Shock waves in the unitary Fermi gas

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Collaboration with:
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1. BCS-BEC crossover and the unitarity limit
2. Thomas-Fermi density functional
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Conclusions
In 2002 the BCS-BEC crossover has been observed$^1$ 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:

- $a_F \rightarrow 0^-$ (BCS regime of weakly-interacting Cooper pairs)
- $a_F \rightarrow \pm \infty$ (unitarity limit of strongly-interacting Cooper pairs)
- $a_F \rightarrow 0^+$ (BEC regime of bosonic dimers)

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

\[ \hat{H} = \sum_{i=1}^{N_\uparrow} \left( \frac{\hat{p}_i^2}{2m} + U(r_i) \right) + \sum_{j=1}^{N_\downarrow} \left( \frac{\hat{p}_j^2}{2m} + U(r_j) \right) + \sum_{i,j} V(r_i - r_j), \]  

where \( U(r) \) is the external confining potential and \( V(r) \) 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:

\[ V(r) = \begin{cases} -V_0 & r < r_0 \\ 0 & r > r_0 \end{cases} \]  

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

\[ a_F = r_0 \left( 1 - \frac{\tan(r_0 \sqrt{mV_0}/\hbar)}{r_0 \sqrt{mV_0}/\hbar} \right). \]
The crossover from a BCS superfluid ($a_F < 0$) to a BEC of molecular pairs ($a_F > 0$) has been investigated experimentally\(^2\), 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

$$r_0 \ll n^{-1/3} \ll |a_F|.$$  \hspace{1cm} (4)

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

$$r_0 = 0 \quad \text{and} \quad a_F = \pm \infty.$$  \hspace{1cm} (5)

The detection of quantized vortices under rotation\(^3\) 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, from simple dimensional arguments, the ground-state energy per volume must be

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

(6)

with \( \epsilon_F \) Fermi energy of the ideal gas, \( n = N/V \) the total density, and \( \xi \) a universal unknown parameter.
Monte Carlo calculations and experimental data with dilute and ultracold atoms suggest\(^4\) that the unitary Fermi gas is a superfluid with \( \xi \simeq 0.4 \).

2. Thomas-Fermi density functional

The Thomas-Fermi (TF) energy functional\(^5\) of the unitary Fermi gas in an external potential \(U(r)\) is

\[
E_{TF} = \int d^3r \left[ \xi \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n^{5/3}(r) + U(r) n(r) \right], \tag{7}
\]

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

\[
N = \int d^3r \ n(r). \tag{8}
\]

By minimizing \(E_{TF}\) one finds

\[
\xi \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n^{2/3}(r) + U(r) = \bar{\mu}, \tag{9}
\]

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

The TF functional **must** be extended to cure the pathological TF behavior at the surface. We add to the energy per particle the gradient term [LS and F. Toigo, Phys. Rev. A 78, 053626 (2008)]

\[
\lambda \frac{\hbar^2}{8m} \frac{(\nabla n)^2}{n^2} = \lambda \frac{\hbar^2}{2m} \frac{(\nabla \sqrt{n})^2}{n}.
\]

(10)

Historically, this term was introduced by von Weizsäcker\(^6\) to treat surface effects in nuclei. Here we consider \(\lambda\) 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, Phys. Rev. A 72, 041603 (2005);

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3. Extended Thomas-Fermi density functional (II)

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

\[
E = \int d^3r \left[ \lambda \frac{\hbar^2}{8m} \left( \nabla n(r) \right)^2 + \xi \frac{3}{5} \frac{\hbar^2}{2m} \left(3\pi^2\right)^{5/3} n(r)^{5/3} + U(r) n(r) \right].
\] (11)

By minimizing the ETF energy functional one gets:

\[
\left[ \lambda \frac{\hbar^2}{2m} \nabla^2 + \xi \frac{\hbar^2}{2m} \left(3\pi^2\right)^{2/3} n(r)^{2/3} + U(r) \right] \sqrt{n(r)} = \bar{\mu} \sqrt{n(r)}.
\] (12)

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

The simple and reasonable choice

\[
\xi = 0.44 \quad \text{and} \quad \lambda = 1/4
\] (13)

fits quite well Monte Carlo data.\(^7\)

\(^7\)Indeed \(\lambda = 1/4\) is the best choice to describe the DC Josephson effect of the unitary Fermi superfluid: see F. Ancilotto, LS, and F. Toigo, Phys. Rev. A 79, 033627 (2009).
Having determined the parameters $\xi$ and $\lambda$ 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 $n(r)$ of the gas in an isotropic harmonic trap

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

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).

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3. Extended Thomas-Fermi density functional (IV)

Unitary Fermi gas under harmonic confinement of frequency $\omega$. 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).]
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\(^{10}\) irrotational and inviscid hydrodynamics:

\[
\frac{\partial n}{\partial t} + \nabla \cdot (nv) = 0 , \quad (15)
\]

\[
m\frac{\partial}{\partial t}v + \nabla \left[ -\lambda \frac{\hbar^2}{2m} \frac{\nabla^2 \sqrt{n}}{\sqrt{n}} + \xi \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3} + U(r) + \frac{m}{2} v^2 \right] = 0 . \quad (16)
\]

They are the simplest extension of the equations of superfluid hydrodynamics of fermions\(^{11}\), where \(\lambda = 0\).

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4. Extended superfluid hydrodynamics (II)

The extended hydrodynamics equations can be written in terms of a superfluid nonlinear Schrödinger equation (superfluid NLSE).\(^{12}\)

In fact, by introducing the complex wave function

\[
\psi(r, t) = n(r, t)^{1/2} \ e^{i\theta(r, t)} \tag{17}
\]

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

\[
v(r, t) = \frac{\hbar^2}{2m} \nabla \theta(r, t), \tag{18}
\]

the equation

\[
i\hbar \frac{\partial}{\partial t} \psi = \left[ -\frac{\hbar^2}{4m} \nabla^2 + U(r) + 2\mu + 2\xi \frac{\hbar^2}{2m} (3\pi^2 |\psi|^2)^{2/3} + (1 - 4\lambda) \frac{\hbar^2}{4m} \frac{\nabla^2 |\psi|}{|\psi|} \right] \psi \tag{19}
\]

is equivalent to the equations of extended superfluid hydrodynamics.

4. Extended superfluid hydrodynamics (III)

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

\[
\Omega_{\text{col}} = c_1 \, q ,
\]

(20)

where \(\Omega_{\text{col}}\) is the collective frequency, \(q\) is the wave number and

\[
c_1 = \sqrt{\frac{\xi}{3}} v_F
\]

(21)

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.

\[
\Omega_{\text{col}} = c_1 \, q \sqrt{1 + \frac{3\lambda}{\xi} \left(\frac{\hbar q}{2mv_F}\right)^2} ,
\]

(22)

which depends on the ratio \(\lambda/\xi\).
One of the basic problems in physics is how density perturbations propagate through a material. In addition to the well-known sound waves, there are shock waves characterized by an abrupt change in the density of the medium: they produce, after a transient time, an extremely large density gradient (the shock). Shock waves are ubiquitous and have been studied in many different physical systems\textsuperscript{13}

Here we investigate the formation and dynamics of shock waves perturbing the uniform unitary Fermi gas by using the zero-temperature equations of generalized superfluid hydrodynamics.\textsuperscript{14}


\textsuperscript{14}LS, \textit{EPL} 96, 40007 (2011)
5. Shock waves perturbing the uniform Fermi gas (II)

To get analytical results we perform the following factorization

\[ n(r) = \bar{n} \rho(z) \quad (23) \]

where \( \rho(z, t) \) is the relative density, i.e. the localized axial modification with respect to the uniform density \( \bar{n} \).

Neglecting the gradient term we find the 1D hydrodynamic equations for the axial dynamics of the superfluid, given by

\[ \dot{\rho} + v \rho' + v' \rho = 0, \quad (24) \]

\[ \dot{v} + vv' + \frac{c_{ls}(\rho)^2}{\rho} \rho' = 0, \quad (25) \]

where dots denote time derivatives, primes space derivatives, and

\[ c_{ls}(\rho) = c_s \rho^{1/3} \quad (26) \]

is the local sound velocity, with \( c_s = c_{ls}(1) = \sqrt{\xi/3} v_F \) the bulk sound velocity, \( v_F = \sqrt{2\epsilon_F/m} \) is bulk Fermi velocity and \( \epsilon_F = \frac{\hbar^2}{2m} \left(3\pi^2 \bar{n}\right)^{2/3} \) the bulk Fermi energy.
5. Shock waves perturbing the uniform Fermi gas (III)

The bulk sound velocity $c_s$ is the speed of propagation of a small perturbation $\tilde{\rho}(z, t)$ with respect to the uniform superfluid of density $\bar{n}$. In fact, setting

$$\rho(z, t) = 1 + \tilde{\rho}(z, t)$$

(27)

with $\tilde{\rho}(z, t) \ll 1$ and $v(z, t)$ of the same order of $\tilde{\rho}(z, t)$, from the linearization of Eqs. (24) and (25) we get the familiar linear wave equation

$$\left( \frac{\partial^2}{\partial t^2} - c_s^2 \frac{\partial^2}{\partial z^2} \right) \tilde{\rho}(z, t) = 0 ,$$

(28)

for $\tilde{\rho}(z, t)$ and a similar equation for $v(z, t)$. Modelling the initial perturbation with a Gaussian shape, i.e.

$$\tilde{\rho}(z, 0) = 2\eta \ e^{-z^2/(2\sigma^2)} ,$$

(29)

one finds from the linearized equations

$$\tilde{\rho}(z, t) = \eta \ e^{-\left(\frac{z-c_s t}{\sigma}\right)^2} + \eta \ e^{-\left(\frac{z+c_s t}{\sigma}\right)^2} ,$$

(30)

with initial condition $\dot{\tilde{\rho}}(z, t = 0) = 0$. Thus, for the conservation of the linear momentum, the initial wave packet splits into two (very small) waves travelling in opposite directions with the speed of sound $c_s$. 
Obviously Eq. (30) is reliable only if $|\eta| \ll 1$. As expected, a small (infinitesimal) perturbation gives rise to sound waves.

What happens with a large (finite) perturbation?

a) **The traveling waves are deformed**: the local velocity depends on the local density.\(^\text{15}\)

b) **The gradient term cannot be neglected**: it is essential during (and after) the formation of the shock.

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\(^{15}\)Analytical details on the local velocity and the period of formation of shock waves can be found in **LS, EPL 96, 40007 (2011)**.
5. Shock waves perturbing the uniform Fermi gas (V)

Time evolution of supersonic shock waves. Initial condition with $\sigma/l_F = 18$ and $\eta = 0.3$. The curves give the relative density profile $\rho(z)$ at subsequent frames, where $l_F = \sqrt{\hbar^2/(m\epsilon_F)}$ is the Fermi length and $\omega_F = \epsilon_F/\hbar$ is the Fermi frequency. [LS, EPL 96, 40007 (2011)]
5. Shock waves perturbing the uniform Fermi gas (VI)

Time evolution of subsonic shock waves. Initial condition with $\sigma/l_F = 18$ and $\eta = -0.2$. The curves give the relative density profile $\rho(z)$ at subsequent frames, where $l_F = \sqrt{\hbar^2/(m\epsilon_F)}$ is the Fermi length and $\omega_F = \epsilon_F/\hbar$ is the Fermi frequency. [LS, EPL 96, 40007 (2011)]
6. Shock waves in colliding Fermi clouds (I)

In 2011 the group of John Thomas (Duke and NCSU) made a remarkable experiment on the collision of two Fermi clouds of $^6$Li atoms at unitarity containing about $10^5$ atoms per spin [Phys. Rev. Lett. **106**, 150401 (2011)].
The experiment of Thomas was nicely reproduced using dissipative hydrodynamic equations with a very large fitting viscosity $\eta$ [Phys. Rev. Lett. 106, 150401 (2011)] which is however unphysical.
The experiment of Thomas is also nicely reproduced using our dispersive hydrodynamic equations (extended superfluid hydrodynamics) without fitting parameters [F. Ancilotto, LS, and F. Toigo, Phys. Rev. A 85, 063612 (2012)].

1D density profiles at different times $t$. Left part: our theory. Right part: experimental data. The normalized density is in units of $10^{-2}/\mu m$ per particle.
Conclusions

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

- Our extended superfluid hydrodynamics, which are equivalent to a nonlinear Schrödinger equation, can be applied to investigate collective modes of the unitary Fermi gas.

- Also shock waves can be studied with our extended superfluid hydrodynamics and we suggest that that the shock waves observed in the collision of two unitary Fermi clouds are dispersive and not dissipative.