Quantum phenomena at ultra-low temperatures, BCS-BEC crossover and the unitarity limit

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Maribor, September 8, 2010

Summary

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Quantum phenomena at ultra-low temperatures

We know that each "elementary" particle has an intrinsic angular momentum, that is called **spin** $\mathbf{S}$.

All particles can be divided into two groups:

– **bosons**, with spin S that is an integer multiplier of the Planck constant $\hbar$:

$$S = n\hbar \,, \quad n = 0, 1, 2, \ldots \,,$$

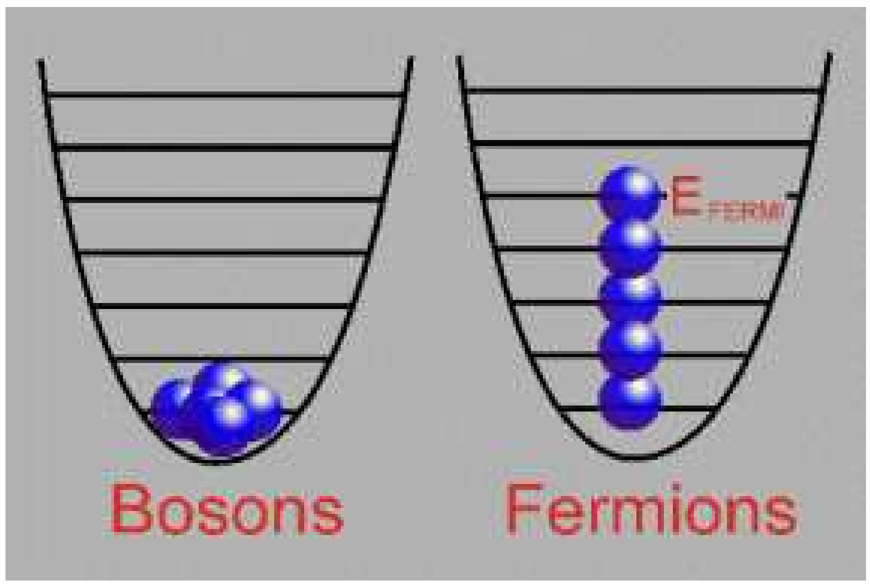
– **fermions**, with spin S that is a semi-integer multiplier of $\hbar$:

$$S = \frac{n}{2}\hbar \,, \quad n = 1, 2, 3, \ldots \,.$$

Examples: ${}^4_2$He is a boson, while ${}^3_2$He, is fermion.

The most intresting experimental result is that
bosons and fermions have a very different behavior!!

– Identical bosons can occupy the same state, i.e. they can stay very close each other; if all bosons are in the same state then there is the so-called **Bose-Einstein condensation**.
– Identical fermions CANNOT occupy the same state, i.e. they must stay far from each other: **Pauli's exclusion principle**.



Bosons and fermions in a harmonic trap.

Quantum statistical mechanics investigates the behavior of bosons and fermions as a function of temperature T.

When the temperature T is high, the statistical distributions of bosons and fermions reduce to the same distribution: the *Maxwell-Boltzmann distribution*, and consequently the statistical effect of spin is not important (**classical statistical mechanics**).

To see the statistical effects of spin and the differences between bosons and fermions (quantum degeneracy) it is necessary to strongly reduce the temperature!!

For N ideal particles in a box of volume V, the critical temperature of quantum degeneracy can be estimated by equating the de Broglie wave length

$$\lambda = \frac{h}{mv} = \frac{h}{m\sqrt{\frac{3k_B T}{m}}} \, , \tag{1}$$

of a particle in the gas at temperature T to the inter-atomic distance

$$d = \frac{1}{n^{1/3}} \, , \tag{2}$$

where $n = N/V$ is the number density. In this way one finds

$$T_c \simeq \frac{\hbar^2}{mK_B} \left(\frac{N}{V} \right)^{2/3} \, . \tag{3}$$

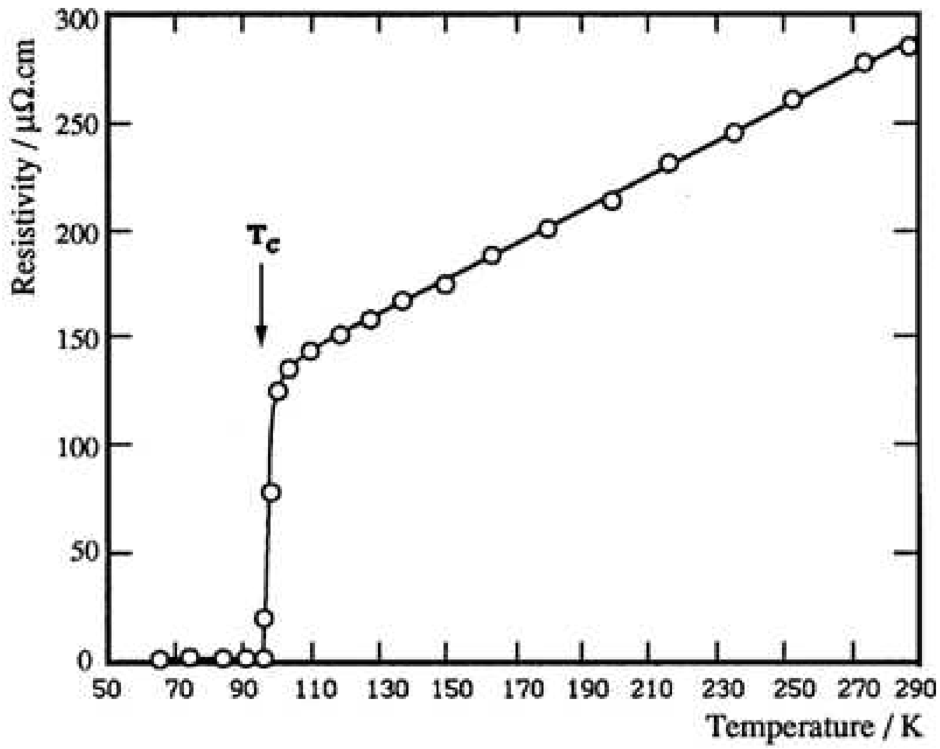
Below this critical temperature T_c the matter has a strange behavior: it can become **supermatter**, where macroscopic quantum phenomena can occur.

The **inter-particle interaction** modifies T_c and can also transform fermions in bosons (BCS theory and BCS-BEC crossover).

Superconductivity in metals and cuprates

In 1911 Heike Kamerlingh Onnes observed that in the mercury (Hg) cooled below $T_c = 4.16$ Kelvin the electrical resistence becomes zero.

Onnes called this phenomenon **superconductivity**.



Electrical resistence as a function of temperature for a superconducting material.

Many materials are superconductors below a critical temperature T_c. But others are not.

Material	**Symbol**	T_c **(Kelvin)**
Aluminium	${}^{27}_{13}Al$	1.19
Tin	${}^{120}_{50}Sn$	3.72
Mercury	${}^{202}_{80}Hg$	4.16
Lead	${}^{208}_{82}Pb$	7.20
Neodymium	${}^{142}_{60}Nb$	9.30

Critical temperature T_c of some superconducting materials, at atmospheric pressure.

In 1957 John Bardeen, Leon Cooper and Robert Schrieffer (BCS theory) suggested that in superconductivity, due to the ionic cristal lattice, pairs of electrons with anti-parallel spins can couple (Cooper pairs), and each pair behaves like a bosonic particle.

In 1986 Karl Alex Müller and Johannes Georg Bednorz descovered *high-temperature superconductors*. These are *cuprates*, namely ceramic materials containing copper oxide. Their critical temperature can reach 133 Kelvin.

Superfluidity in helium 4

In 1937 Pyotr Leonidovich Kapitza descovered that below $T_c = 2.16$ Kelvin helium 4 (^{4}He) remains liquid but it shows zero viscosity.

Kapitza called this phenomenon **superfluidity**.

Example: a macroscopic object immersed in superfluid helium moves without viscosity if its velocity v è below a critical value v_c.

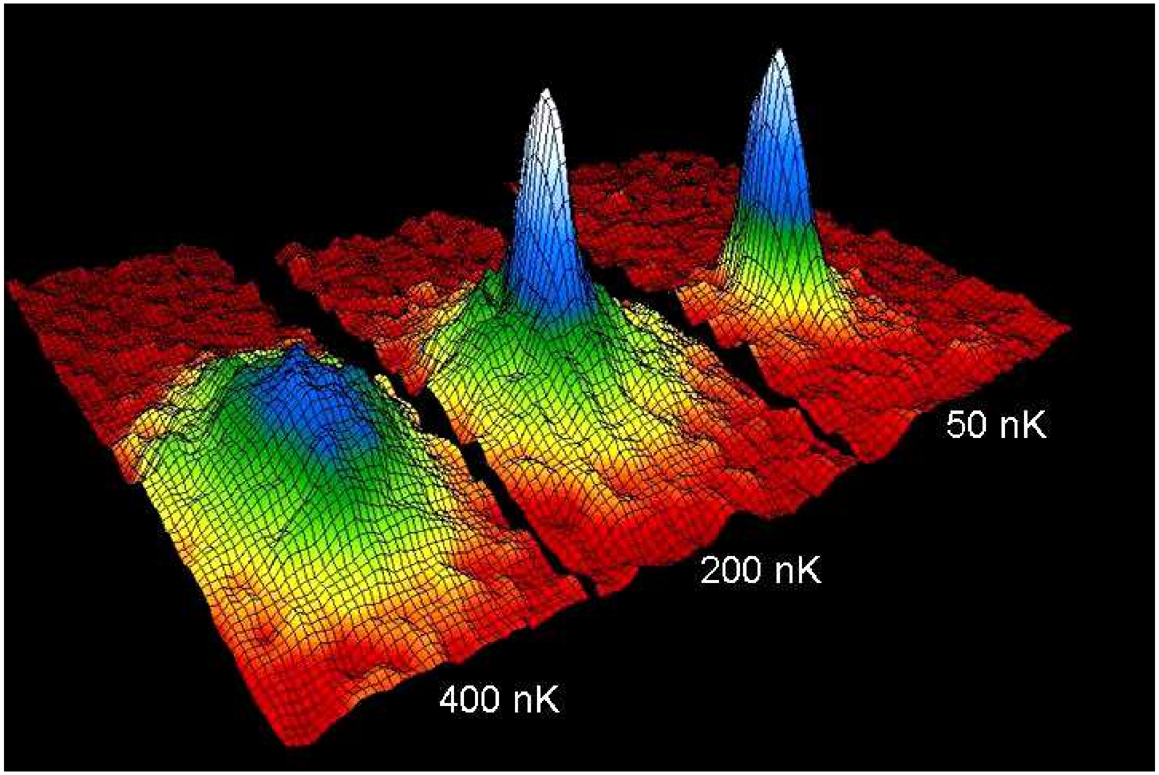
In 1938 Fritz London gave a theoretical explanation of superfluidity of helium 4 on the basis of Bose-Einstein condensation.

London observed that ^{4}He is a boson and that the critical temperature T_c of Bose-Einstein condensation for an ideal Bose gas is in good agreement with the T_c of helium 4.

Bose-Einstein condensation in dilute atomic gases

In 1995 Eric Cornell, Carl Wieman and Wolfgang Ketterle achieved the Bose-Einstein condensation with ultra-dilute and ultra-cold atomic vapors (^{87}Rb and ^{23}Na).

The critical temperature is about $T_c \simeq 100$ nanoKelvin.



Density profiles of the atomic gas of Rubidium.

In these experiments ultracold atoms are confined in a harmonic trap

$$U(\mathbf{r}) = \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2) \tag{4}$$

produced by magnetic (magnetic-dipole-moment interaction) or electric fields (electric-dipole-moment interaction).

The critical temperature of Bose-Einstein condensation for an ideal Bose gas in a harmonic trap is

$$k_B T_c \simeq \hbar\omega \ N^{1/3} \ , \tag{5}$$

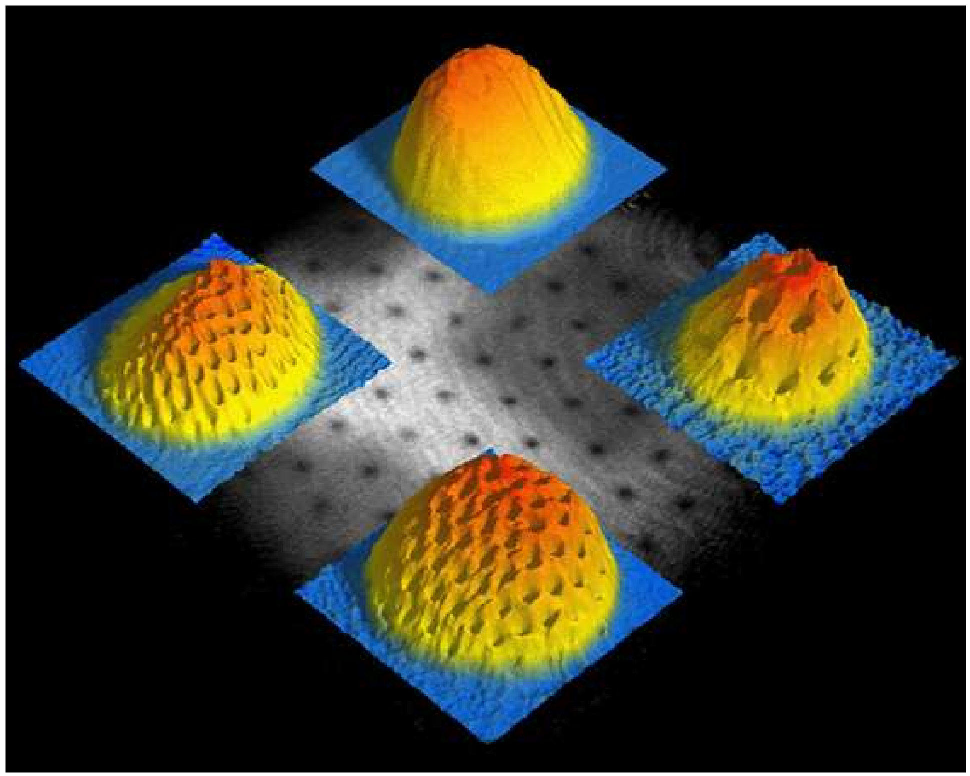
and the condensate fraction reads

$$f_0 = 1 - \left(\frac{T}{T_c}\right)^3 \ . \tag{6}$$

In real systems the zero-temperature condensate fraction is
- ultra-dilute atomic gases: $f_0 \simeq 99\%$
– liquid helium 4: $f_0 \simeq 10\%$
– metallic superconductors : $f_0 \simeq 0.01\%$

An interesting consequence of Bose-Einstein condensation in ultra-cold atoms and helium 4 is the possibility of obtaining **quantized vortices**, where the fluid velocity follows the law

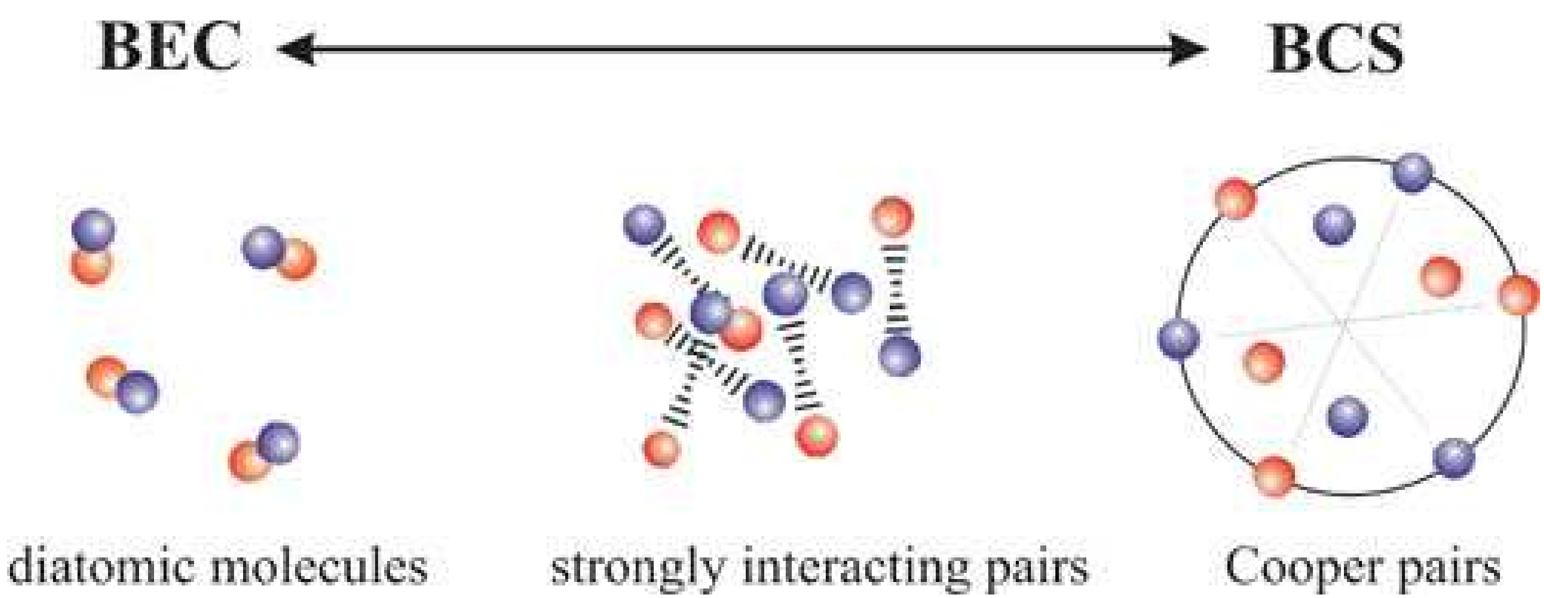
$$v = \frac{\hbar}{m} \frac{k}{r_\perp}, \qquad k = 0, 1, 2, ...$$



Formation of quantized vortices in Bose-condensed gas of ^{87}Rb atoms. The number of vortices increases by increasing the rotational frequency of the system.

BCS-BEC crossover and the unitarity limit

In 2002 the BCS-BEC crossover has been observed* with ultracold gases made of fermionic alkali-metal atoms.



This crossover is obtained by changing (with a Feshbach resonance) the s-wave scattering length a_F of the inter-atomic potential:

– $a_F \to 0^-$ (BCS regime of weakly-interacting Cooper pairs)

– $a_F \to \pm\infty$ (unitarity limit of strongly-interacting Cooper pairs)

– $a_F \to 0^+$ (BEC regime of bosonic dimers)

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

Unitary Fermi gas

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

$$\hat{H} = \sum_{i=1}^{N_\uparrow} \left(\frac{\hat{p}_i^2}{2m} + U(\mathbf{r}_i) \right) + \sum_{j=1}^{N_\downarrow} \left(\frac{\hat{p}_j^2}{2m} + U(\mathbf{r}_j) \right) + \sum_{i,j} V(\mathbf{r}_i - \mathbf{r}_j) \ , \tag{7}$$

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 gas can be modelled by a square well potential:

$$V(r) = \begin{cases} -V_0 & r < r_0 \\ 0 & r > r_0 \end{cases} \tag{8}$$

By varying the depth V_0 of the potential one changes the s-wave scattering length

$$a_F = r_0 \left(1 - \frac{tan(r_0 \sqrt{m V_0}/\hbar)}{r_0 \sqrt{m V_0}/\hbar} \right) \ . \tag{9}$$

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

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

$$r_0 \ll n^{-1/3} \ll |a_F| \; . \tag{10}$$

Under these conditions the Fermi gas is called unitary Fermi gas. Ideally, the unitarity limit corresponds to

$$r_0 = 0 \qquad \text{and} \qquad a_F = \pm\infty \; . \tag{11}$$

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

*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 **442**, 54 (2006)

The only length characterizing the uniform unitary Fermi gas is the average distance between particles $d = n^{-1/3}$.

In this case, from simple dimensional arguments, the ground-state energy per volume must be

$$\frac{E_0}{V} = \xi \frac{3}{5} \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n^{5/3} = \xi \, \frac{3}{5} \, \epsilon_F \, n \, , \tag{12}$$

with ϵ_F Fermi energy of the ideal gas, $n = N/V$ the total density, and ξ a universal unknown parameter.

Monte Carlo calculations and experimental data with dilute and ultracold atoms suggest* that the unitary Fermi gas is a superfluid with $\xi \simeq 0.4$.

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

Extended Thomas-Fermi density functional

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

$$E_{TF} = \int d^3\mathbf{r}\ [\xi \frac{3}{5}\frac{\hbar^2}{2m}(3\pi^2)^{2/3} n^{5/3}(\mathbf{r}) + U(\mathbf{r}) n(\mathbf{r})]\ , \qquad (13)$$

with $n(\mathbf{r}) = n_\uparrow(\mathbf{r}) + n_\downarrow(\mathbf{r})$ total local density. The total number of fermions is

$$N = \int d^3\mathbf{r}\ n(\mathbf{r})\ . \qquad (14)$$

By minimizing E_{TF} one finds

$$\xi \frac{\hbar^2}{2m}(3\pi^2)^{2/3} n^{2/3}(\mathbf{r}) + U(\mathbf{r}) = \bar{\mu}\ , \qquad (15)$$

with $\bar{\mu}$ chemical potential of the non uniform system.

*S. Giorgini, L.P. Pitaevskii, and S. Stringari, RMP **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

$$\lambda \frac{\hbar^2}{8m} \frac{(\nabla n)^2}{n^2} = \lambda \frac{\hbar^2}{2m} \frac{(\nabla \sqrt{n})^2}{n} . \tag{16}$$

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

$$E = \int d^3\mathbf{r} \ \left[\lambda \frac{\hbar^2}{8m} \frac{(\nabla n(\mathbf{r}))^2}{n(\mathbf{r})} + \xi \frac{3}{5} \frac{\hbar^2}{2m} (3\pi^2)^{5/3} n(\mathbf{r})^{2/3} + U(\mathbf{r}) n(\mathbf{r}) \right] \ . \tag{17}$$

By minimizing the ETF energy functional one gets:

$$\left[\lambda \frac{\hbar^2}{2m} \nabla^2 + \xi \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n(\mathbf{r})^{2/3} + U(\mathbf{r}) \right] \sqrt{n(\mathbf{r})} = \bar{\mu} \ \sqrt{n(\mathbf{r})} \ . \tag{18}$$

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

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

$$\xi = 0.44 \qquad \text{and} \qquad \lambda = 1/4 \ . \tag{19}$$

To better fix 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 $U(\mathbf{r}) = m\omega^2 r^2/2$.

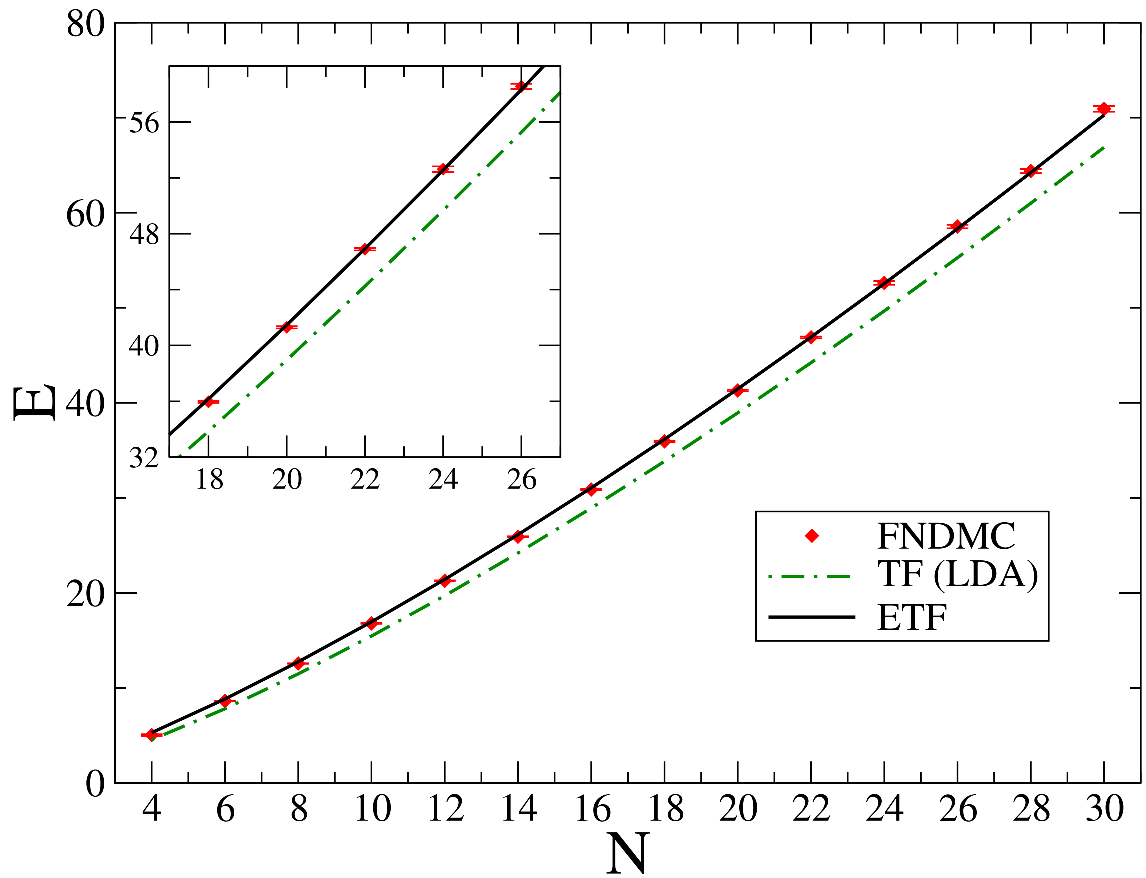
After a systematic analysis [L.S. and F. Toigo, PRA **78**, 053626 (2008)] we find

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

as the best fitting parameters in the unitary regime (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, PRA **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, PRA **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.

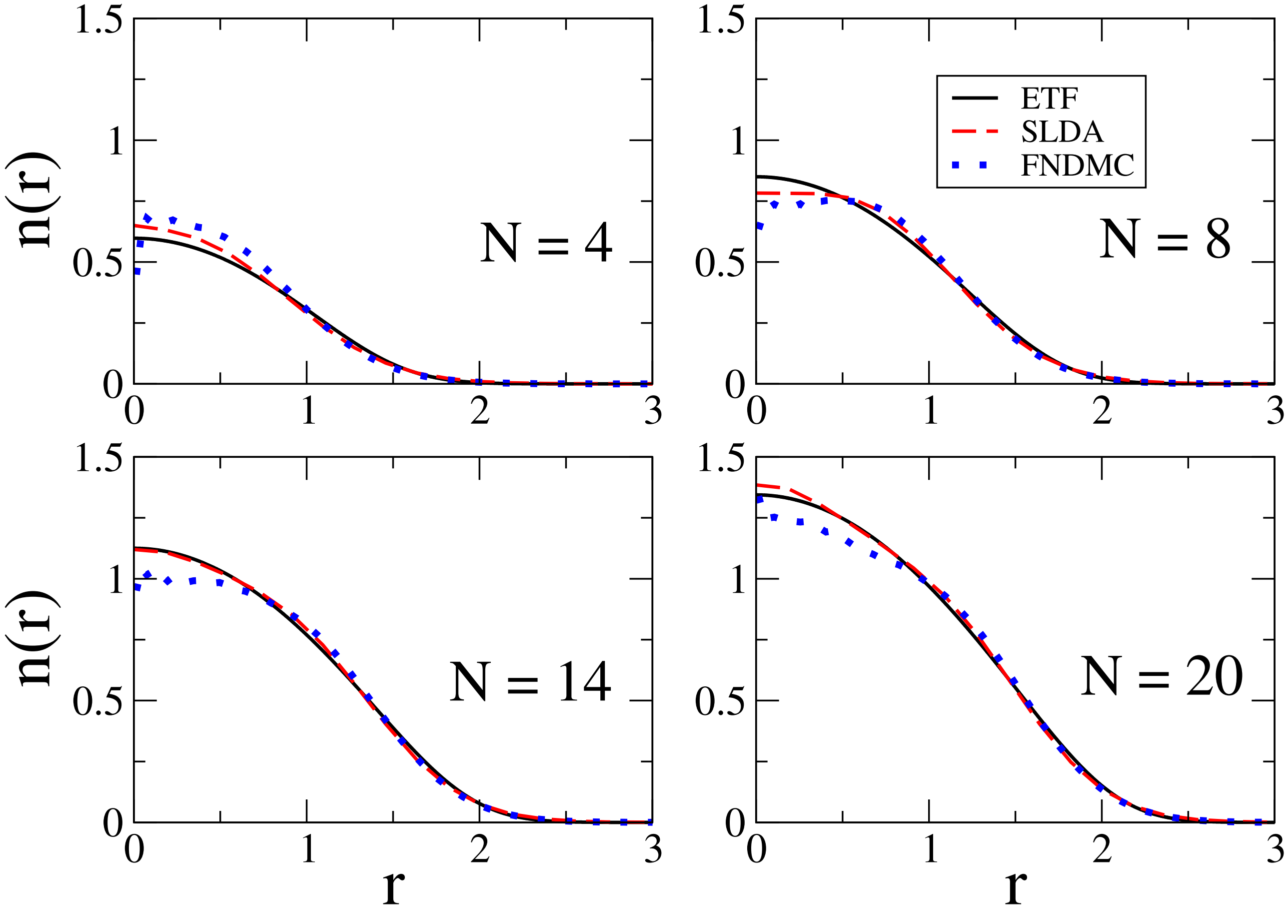
We calculate numerically (by solving with a finite-difference Crank-Nicolson method the stationary 3D NLSE) the density profile $n(\mathbf{r})$ of the gas in a isotropic harmonic trap

$$U(\mathbf{r}) = \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2) \ . \tag{20}$$

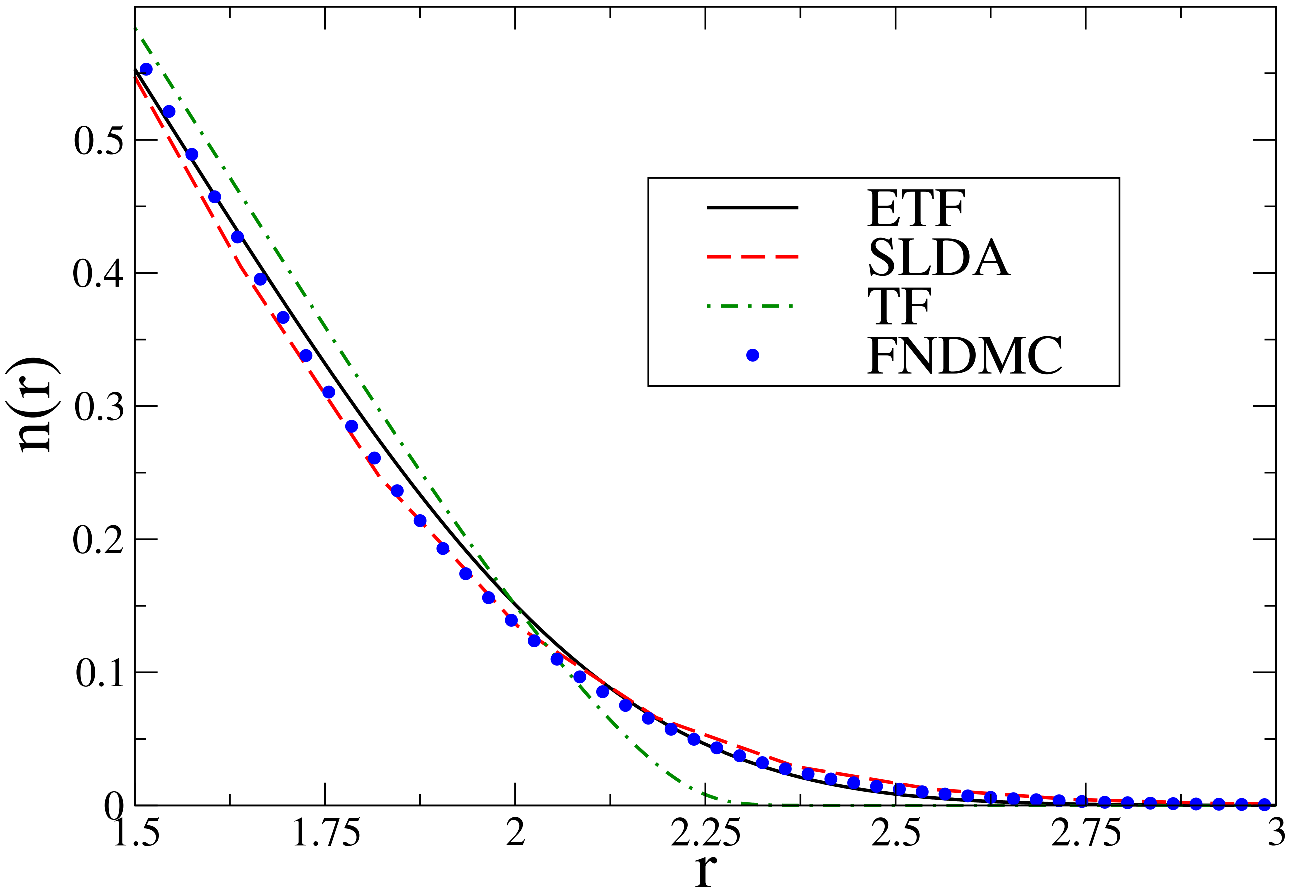
We compare our results with those obtained by Doerte Blume* with her FNDMC code. For completeness we consider also the density profiles obtained by Aurel Bulgac† using his multi-orbital density functional (SLDA).

*D. Blume, J. von Stecher, C.H. Greene, PRL **99**, 233201 (2007); J. von Stecher, C.H. Greene and D. Blume, PRA **77** 043619 (2008); D. Blume, unpublished.

†A. Bulgac, PRA **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, LPL **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, LPL **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:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0 \ , \qquad (21)$$

$$m\frac{\partial}{\partial t}\mathbf{v} + \nabla[-\lambda\frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{n}}{\sqrt{n}} + \xi\frac{\hbar^2}{2m}(3\pi^2 n)^{2/3} + U(\mathbf{r}) + \frac{m}{2}v^2] = 0 \ . \qquad (22)$$

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, RMP **80**, 1215 (2008).

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

$$\Omega_{col} = c_1 \; q \; , \tag{23}$$

where Ω_{col} is the collective frequency, q is the wave number and

$$c_1 = \sqrt{\frac{\xi}{3}} v_F \tag{24}$$

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, PRA **78**, 053626 (2008)] also a correcting term, i.e.

$$\Omega_{col} = c_1 \; q \; \sqrt{1 + \frac{3\lambda}{\xi} (\frac{\hbar q}{2 m v_F})^2} \, , \tag{25}$$

which depends on the ratio λ/ξ.

In the case of harmonic confinement

$$U(\mathbf{r}) = \frac{1}{2} m\omega^2 r^2 \tag{26}$$

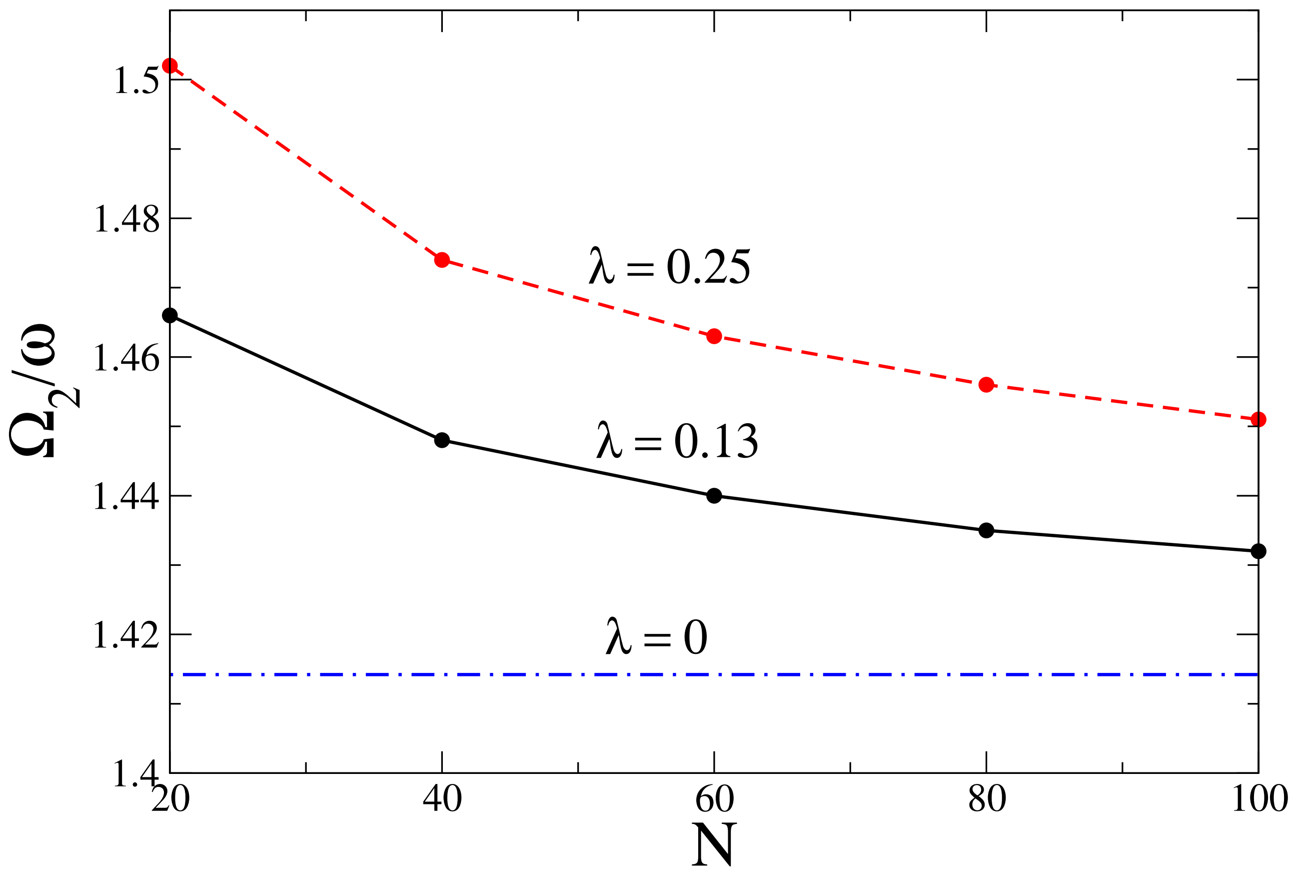
we study numerically the collective modes of the unitary Fermi gas by increasing the number N of atoms.

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:

$$\Omega_0 = 2\omega \qquad \text{and} \qquad \Omega_1 = \omega \; , \tag{27}$$

as predicted by Y. Castin [CRP **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, LPL **7**, 78 (2010).]

Conclusions

- Macroscopic quantum phenomena at ultra-low temperature are strongly related to Bose-Einstein condensation.

- In dilute gases of alkali-metal atoms it has been observed BEC (with bosons) but also the BCS-BEC crossover (with fermions).

- Very interesting is the unitarity limit of the BCS-BEC crossover and the corresponding unitary Fermi gas.

- Our ETF functional of the unitary Fermi gas can be used to study ground-state density profiles in a generic external potential $U(\mathbf{r})$.

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