The unitary Fermi gas at zero and finite temperature

Luca Salasnich

CNR-INFM and CNISM, Department of Physics, University of Padua, Italy

Collaboration with:
Francesco Ancilotto and Flavio Toigo

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Summary

- Unitary Fermi gas
- Extended Thomas-Fermi density functional
- Extended superfluid hydrodynamics
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- Low-temperature thermodynamics
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Unitary Fermi gas

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

The system is dilute 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 unitarity regime 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 $a = \pm\infty$.

For a dilute gas 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 practically 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. Mod. Phys. **80**, 1215 (2008).

The TF functional must 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 phenomenological parameter 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

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

By minimizing the ETF energy functional one gets:

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

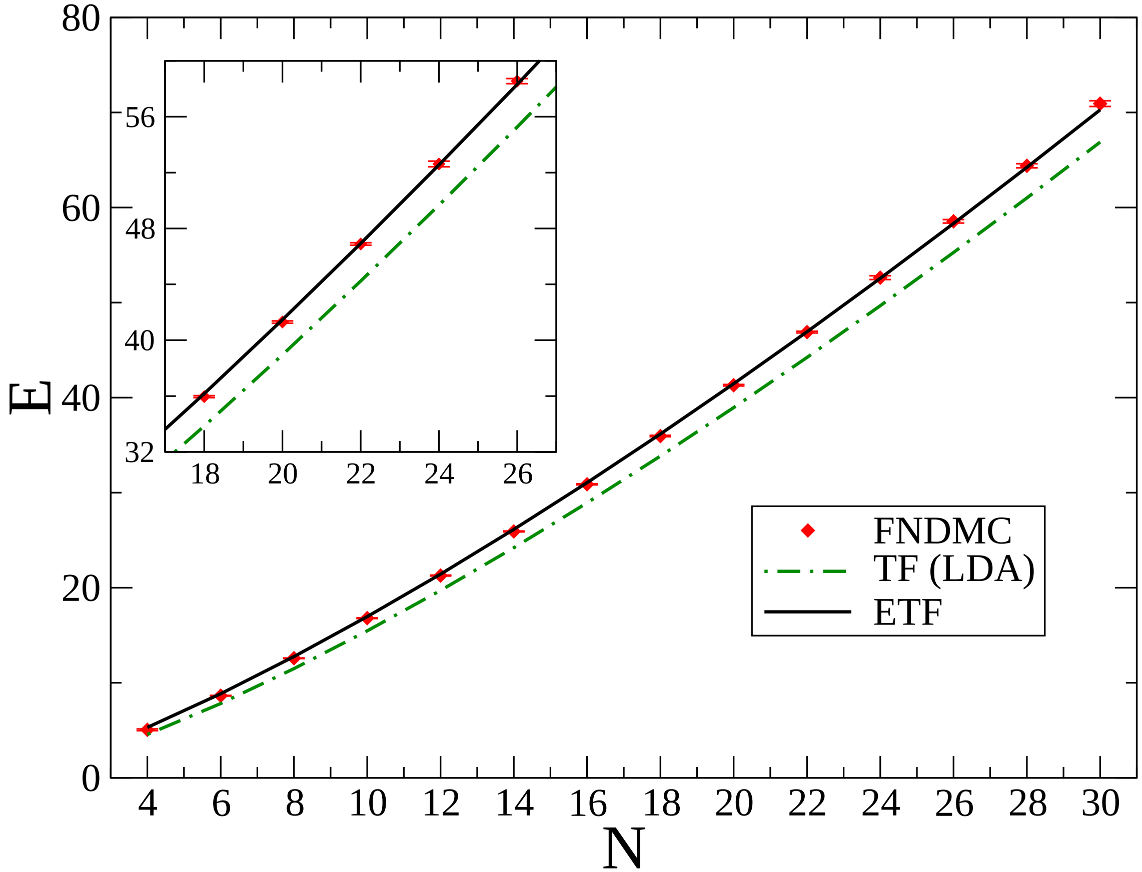
This is a sort of stationary 3D nonlinear Schrödinger equation (NLSE).

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

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

as the best fitting parameters in the unitary regime (A. Perali, P. Pieri, and G.C. Strinati, PRL **93**, 100404 (2004) got the same ξ). 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 trapped unitary Fermi gas.

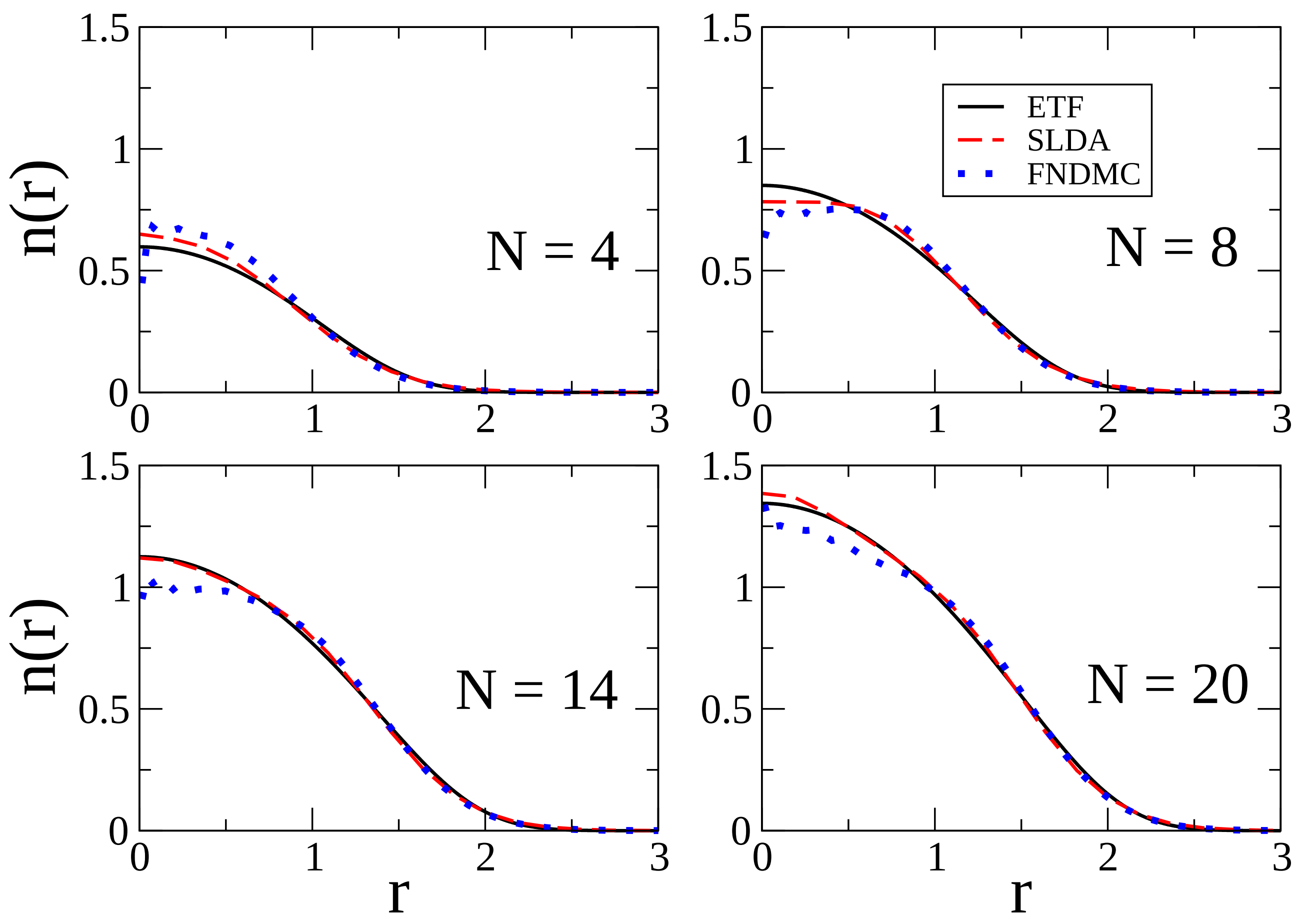
We calculate numerically (by solving with a finite-difference Crank-Nicolson method the stationary 3D NLSE) the density profile $n(\mathbf{r})$ of the gas in a isotropic harmonic trap

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

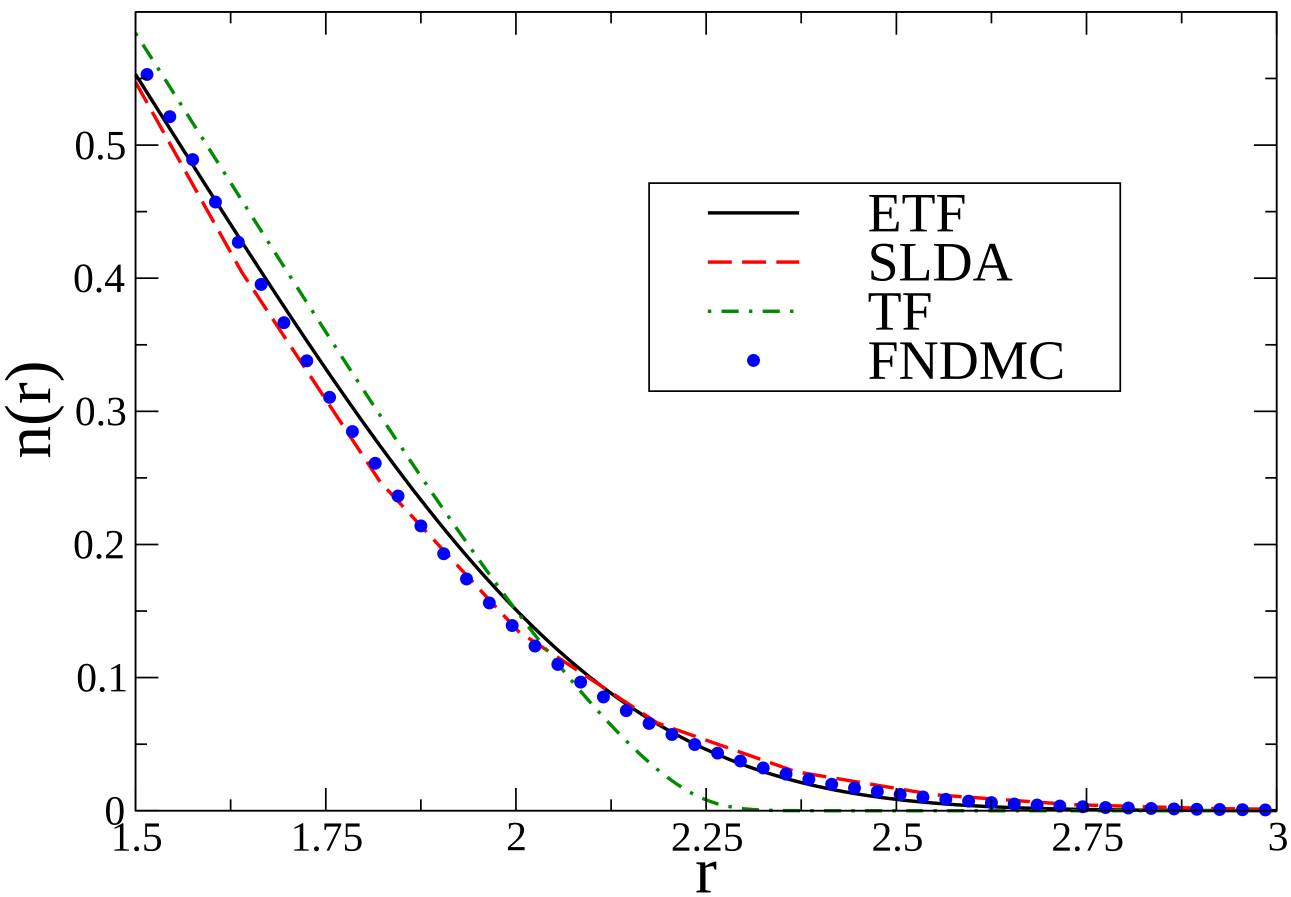
We compare our results with those obtained by Doerte Blume* with her FNDMC code. For completeness we consider also the density profiles obtained by Aurel Bulgac† using his multi-orbital density functional (SLDA).

*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, Laser Phys. Lett. **7**, 78 (2010).]



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, Laser Phys. Lett. **7**, 78 (2010).]

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:

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

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

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

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

$$\Omega = c_1 \; q \; , \tag{22}$$

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

$$c_1 = \sqrt{\frac{\xi}{3}} v_F \tag{23}$$

is the first sound velocity, with $v_F = \sqrt{\frac{2\epsilon_F}{m}}$ 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.

$$\Omega = c_1 \; q \; \sqrt{1 + \frac{3\lambda}{\xi} (\frac{\hbar q}{2 m v_F})^2} \; , \tag{24}$$

which depends on the ratio λ/ξ.

In the case of harmonic confinement

$$U(\mathbf{r}) = \frac{1}{2} m\omega^2 r^2 \tag{25}$$

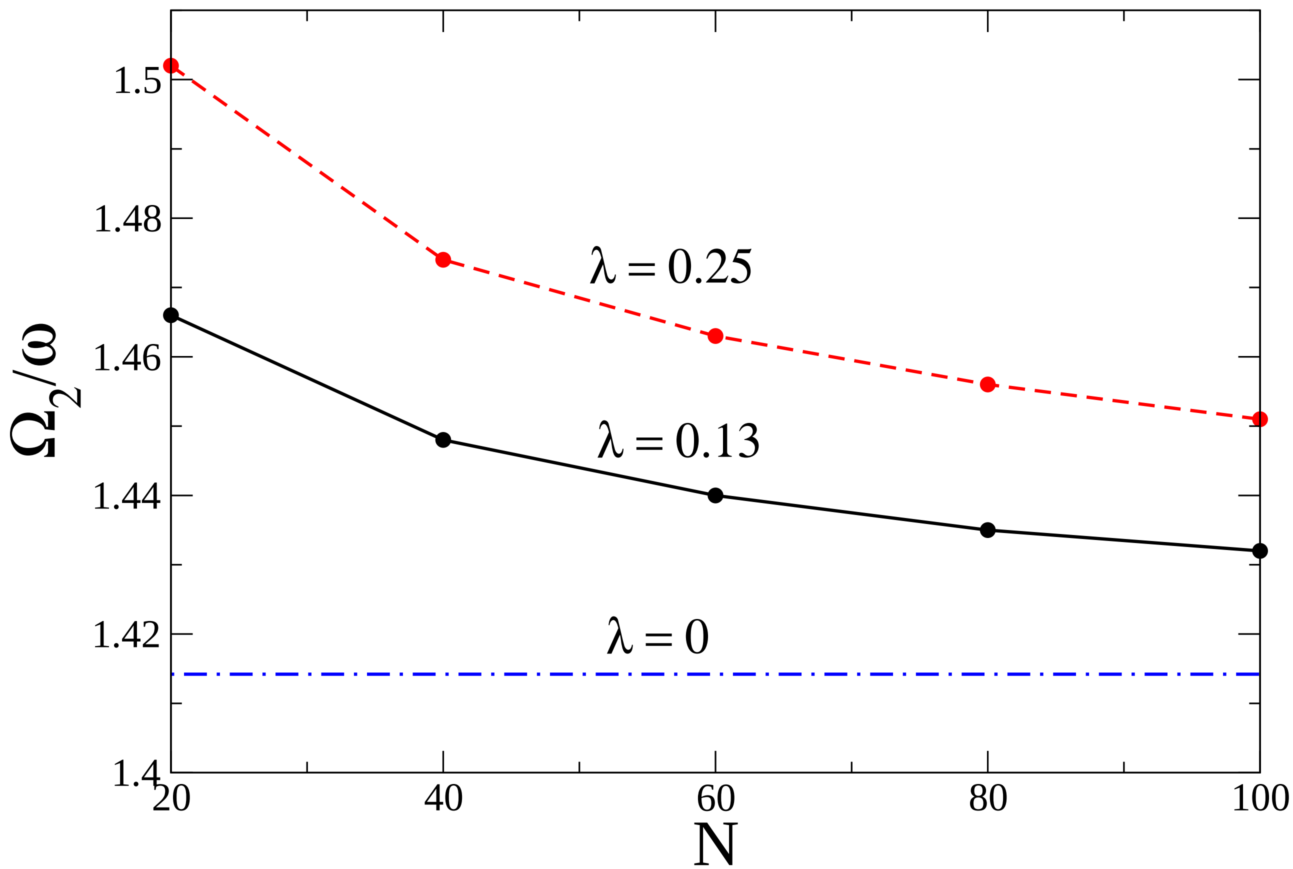
we study numerically the collective modes of the unitary Fermi gas by increasing the number N of atoms.

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:

$$\Omega_0 = 2\omega \qquad \text{and} \qquad \Omega_1 = \omega \; , \tag{26}$$

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

We find instead that the frequency Ω_2 of the quadrupole ($l=2$) mode depends 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, Laser Phys. Lett. **7**, 78 (2010).]

Low-temperature thermodynamics

We model the many-body quantum Hamiltonian $\hat{H}$ of the uniform unitary Fermi gas with the simple effective Hamiltonian

$$\hat{H}_{eff} = E_0 + \sum_{\mathbf{q}} \epsilon_{col}(q)\ \hat{b}^{+}_{\mathbf{q}} \hat{b}_{\mathbf{q}} + 2 \sum_{\mathbf{p}} \epsilon_{sp}(p)\ \hat{c}^{+}_{\mathbf{p}} \hat{c}_{\mathbf{p}}\ , \tag{27}$$

where

$$E_0 = \frac{3}{5} \xi N \epsilon_F \tag{28}$$

is the ground-state energy,

$$\epsilon_{col}(q) = \sqrt{c_1^2 q^2 + \frac{\lambda}{4m^2} q^4} \simeq c_1 q + \frac{\lambda}{8m^2 c_1} q^3 \tag{29}$$

is the energy of the bosonic collective excitations, and

$$\epsilon_{sp}(p) = \sqrt{(\frac{p^2}{2m} - \zeta \epsilon_F)^2 + \Delta_0^2} \simeq \Delta_0 + \frac{1}{2m_0}(p - p_0)^2 \tag{30}$$

is the energy of the fermionic single-particle excitations, with $m_0 = \frac{m\Delta_0}{2\zeta\epsilon_F}$ and $p_0 = \sqrt{2m\mu} = \zeta^{1/2} p_F$.

The Helmholtz free energy F of a thermodynamic system with Hamiltonian $\hat{H}_{eff}$ is given by

$$F = -k_B T \ln \left\{ Tr[e^{-\hat{H}_{eff}/k_B T}] \right\} \ . \tag{31}$$

For the uniform unitary Fermi gas in a volume V we find

$$F = F_0 + F_{col} + F_{sp} \tag{32}$$

where

$$\frac{F_0}{V} = \frac{3}{5} \xi n \epsilon_F \tag{33}$$

is the free energy of the ground-state,

$$\frac{F_{col}}{V} = -\frac{\pi^2}{90} \frac{(k_B T)^4}{(\hbar c_1)^3} + \frac{\lambda \pi^4}{756} \frac{(k_B T)^6}{(\hbar c_1)^3 (m c_1^2)^2} \tag{34}$$

is the free energy of the bosonic collective excitations, and

$$\frac{F_{sp}}{V} = -k_B T \frac{4 p_0^2 (m_0 k_B T)^{1/2}}{(2\pi)^{3/2} \hbar^3} e^{-\Delta_0/k_B T} \tag{35}$$

is the free energy of fermionic single-particle excitations.

In our low-temperature thermodynamics (LTT) the total Helmholtz free energy F of the low-temperature unitary Fermi gas can be then written as

$$F = N \ \epsilon_F \ \Phi\left(\frac{T}{T_F}\right) \ , \tag{36}$$

where N is the total number of atoms in the unitary gas and $\Phi(x)$ is a function of the scaled temperature $x = T/T_F$, with $T_F = \epsilon_F/k_B$, given by

$$\Phi(x) = \frac{3}{5}\xi - \frac{\pi^4\sqrt{3}}{80 \ \xi^{3/2}}x^4 + \frac{\lambda\pi^6 3\sqrt{3}}{896 \ \xi^{7/2}}x^6 - \frac{3\sqrt{2\pi}}{2}\zeta^{1/2}\gamma^{1/2}x^{3/2}e^{-\gamma/x} \ , \tag{37}$$

where $\gamma = \Delta_0/\epsilon_F$. From the Helmholtz free energy F we can easily obtain all the thermodynamic functions. For instance, the chemical potential

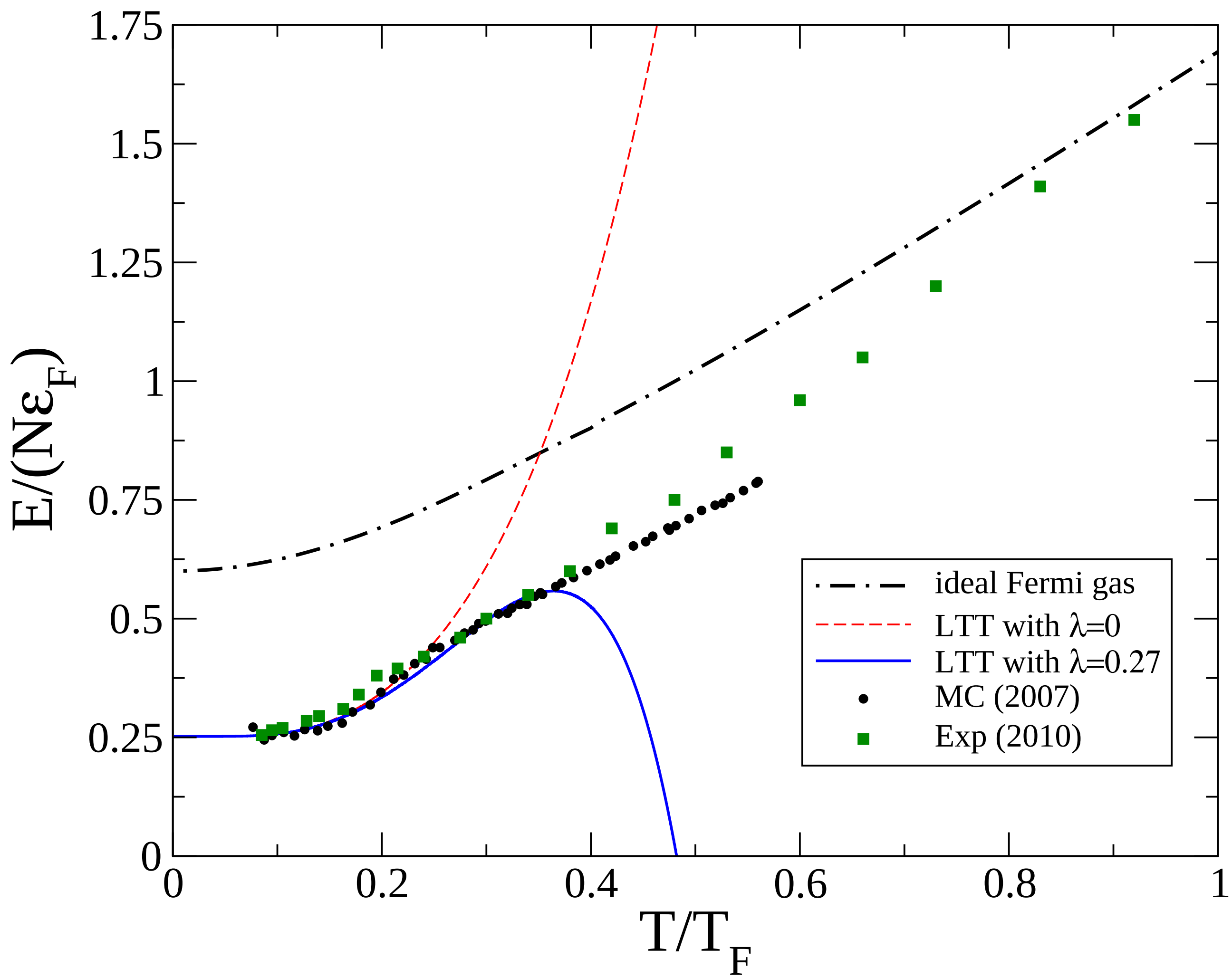
$$\mu = \left(\frac{\partial F}{\partial N}\right)_{T,V} \ , \tag{38}$$

the entropy

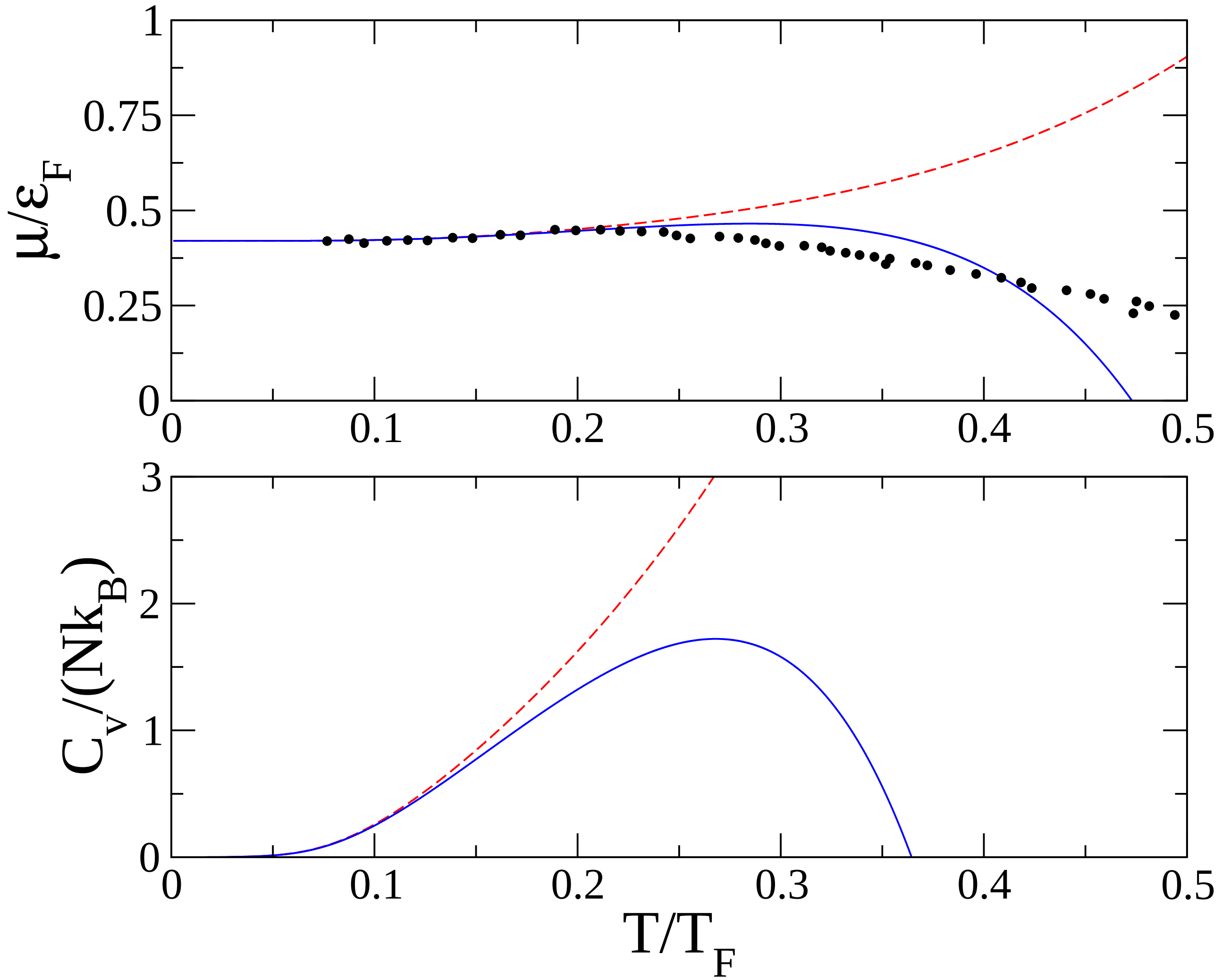
$$S = -\left(\frac{\partial F}{\partial T}\right)_{N,V} \ , \tag{39}$$

the internal energy

$$E = F + TS \ . \tag{40}$$



Internal energy E of the unitary Fermi gas as a function of the temperature T. Circles: Monte Carlo results of A. Bulgac, J.E. Drut, and P. Magierski, PRL **99**, 120401 (2007). Squares: Experimental data of M. Horikoshi, S. Nakajima, M. Ueda, and T. Mukaiyama, Science **327**, 442 (2010). [L.S. and F. Toigo, very preliminary results.]



Chemical potential E and heat capacity C_v of the unitary Fermi gas as a function of the temperature T. Dashad line: ST with $\lambda = 0$. Solid line: ST with $\lambda = 0.27$. Circles: Monte Carlo results of A. Bulgac, J.E. Drut, and P. Magierski, PRL **99**, 120401 (2007). [L.S. and F. Toigo, very preliminary results.]

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 $U(\mathbf{r})$.

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

- Low-temperature thermodynamics can be obtained by using the zero-temperature elementary excitations.