Dynamical properties of the unitary Fermi gas: collective modes and shock waves

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Summary

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- 2. Thomas-Fermi density functional
- 3. Extended Thomas-Fermi density functional
- 4. Generalized superfluid hydrodynamics
- 5. Shock waves
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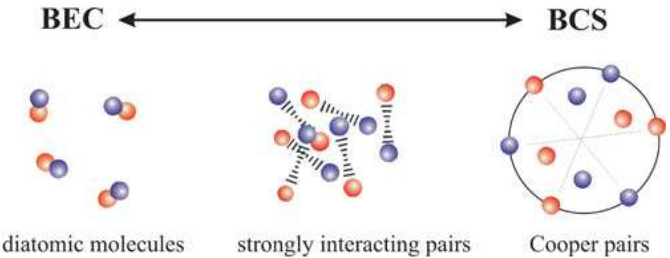
1. BCS-BEC crossover and the unitarity limit (I)

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:

– $a_F \to 0^-$ (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)

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

1. BCS-BEC crossover and the unitarity limit (II)

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

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

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:

$$V(r) = \begin{cases} -V_0 & r < r_0 \\ 0 & r > r_0 \end{cases} \quad (2)$$

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

$$a_F = r_0 \left(1 - \frac{tan(r_0\sqrt{mV_0}/\hbar)}{r_0\sqrt{mV_0}/\hbar} \right) \, . \quad (3)$$

1. BCS-BEC crossover and the unitarity limit (III)

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

$$r_0 \ll n^{-1/3} \ll |a_F| \, . \tag{4}$$

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

$$r_0 = 0 \qquad \text{and} \qquad a_F = \pm\infty \, . \tag{5}$$

The detection of quantized vortices under rotation[3] has clarified that the unitary Fermi gas is superfluid.

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

[3] M.W. Zwierlein *et al.*, Science **311**, 492 (2006); M.W. Zwierlein *et al.*, Nature **442**, 54 (2006)

1. BCS-BEC crossover and the unitarity limit (IV)

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

$$\frac{E_0}{V} = \xi \frac{3}{5} \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n^{5/3} = \xi \; \frac{3}{5} \; \epsilon_F \; n \; , \tag{6}$$

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[4] that the unitary Fermi gas is a superfluid with $\xi \simeq 0.4$.

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

2. Thomas-Fermi density functional

The Thomas-Fermi (TF) energy functional[5] of the unitary Fermi gas in an external potential $U(\mathbf{r})$ is

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

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

$$N = \int d^3\mathbf{r} \; n(\mathbf{r}) \, . \tag{8}$$

By minimizing E_{TF} one finds

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

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

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

3. Extended Thomas-Fermi density functional (I)

The TF functional must be extended to cure the pathological TF behavior at the surface.
We add to the energy per particle the term

$$\lambda \frac{\hbar^2}{8m} \frac{(\nabla n)^2}{n^2} = \lambda \frac{\hbar^2}{2m} \frac{(\nabla \sqrt{n})^2}{n} \ . \tag{10}$$

Historically, this term was introduced by von Weizsäcker[6] 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).

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

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

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

By minimizing the ETF energy functional one gets:

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

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:

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

which fits quite well Monte Carlo data.

3. Extended Thomas-Fermi density functional (III)

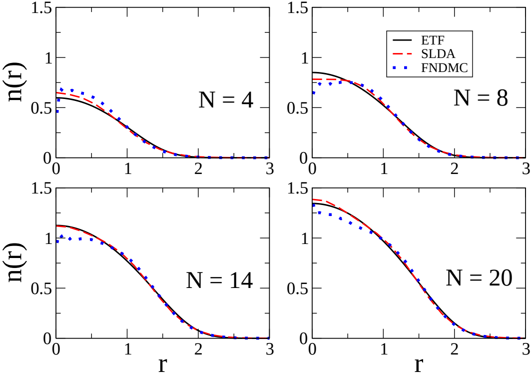
Having determined the parameters ξ and λ we can now use our single-orbital density functional to calculate various properties of the trapped unitary Fermi gas.
We calculate numerically (by solving with a finite-difference Crank-Nicolson method the stationary 3D NLSE) the density profile $n(\mathbf{r})$ of the gas in a isotropic harmonic trap

$$U(\mathbf{r}) = \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2) \ . \tag{14}$$

We compare our results with those obtained by Doerte Blume[7] with her FNDMC code. For completeness we consider also the density profiles obtained by Aurel Bulgac[8] using his multi-orbital density functional (SLDA).

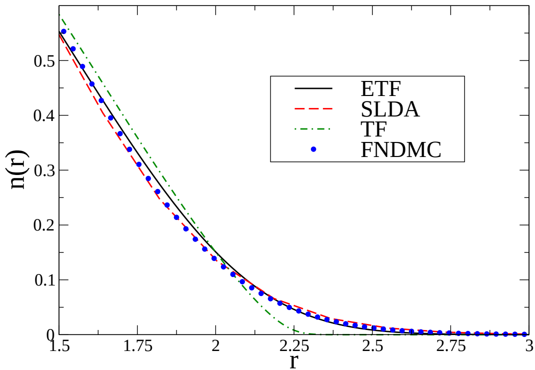
[7] D. Blume, J. von Stecher, C.H. Greene, PRL **99**, 233201 (2007); J. von Stecher, C.H. Greene and D. Blume, PRA **77** 043619 (2008); D. Blume, unpublished.
[8] A. Bulgac, PRA **76**, 040502(R) (2007).

3. Extended Thomas-Fermi density functional (IV)



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).]

3. Extended Thomas-Fermi density functional (V)



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).]

4. Generalized superfluid hydrodynamics (I)

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[9] irrotational and inviscid hydrodynamics:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0 \,, \quad (15)$$

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

They are the simplest extension of the equations of superfluid hydrodynamics of fermions[10], where $\lambda = 0$.

[9] 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).
[10] S. Giorgini, L.P. Pitaevskii, and S. Stringari, RMP **80**, 1215 (2008).

4. Generalized superfluid hydrodynamics (II)

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

$$\Omega_{col} = c_1 \ q \ , \tag{17}$$

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

$$c_1 = \sqrt{\frac{\xi}{3}} v_F \tag{18}$$

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.

$$\Omega_{col} = c_1 \ q \ \sqrt{1 + \frac{3\lambda}{\xi} \left(\frac{\hbar q}{2 m v_F}\right)^2} \ , \tag{19}$$

which depends on the ratio λ/ξ.

4. Generalized superfluid hydrodynamics (III)

In the case of harmonic confinement

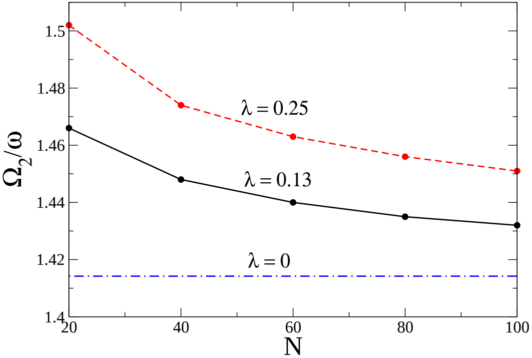
$$U(\mathbf{r}) = \frac{1}{2} m\omega^2 r^2 \tag{20}$$

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:

$$\Omega_0 = 2\omega \qquad \text{and} \qquad \Omega_1 = \omega \ , \tag{21}$$

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.

4. Generalized superfluid hydrodynamics (IV)



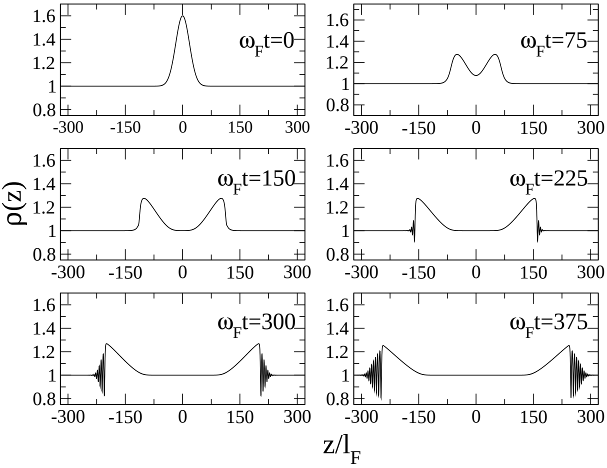
Quadrupole frequency Ω_2 of the unitary Fermi gas ($\xi = 0.455$) with N atoms under harmonic confinement of frequency ω. Three different values of the gradient coefficient λ. For $\lambda = 0$ (TF limit): $\Omega_2 = \sqrt{2}\omega$. [L.S., F. Ancilotto and F. Toigo, LPL **7**, 78 (2010).]

5. Shock waves (I)

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[11]
Here we investigate the formation and dynamics of shock waves in the unitary Fermi gas by using the zero-temperature equations of generalized superfluid hydrodynamics.

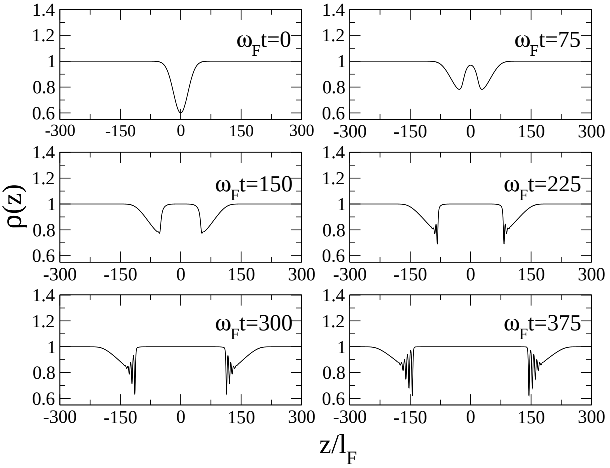
[11] L.D. Landau and E.M. Lifshitz, *Fluid Mechanics* (Pergamon Press, London, 1987); G.G. Whitham, *Linear and Nonlinear Waves* (Wiley, New York, 1974).

5. Shock waves (II)



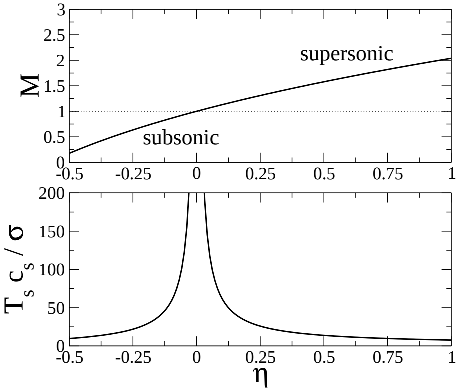
Time evolution of supersonic shock waves. Initial condition with $\sigma/l_F = 18$ and $\eta = 0.3$. The curves give the relative density profile $\rho(z)$ at subsequent frames, where $l_F = \sqrt{\hbar^2/(m\epsilon_F)}$ is the Fermi length and $\omega_F = \epsilon_F/\hbar$ is the Fermi frequency.

5. Shock waves (III)



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.

5. Shock waves (IV)



Properties of the shock waves. Upper panel: Mach number $M = v_{max}/c_s$ as a function of the amplitude η of the perturbation (solid line). Lower panel: period T_s of formation (breaking time) of the shock-wave front as a function of the amplitude η of the perturbation. T_s is in units of σ/c_s, where σ is the width of the perturbation and $c_s = \sqrt{\xi/3}v_F$ is the bulk speed of sound, with v_F the Fermi velocity.

Conclusions

- 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 generalized superfluid hydrodynamics can be applied to investigate collective modes of the unitary Fermi gas in a generic external potential $U(\mathbf{r})$.
- Also shock waves can be studied with our generalized superfluid hydrodynamics if $T \ll T_c$, with T_c the critical temperature of the superfluid-normal phase transition ($T_c \simeq 0.2\ T_F$, and $T_F \simeq 10^{-7}$ Kelvin for dilute alkali-metal atoms).