi) = \xi\frac{3}{5}\frac{\hbar^2}{2m}(3\pi^2)^{2/3}n^{2/3} = \xi\,\frac{3}{5}\,\epsilon_F , \tag{8}$$

with ϵ_F Fermi energy of the ideal gas and ξ a universal unknown parameter (Monte Carlo calculations suggest $\xi \simeq 0.4$).

*K.M. O'Hara *et al.*, Science **298**, 2179 (2002).

†M.W. Zwierlein *et al.*, Science **311**, 492 (2006); M.W. Zwierlein *et al.*, Nature (London) **442**, 54 (2006)

Extended Thomas-Fermi density functional

The Thomas-Fermi (TF) energy functional* of the unitary Fermi gas trapped by an external potential $U(\mathbf{r})$ is

$$E = \int d^3\mathbf{r} \; n(\mathbf{r}) \left[\xi \frac{3}{5} \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n(\mathbf{r})^{2/3} + U(\mathbf{r}) \right] \; . \tag{9}$$

with $n(\mathbf{r})$ the local density. The total number of fermions is

$$N = \int d^3\mathbf{r} \; n(\mathbf{r}) \; . \tag{10}$$

By minimizing E_{TF} one finds

$$\xi \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n(\mathbf{r})^{2/3} + U(\mathbf{r}) = \bar{\mu} \; , \tag{11}$$

with $\bar{\mu}$ chemical potential of the non-uniform system. In this way

$$n(\mathbf{r}) = \frac{(2m)^{3/2}}{3\pi^2 (\xi \hbar^2)^{3/2}} (\bar{\mu} - U(\mathbf{r}))^{3/2} \; . \tag{12}$$

*S. Giorgini, L.P. Pitaevskii, and S. Stringari, Rev. Mov. Phys. **80**, 1215 (2008).

The TF functional <u>must</u> be extended to cure the pathological TF behavior at the surface.

We add to the energy per particle the term

$$\lambda \frac{\hbar^2}{8m} \frac{(\nabla n)^2}{n^2} = \lambda \frac{\hbar^2}{2m} \frac{(\nabla \sqrt{n})^2}{n} \; . \tag{13}$$

Historically, this term was introduced by von Weizsäcker[†] to treat surface effects in nuclei. Here we consider λ as a <u>phenomenological parameter</u> accounting for the increase of kinetic energy due the spatial variation of the density.

There are also multi-orbital density functionals for unitary Fermi gas:
– the Kohn-Sham density functional of Papenbrock,
Phys. Rev. A **72**, 041603 (2005);
– the Bogoliubov-de Gennes superfluid local-density approximation (SLDA) of Bulgac, Phys. Rev. A **76**, 040502(R) (2007).

[†]C.F. von Weizsäcker, Z. Phys. **96**, 431 (1935).

The new energy functional, that is the extended Thomas-Fermi (ETF) functional of the unitary Fermi gas, reads

$$E = \int d^3\mathbf{r}\ n(\mathbf{r}) \left[\lambda \frac{\hbar^2}{8m} \frac{(\nabla n(\mathbf{r}))^2}{n(\mathbf{r})^2} + \xi \frac{3}{5} \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n(\mathbf{r})^{2/3} + U(\mathbf{r}) \right] \ . \quad (14)$$

By minimizing the ETF energy functional one gets:

$$\left[-\lambda \frac{\hbar^2}{2m} \nabla^2 + \xi \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n(\mathbf{r})^{2/3} + U(\mathbf{r}) \right] \sqrt{n(\mathbf{r})} = \bar{\mu} \sqrt{n(\mathbf{r})} . \quad (15)$$

This is a sort of stationary 3D nonlinear Schrödinger equation (NLSE).

To determine ξ and λ we look for the values of the two parameters which lead to the best fit of the ground-state energies obtained with the fixed-node diffusion Monte Carlo (FNDMC) method[‡] in a harmonic trap $U(\mathbf{r}) = m\omega^2 r^2 / 2$. After a systematic analysis [L.S. and F. Toigo, Phys. Rev. A **78**, 053626 (2008)] we find

$$\xi = 0.455 \quad \text{and} \quad \lambda = 0.13$$

as the best fitting parameters in the unitary regime. See the next figure.

[‡]J von Stecher, C.H. Greene and D. Blume, Phys. Rev. A **77** 043619 (2008)
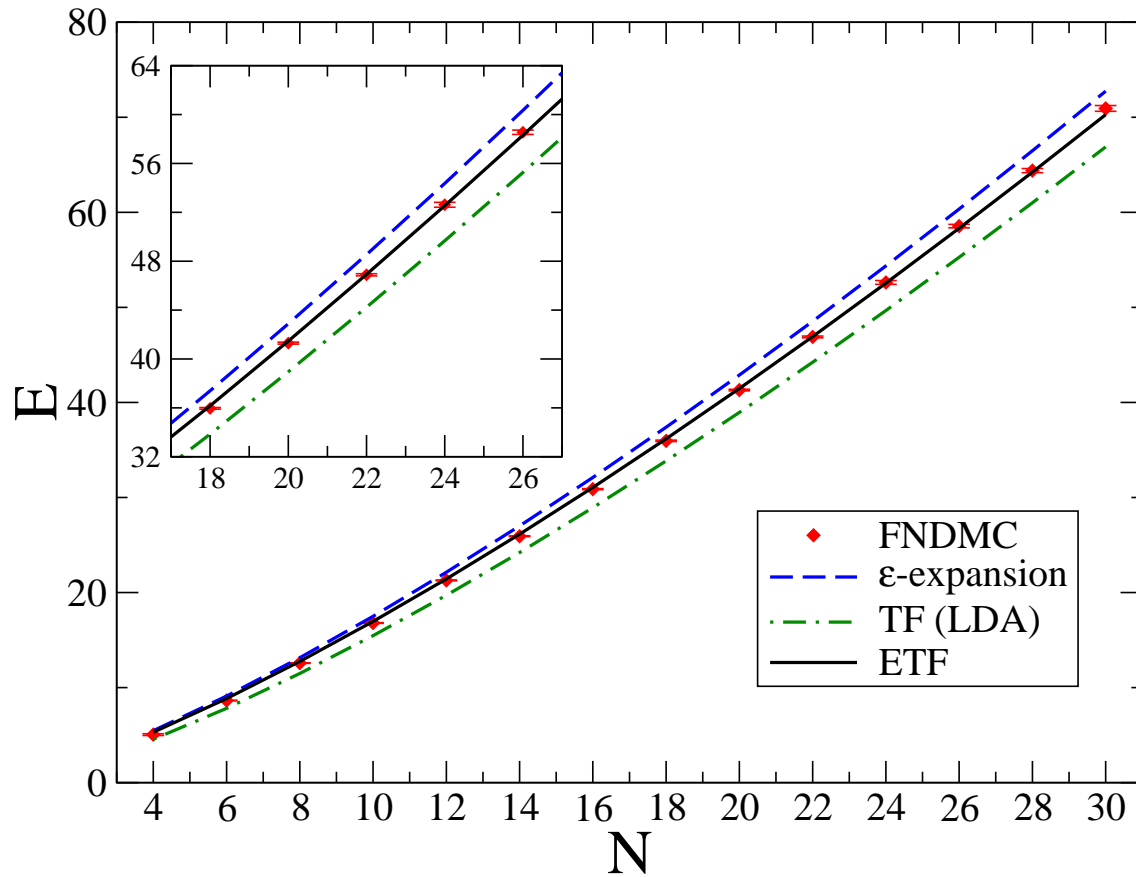
Ground-state energy E for the unitary Fermi gas of N atoms under harmonic confinement of frequency ω. Energy in units of $\hbar\omega$. [Adapted from L.S. and F. Toigo, Phys. Rev. A **78**, 053626 (2008)]

Having determined the parameters ξ and λ we can now use our single-orbital density functional to calculate various properties of the trappeed unitary Fermi gas.

We calculate numerically (by solving with a finite-difference Crank-Nicolson method the stationary 3D NLSE) the density profile $n(\mathbf{r})$ of the gas in a isotropic harmonic trap

$$U(\mathbf{r}) = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2) \,. \tag{16}$$

We compare our results with those obtained by Doerte Blume[§] with her FNDMC code. For completeness we consider also the density profiles obtained by Aurel Bulgac[¶] using his multi-orbital density functional (SLDA).

[§]D. Blume, J. von Stecher, C.H. Greene, Phys. Rev. Lett. **99**, 233201 (2007); J. von Stecher, C.H. Greene and D. Blume, Phys. Rev. A **77** 043619 (2008); D. Blume, unpublished.

[¶]A. Bulgac, Phys. Rev. A **76**, 040502(R) (2007).
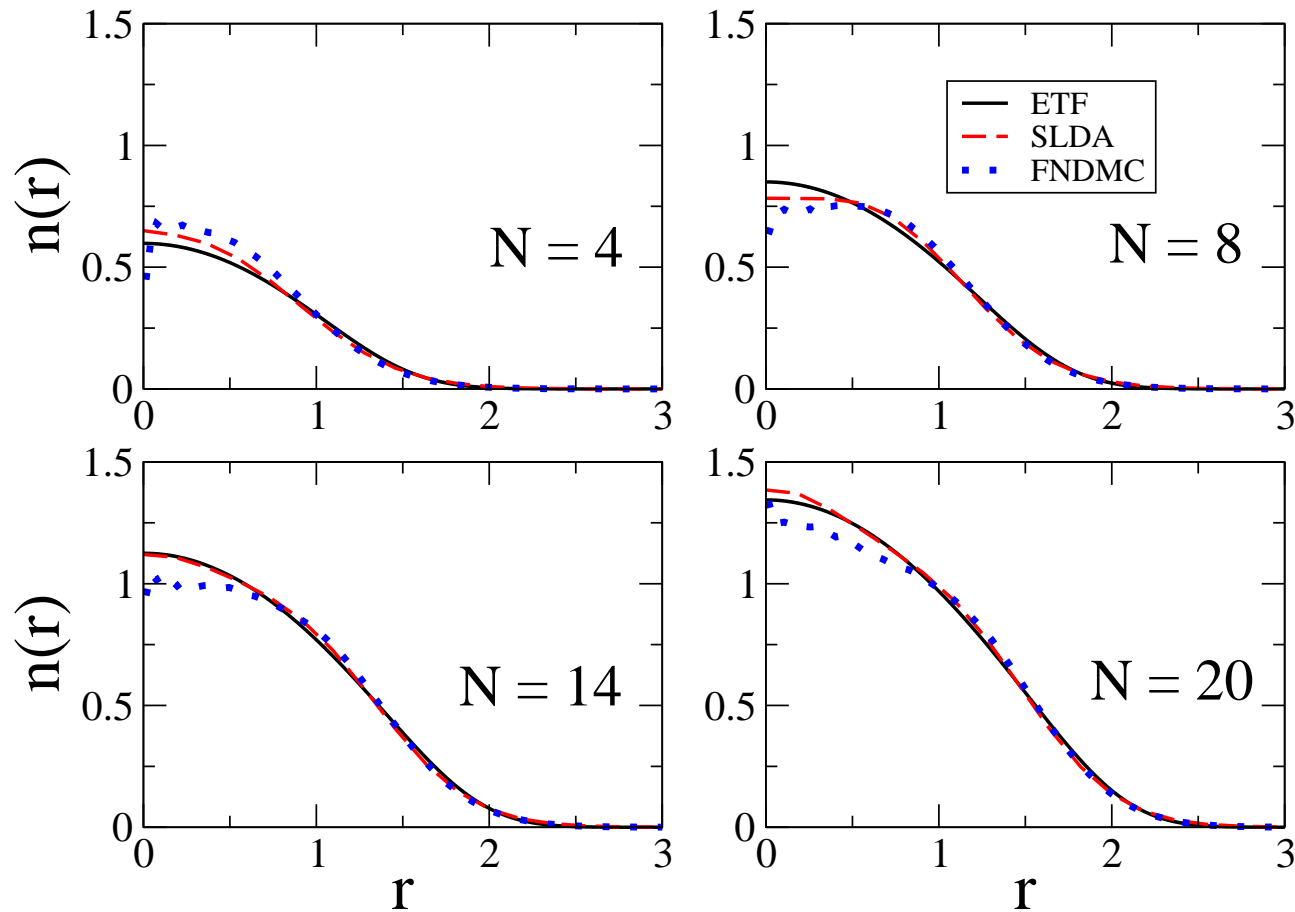
Unitary Fermi gas under harmonic confinement of frequency ω. Density profiles $n(r)$ for N (even) fermions obtained with our ETF (solid lines), Bulgac's SLDA (dashed lines) and FNDMC (circles). Lengths in units of $a_H = \sqrt{\hbar/(m\omega)}$. [L.S., F. Ancilotto and F. Toigo, to be published in Laser Phys. Lett.]
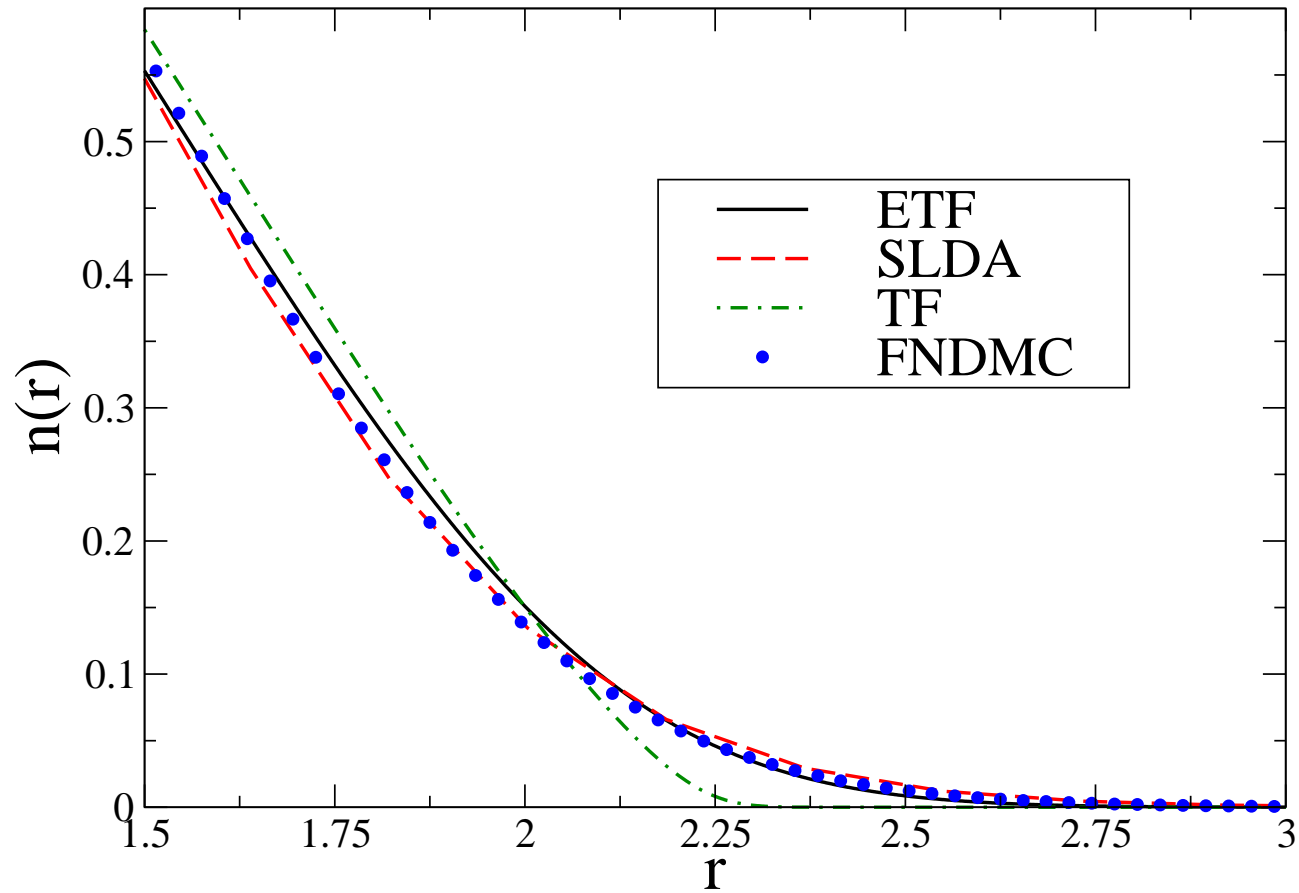
Zoom of the density profile $n(r)$ for $N = 20$ fermions near the surface obtained with our ETF (solid lines), Bulgac's SLDA (circles) and FNDMC (circles). Lengths in units of $a_H = \sqrt{\hbar/(m\omega)}$. [L.S., F. Ancilotto and F. Toigo, to be published in Laser Phys. Lett.]

Extended superfluid hydrodynamics

Let us now analyze the effect of the gradient term on the dynamics of the superfluid unitary Fermi gas.

At zero temperature the low-energy collective dynamics of this fermionic gas can be described by the equations of extended* irrotational and inviscid hydrodynamics:

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

$$m\frac{\partial}{\partial t}\mathbf{v} + \nabla[-\lambda\frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{n}}{\sqrt{n}} + \mu(n;\xi) + U(\mathbf{r}) + \frac{m}{2}v^2] = 0 , \tag{18}$$

where $\mu(n;\xi) = \xi\epsilon_F$ is the bulk chemical potential, with $\epsilon_F = \hbar^2(3\pi^2 n)^{1/3}/(2m)$ the Fermi energy.

They are the simplest extension of the equations of superfluid hydrodynamics of fermions[†], where $\lambda = 0$.

*Quantum hydrodynamics of electrons: N. H. March and M. P. Tosi, Proc. R. Soc. A **330**, 373 (1972); E. Zaremba and H.C. Tso, PRB **49**, 8147 (1994).

[†]S. Giorgini, L.P. Pitaevskii, and S. Stringari, Rev. Mov. Phys. **80**, 1215 (2008).

The extended hydrodynamics equations can be written in terms of a time-dependent NLSE, which is Galilei-invariant.[‡]

In fact, by introducing the complex wave function

$$\psi(\mathbf{r},t) = \sqrt{n(\mathbf{r},t)}\ e^{i\theta(\mathbf{r},t)}\ , \tag{19}$$

which is normalized to the total number N of superfluid atoms, and taking into account the correct phase-velocity relationship

$$\mathbf{v}(\mathbf{r},t) = \frac{\hbar}{2m}\nabla\theta(\mathbf{r},t)\ , \tag{20}$$

where $\theta(\mathbf{r},t)$ is the phase of the condensate wavefunction of Cooper pairs, the equation

$$i\hbar\frac{\partial}{\partial t}\psi = [-\frac{\hbar^2}{4m}\nabla^2 + 2U(\mathbf{r}) + 2\mu(|\psi|^2;\xi) + (1-4\lambda)\frac{\hbar^2}{4m}\frac{\nabla^2|\psi|}{|\psi|}]\psi\ , \tag{21}$$

is strictly equivalent to the equations of extended hydrodynamics.

[‡]F. Guerra and M. Pusterla, Lett. Nuovo Cim. **34**, 351 (1982); H.-D. Doebner and G.A. Goldin, Phys. Rev. A **54**, 3764 (1996).

The extended hydrodynamics equations are the Euler-Lagrange equation of the following Lagrangian density

$$\mathcal{L} = -n\left(\dot{\theta} + \frac{\hbar^2}{8m}(\nabla\theta)^2 + U(\mathbf{r}) + \varepsilon(n;\xi) + \lambda\frac{\hbar^2}{8m}\frac{(\nabla n)^2}{n^2}\right) , \qquad (22)$$

which depends on the total number density $n(\mathbf{r},t)$ and the phase $\theta(\mathbf{r},t)$ [L.S. and F. Toigo, Phys. Rev. A **78**, 053626 (2008)].

In the case $\lambda = 0$ it is called the Popov Lagrangian of superfluid hydrodynamics [V.N. Popov, *Functional Integrals in Quantum Field Theory and Statistical Physics* (Reidel, Dordrecht, 1983)].

Setting, as previously,

$$\psi(\mathbf{r},t) = \sqrt{n(\mathbf{r},t)} \ e^{i\theta(\mathbf{r},t)} , \qquad (23)$$

the extended Popov Lagrangian (22) is equivalent to the following one:

$$\mathcal{L} = \psi^*\left(i\frac{\hbar}{2}\frac{\partial}{\partial t} + \frac{\hbar^2}{8m}\nabla^2 - U(\mathbf{r}) - \varepsilon(|\psi|^2;\xi)\right)\psi + (1-4\lambda)\frac{\hbar^2}{8m}(\nabla|\psi|)^2 . \qquad (24)$$

Sound velocity and collective modes

From the equations of superfluid hydrodynamics one finds the dispersion relation of low-energy collective modes of the uniform ($U(\mathbf{r}) = 0$) unitary Fermi gas in the form

$$\frac{\Omega}{q} = \sqrt{\frac{\xi}{3}} v_F \, , \qquad (25)$$

where Ω is the collective frequency, q is the wave number and

$$v_F = \sqrt{\frac{2\epsilon_F}{m}} \qquad (26)$$

is the Fermi velocity of a noninteracting Fermi gas.

The equations of extended superfluid hydrodynamics (or the superfluid NLSE) give [L.S. and F. Toigo, Phys. Rev. A **78**, 053626 (2008)] also a correcting term, i.e.

$$\frac{\Omega}{q} = \sqrt{\frac{\xi}{3}} v_F \sqrt{1 + \frac{3\lambda}{\xi} (\frac{\hbar q}{2 m v_F})^2} \, , \qquad (27)$$

which depends on the ratio λ/ξ.

In the case of harmonic confinement

$$U(\mathbf{r}) = \frac{1}{2}m\omega^2 r^2 \tag{28}$$

we study numerically the collective modes of the unitary Fermi gas by increasing the number N of atoms.

By solving the superfluid NLSE we find that the frequency Ω_0 of the monopole mode ($l = 0$) and the frequency Ω_1 dipole mode ($l = 1$) do not depend on N:

$$\Omega_0 = 2\omega \qquad \text{and} \qquad \Omega_1 = \omega , \tag{29}$$

as predicted by Y. Castin [Comptes Rendus Physique **5**, 407 (2004)].

We find instead that the frequencies Ω_2 and Ω_3 of quadrupole ($l = 2$) and octupole ($l = 3$) modes depend on N and on the choice of the gradient coefficient λ.
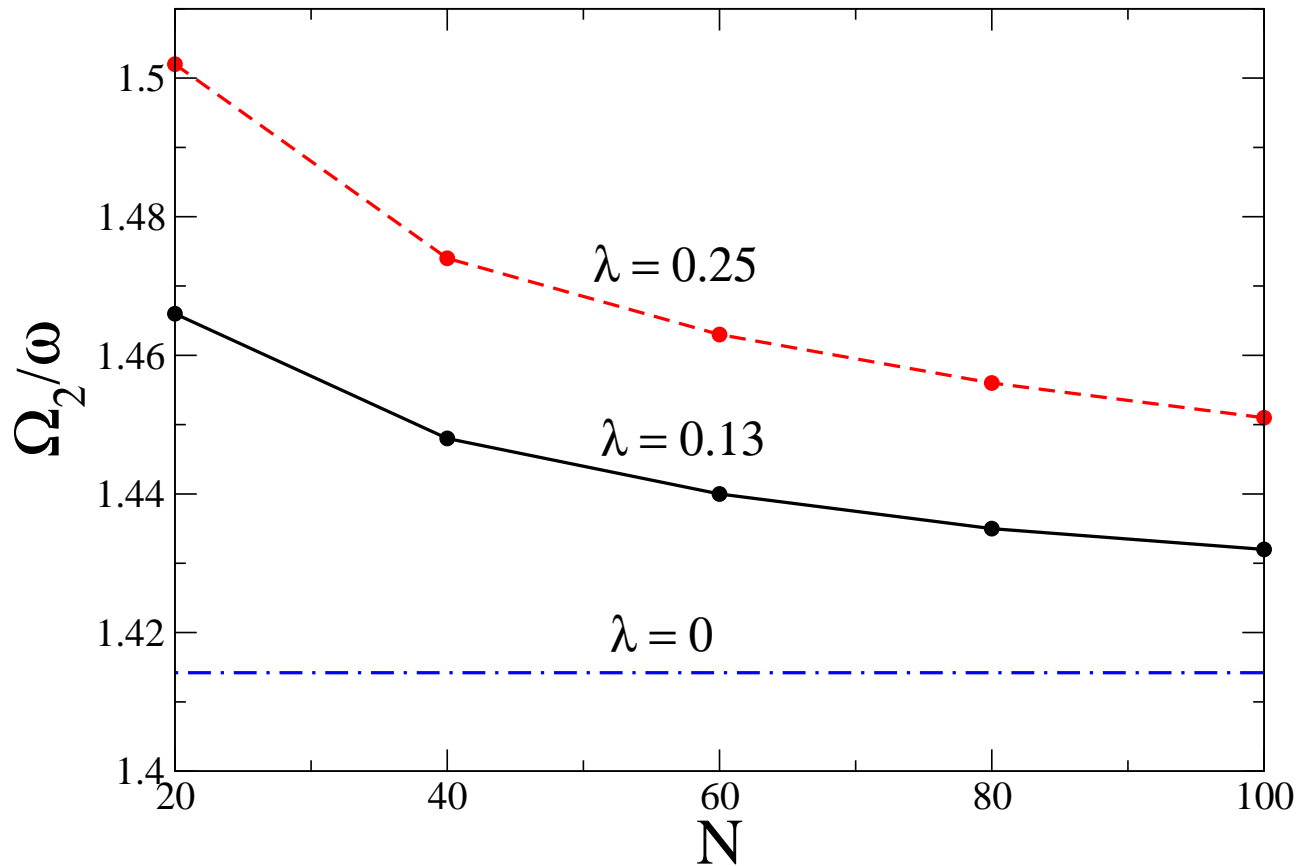
Quadrupole frequency Ω_2 of the unitary Fermi gas ($\xi = 0.455$) with N atoms under harmonic confinement of frequency ω. Three different values of the gradient coefficient λ. For $\lambda = 0$ (TF limit): $\Omega_2 = \sqrt{2}\omega$. [L.S., F. Ancilotto and F. Toigo, to be published in Laser Phys. Lett.]
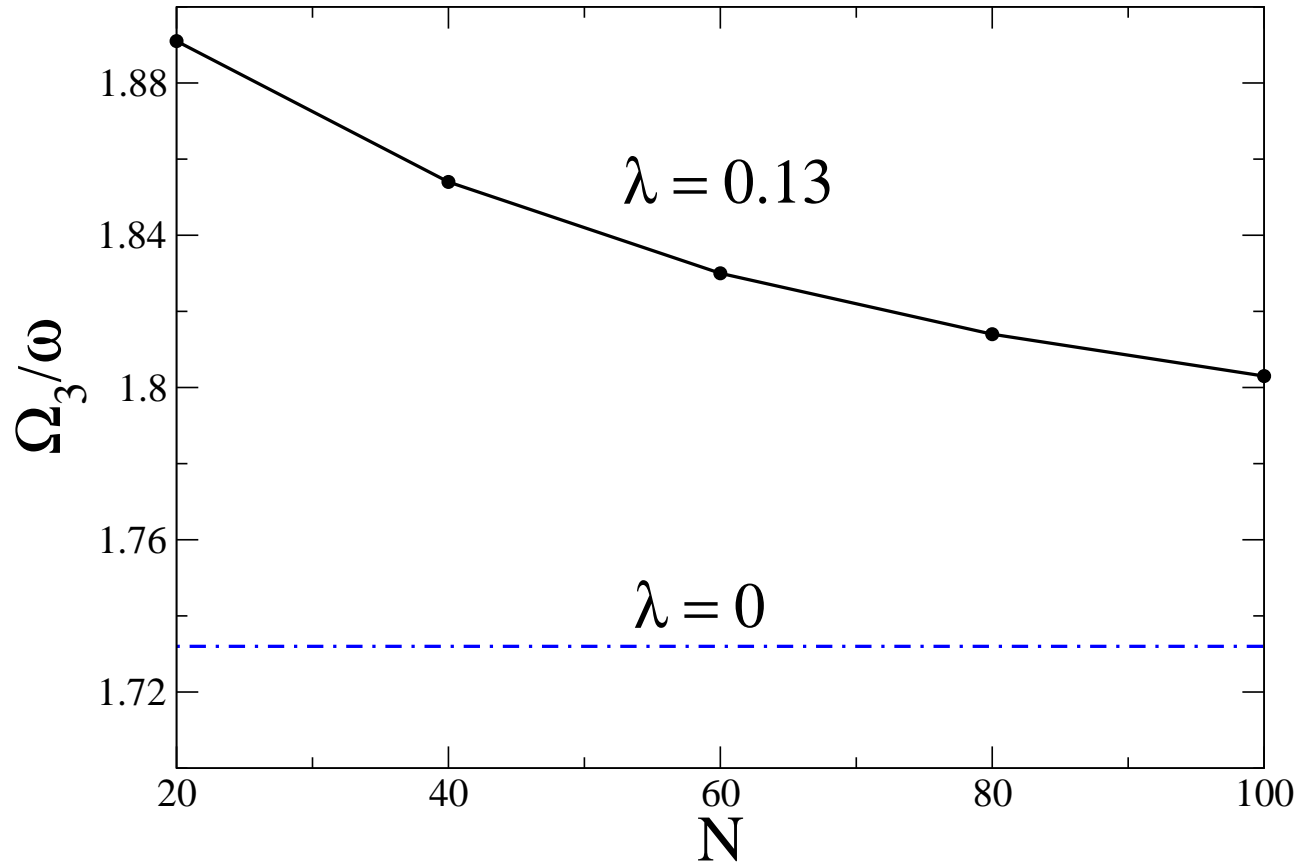
Octupole frequency Ω_3 of the unitary Fermi gas ($\xi = 0.455$) with N atoms under harmonic confinement of frequency ω. Two different values of the gradient coefficient λ. For $\lambda = 0$ (TF limit): $\Omega_3 = \sqrt{3}\omega$. [L.S., F. Ancilotto and F. Toigo, to be published in Laser Phys. Lett.]

Conclusions

- We have introduced an extended Thomas-Fermi (ETF) functional for the trapped unitary Fermi gas.

- ETF functional be used to study ground-state density profiles in a generic external potential $U(\mathbf{r})$.

- We have also introduced a time-dependent version of the ETF functional: the extended superfluid hydrodynamics.

- Extended superfluid hydrodynamics can be applied to investigate collective modes of the unitary gas in a generic external potential $U(\mathbf{r})$.

- Our extended hydrodynamics has been recently used to study the transition from multi vortices to a giant vortex in quadratic-quartic potential by Alberto Cetoli and Emil Lundh [Phys. Rev. A **80**, 023610 (2009)].