Surface effects in the Unitary Fermi Gas

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- Finding the universal parameters of the ETF functional
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Extended Thomas-Fermi density functional

The Thomas-Fermi (TF) energy functional* of a dilute and ultracold two-component Fermi gas trapped by an external potential $U(\mathbf{r})$ is

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

with $\varepsilon(n; a_F)$ energy per particle, $n(\mathbf{r})$ total density and a_F the s-wave scattering length. The total number of fermions is

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

By minimizing E_{TF} one finds

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

with $\mu(n; a_F) = \frac{\partial(n\varepsilon(n;a_F))}{\partial n}$ bulk chemical potential of a uniform system and $\bar{\mu}$ chemical potential of the non uniform system.

*S. Giorgini, L.P. Pitaevskii, and S. Stringari, RMP **80**, 1215 (2008).

For the uniform unitary Fermi gas[†] the s-wave scattering length a_F diverges:

$$a_F \to \pm\infty \ , \tag{4}$$

and the only length characterizing the uniform system is the average distance between particles $n^{-1/3}$. In this case:

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

with ϵ_F Fermi energy of the ideal gas and ξ a universal parameter.

The bulk chemical potential associated to Eq. (5) is

$$\mu(n;\xi) = \frac{\partial(n\varepsilon(n))}{\partial n} = \xi \frac{\hbar^2}{2m}(3\pi^2)^{2/3} n^{2/3} = \xi \ \epsilon_F \ . \tag{6}$$

[†] "The Many-Body X Challenge Problem", formulated by G.F. Bertsch, see R. A. Bishop, IJMP B **15**, iii (2001).

The TF functional must be extended to cure the pathological TF behavior at the surface.

We add to the energy per particle the term

$$\lambda \frac{\hbar^2}{8m} \frac{(\nabla n)^2}{n^2} = \lambda \frac{\hbar^2}{2m} \frac{(\nabla \sqrt{n})^2}{n} \ . \tag{7}$$

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.

Other recent density-functional methods for unitary Fermi gas:
– the Kohn-Sham density functional approach of Papenbrock,
PRA **72**, 041603 (2005);
– the superfluid local-density approximation of Bulgac,
PRA **76**, 040502(R) (2007).

[‡]C.F. von Weizsäcker, ZP **96**, 431 (1935).

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

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

By minimizing the ETF energy functional one gets:

$$\left[\lambda \frac{\hbar^2}{2m} \nabla^2 + \xi \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n(\mathbf{r})^{2/3} + U(\mathbf{r}) \right] \sqrt{n(\mathbf{r})} = \bar{\mu}\ \sqrt{n(\mathbf{r})}\ . \tag{9}$$

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

The constants ξ and λ should be universal i.e. independent on the confining potential $U(\mathbf{r})$.

In a recent paper [S.K. Adhikari and L.S., PRA **78**, 043616 (2008)] we have used this simple choice

$$\xi = 0.44 \qquad \text{and} \qquad \lambda = 1/4 \, , \tag{10}$$

for the unitary Fermi gas in a spherical harmonic potential

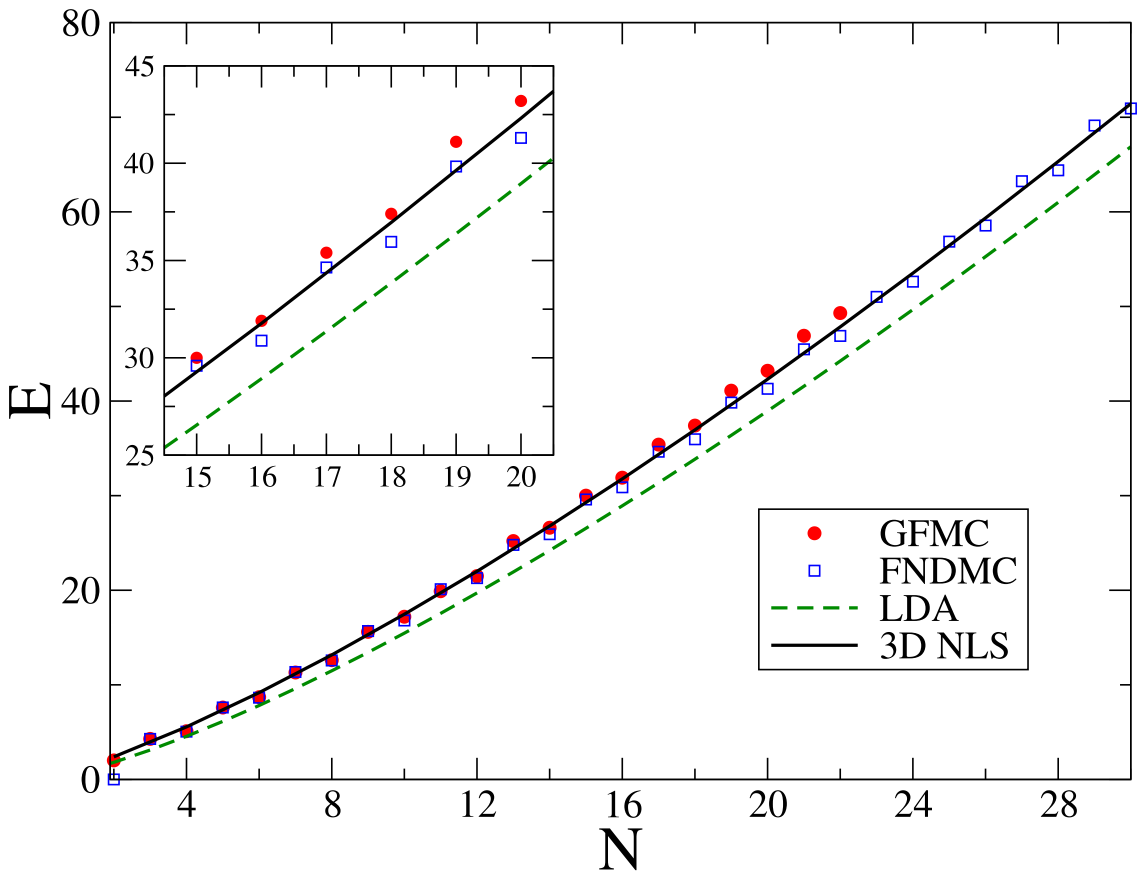
$$U(\mathbf{r}) = \frac{1}{2} m \omega^2 r^2 \, . \tag{11}$$

$\xi = 0.44$ is a MC prediction for uniform unitary Fermi gas [Carlson et al. PRL **91** 050401 (2003)].

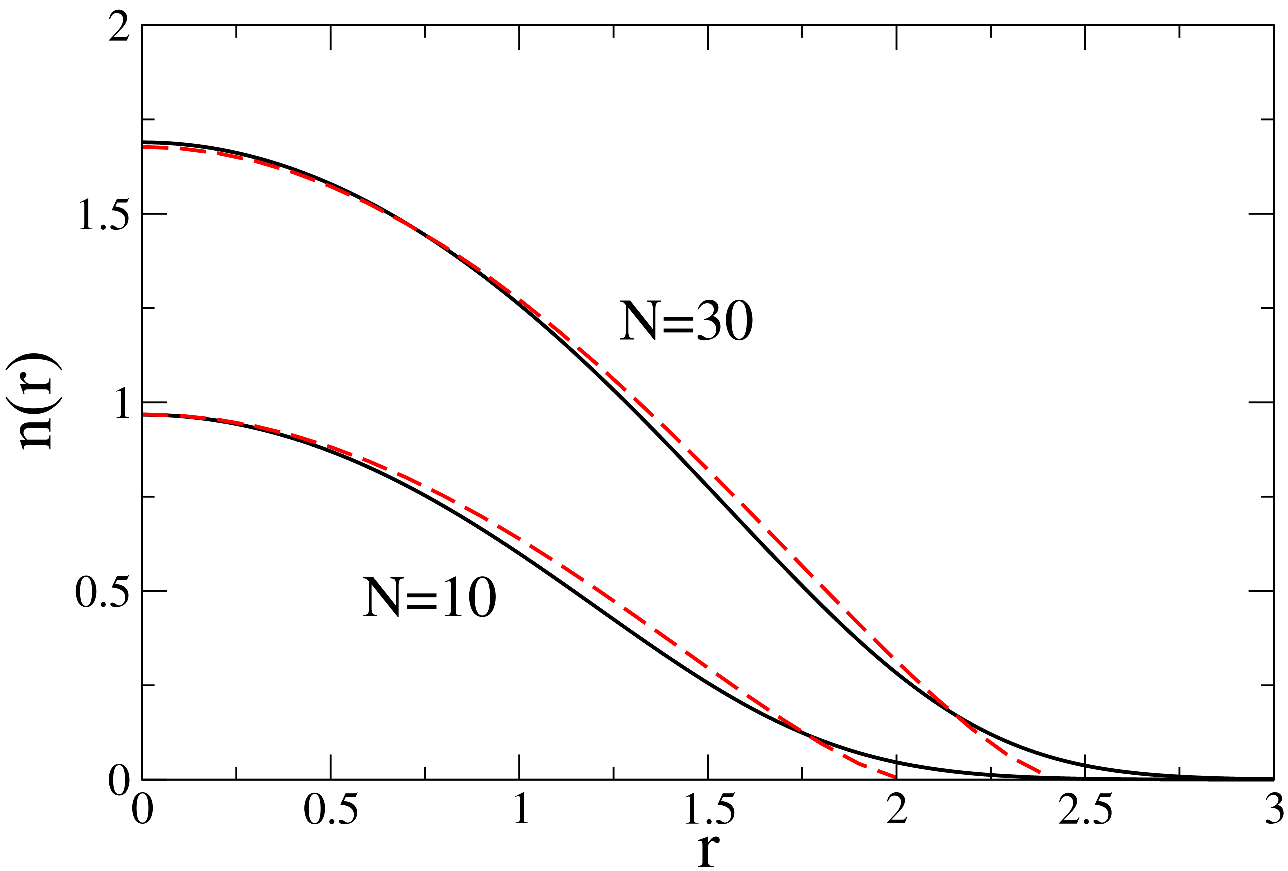
$\lambda \simeq 0.25$ is the prediction at unitarity of effective field theory [G. Rupak and T. Schäfer, NP A **816**, 52 (2009)].

We compare the results of our 3D NLS equation with recent Monte Carlo data[§]:
– Green-function Monte Carlo (GFMC) of Chang and Bertsch,
PRA **76** 021603(R) (2007);
– Fixed-node diffusion Monte Carlo (FNDMC) of Dörte Blume *et al.*
PRL **99**, 233201 (2007).

[§]They compare their MC data with an approximate N-expansion using $\lambda = \xi/9 \simeq 0.05$.



Ground-state energy E (in units of $\hbar\omega$) versus N. Solid line: ETF functional with $\xi = 0.44$ and $\lambda = 1/4$. Dashed line: local density approximation (LDA), i.e. the Thomas-Fermi model ($\lambda = 0$). The results of Green-function Monte Carlo (GFMC) and fixed-node diffusion Monte Carlo (FNDMC) are shown for a comparison (symbols). [S.K. Adhikari and L.S., NJP **11**, 023011 (2009)]



Unitary Fermi gas under harmonic confinement of frequency ω. Density profiles $n(r)$ for $N = 10$ and $N = 30$ fermions obtained with ETF (solid lines) and TF (dashed lines). In all calculations: universal parameter $\xi = 0.44$ and gradient coefficient $\lambda = 1/4$. Lengths in units of $a_H = \sqrt{\hbar/(m\omega)}$. [L.S. and F. Toigo, PRA **78**, 053626 (2008)]

Finding the universal parameters of the ETF functional

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 by Monte Carlo data.

We use the **more recent and reliable** Monte Carlo results with N even (complete superfluidity): the fixed-node diffusion Monte Carlo (FNDMC) of J von Stecher, C.H. Greene and D. Blume, PRA **77** 043619 (2008).

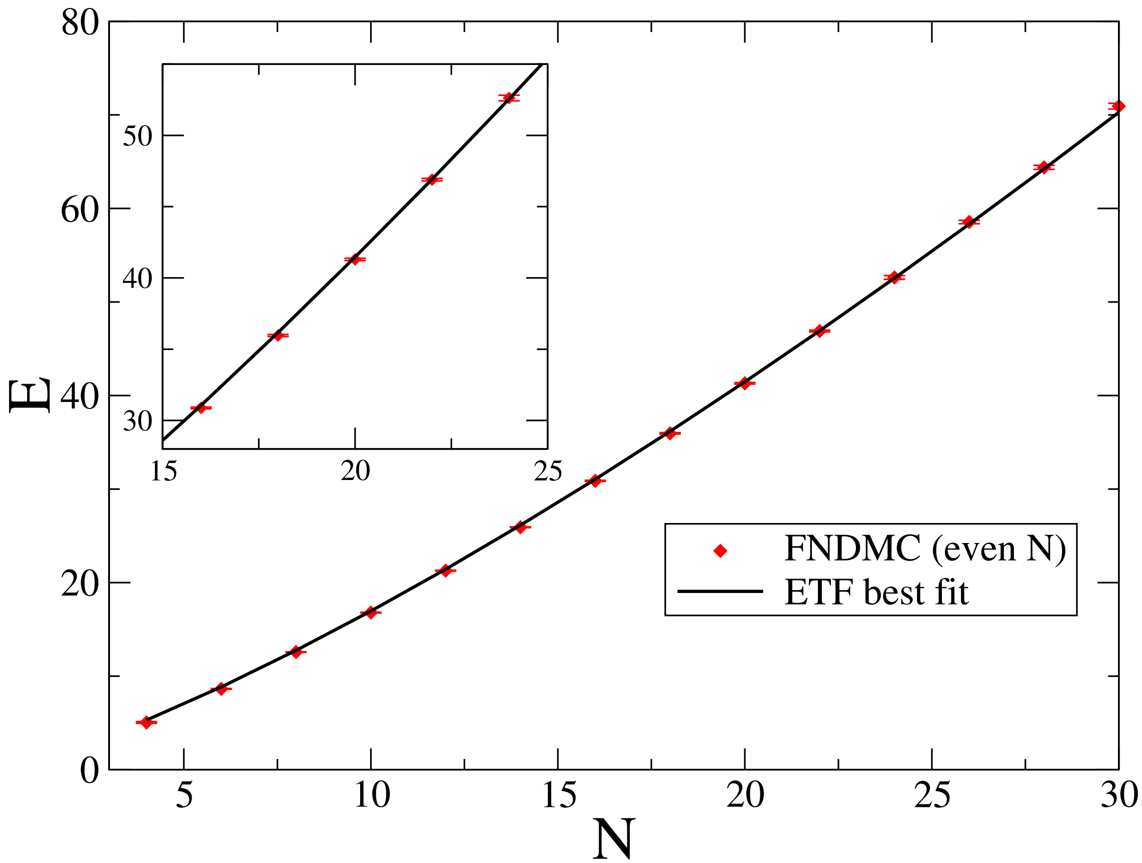
After a systematic analysis [L.S. and F. Toigo, PRA **78**, 053626 (2008)] we find

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

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

Fixing $\xi = 0.44$ we find instead $\lambda = 0.18$.

¶The value $\xi = 0.455$ coincides with that obtained by A. Perali, P. Pieri, and G.C. Strinati, PRL **93**, 100404 (2004) with beyond-mean-field extended BCS theory.



Ground-state energy E for the unitary Fermi gas of N atoms under harmonic confinement of frequency ω. Symbols: FNDMC data with even N; solid line: ETF results with best fit ($\xi = 0.455$ and $\lambda = 0.13$). Energy in units of $\hbar\omega$. [L.S. and F. Toigo, PRA **78**, 053626 (2008)]

Odd-even splitting

In our determination of ξ and λ we have analyzed the unitary gas with an even number N of particles.

Monte Carlo calculations show a clear odd-even effect (zig-zag effect): the ground state energy of N odd particles in the isotropic harmonic trap is

$$E_N = \frac{1}{2}(E_{N-1} + E_{N+1}) + \Delta_N \; , \tag{12}$$

where the splitting Δ_N is always positive.

Dam Thanh Son has suggested[‖] that, 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.

[‖] D.T. Son, e-preprint arXiv:0707.1851.

Dam Thanh Son has also found that, for fermions at unitarity, confined by a harmonic potential with frequency ω, the odd-even splitting grows as

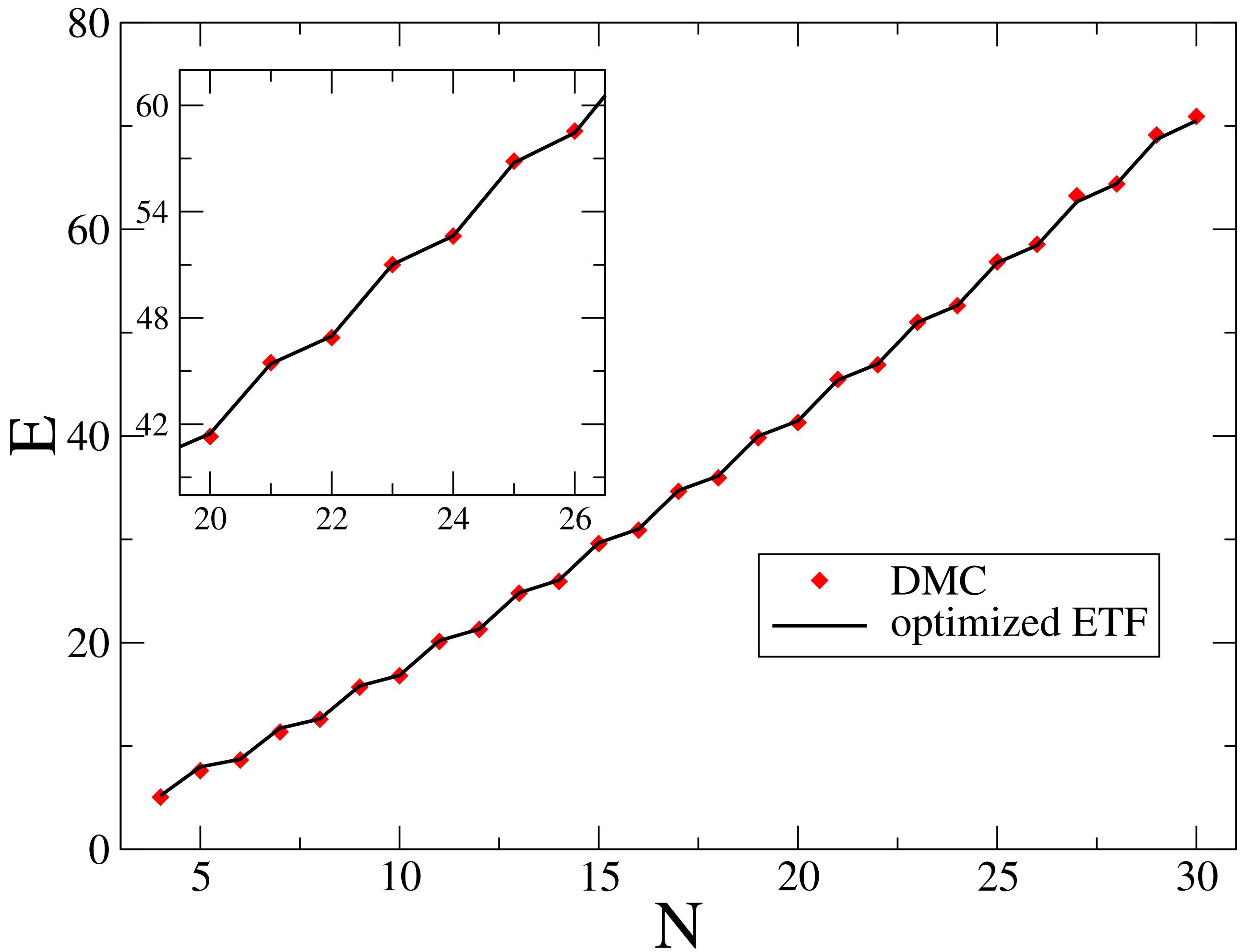
$$\Delta E_N = \gamma \; N^{1/9} \; \hbar\omega \; , \tag{13}$$

where γ is an unknown dimensionless constant.

After a systematic investigation of the FNDMC data we find that

$$\gamma = 0.856$$

gives the best fit. See the next figure.



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; solid line: optimized ETF results ($\xi = 0.455$, $\lambda = 0.13$, $\gamma = 0.856$). Energy in units of $\hbar\omega$. [L.S. and F. Toigo, PRA **78**, 053626 (2008)]

Generalized superfluid hydrodynamics

Let us now analyze the effect of the gradient term 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[**] irrotational hydrodynamics:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0 \,, \qquad (14)$$

$$m\frac{\partial}{\partial t}\mathbf{v} + \nabla\left[-\lambda \frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{n}}{\sqrt{n}} + \mu(n;\xi) + U(\mathbf{r})\right] = 0 \,. \qquad (15)$$

They are the simplest generalization 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, RMP **80**, 1215 (2008).

The generalized hydrodynamics equations can be written in terms of a superfluid nonlinear Schrödinger equation (NLSE), which is Galilei-invariant.[‡‡]

In fact, by introducing the complex wave function

$$\psi(\mathbf{r},t) = \sqrt{n(\mathbf{r},t)}\; e^{i\theta(\mathbf{r},t)} \; , \tag{16}$$

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

$$\mathbf{v}(\mathbf{r},t) = \frac{\hbar}{2m}\nabla\theta(\mathbf{r},t) \; , \tag{17}$$

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

$$i\hbar\frac{\partial}{\partial t}\psi = [-\frac{\hbar^2}{4m}\nabla^2 + 2U(\mathbf{r}) + 2\mu(|\psi|^2;\xi) + (1-4\lambda)\frac{\hbar^2}{4m}\frac{\nabla^2|\psi|}{|\psi|}]\psi \; , \tag{18}$$

is strictly equivalent to the equations of generalized hydrodynamics.

[‡‡]H.-D. Doebner and G.A. Goldin, PRA **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

$$\frac{\Omega}{q} = \sqrt{\frac{\xi}{3}} v_F \, , \tag{19}$$

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

$$v_F = \sqrt{\frac{2\epsilon_F}{m}} \tag{20}$$

is the Fermi velocity of a noninteracting Fermi gas.

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

$$\frac{\Omega}{q} = \sqrt{\frac{\xi}{3}} v_F \sqrt{1 + \frac{3\lambda}{\xi} (\frac{\hbar q}{2 m v_F})^2} \, , \tag{21}$$

which depends on the ratio λ/ξ.

In the case of harmonic confinement

$$U(\mathbf{r}) = \frac{1}{2} m \omega^2 r^2 \tag{22}$$

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:

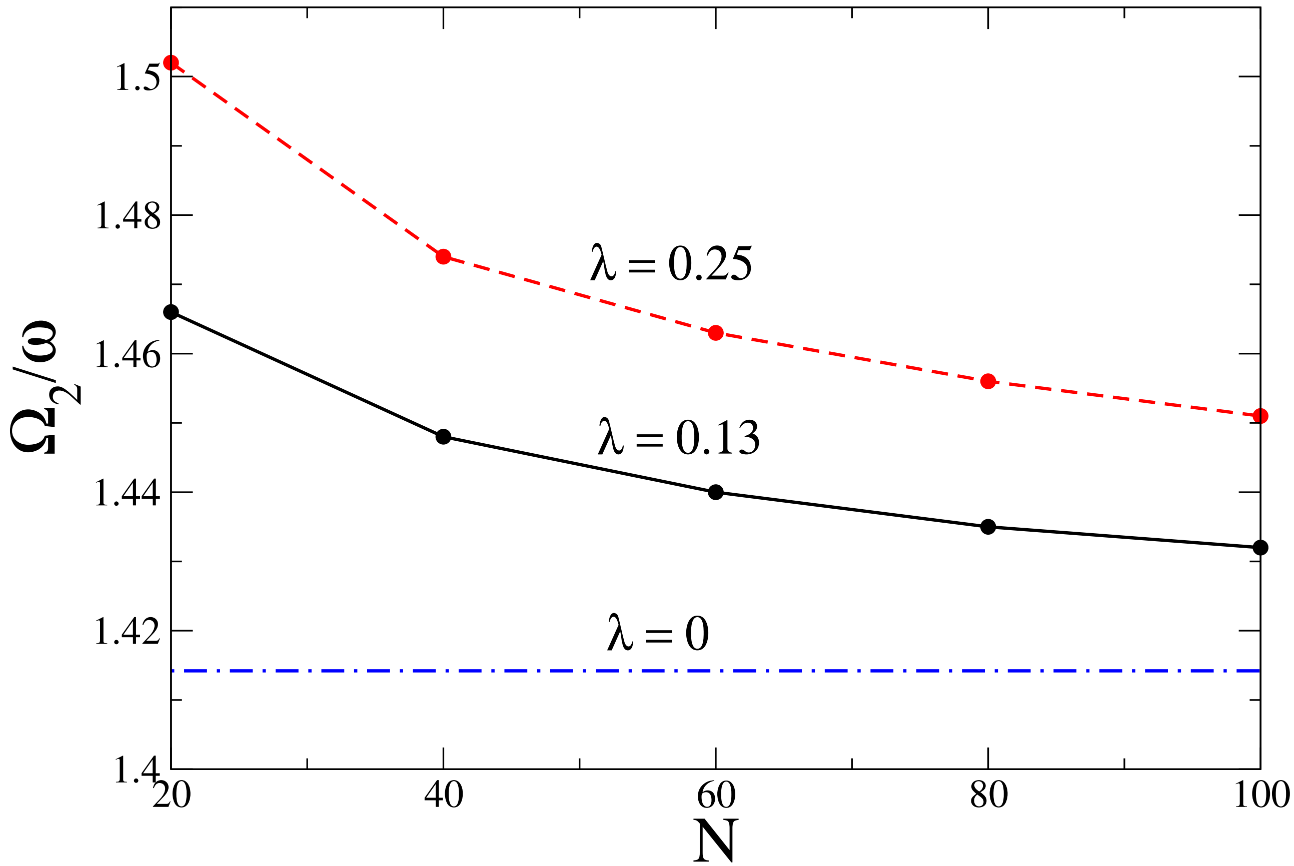
$$\Omega_0 = 2\omega \qquad \text{and} \qquad \Omega_1 = \omega \; . \tag{23}$$

We find instead that the frequency Ω_2 of the quadrupole mode ($l = 2$) depends on N and on the choice of the gradient coefficient λ.

Initial wave function to excite the quadrupole mode:

$$\psi_{in}(\mathbf{r}) = \psi_{gs}(r) \; e^{i\epsilon(2z^2 - x^2 - y^2)} \; , \tag{24}$$

where $\psi_{gs}(r)$ is the ground-state wave function and ϵ is a small parameter.



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, preliminary results]

Conclusions

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

- By fitting FNDMC calculations we have determined the universal parameters ξ and λ of ETF functional.

- ETF functional can 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 generalized superfluid hydrodynamics (or superfluid NLSE).

- The superfluid NLSE can be used to investigate collective modes also for a small number of atoms.