Study of a density functional for a unitary Fermi gas

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Abstract

In this thesis, following L. Salasnich and F. Toigo [Phys. Rev. A 78, 053626 (2008)] we use an extended Thomas-Fermi (TF) density functional to describe a gas of interacting fermions composed of an even number $N$ of particle in the unitary regime confined by a spherically symmetric harmonic trap. The great advantage in taking such a functional, relative to functionals based on single-fermion wave functions, is to depend only on the density number $n$ and on its derivatives, so that the numerical load is independent of the number of particles. By minimizing the ETF functional with respect to the density we obtain a time-independent non-linear Schrödinger equation which we solve using the imaginary time propagation method, by integrating numerically the corresponding time-dependent Schrödinger equation. We determine the two characteristic parameters of the functionals $\xi$ and $\lambda$ by fitting the Monte Carlo total energy data obtained by D. Blume et al. [Phys. Rev. Lett. 99, 233201 (2007)]. We obtain the values $\xi = 0.469$ and $\lambda = 0.082$ leading to a $\chi^2 = 42$. These values are to be compared with $\xi = 0.455$ and $\lambda = 0.13$, leading to a $\chi^2 = 282$ as proposed by Salasnich and Toigo. We also study the dependence of the ground-state density profile on the values of the two parameters, finding that $\xi$ enhances the width of the profile, while increasing $\lambda$ smooths out the outer boundary of the fermionic cloud.

Advisor: Dr. Nicola Manini
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1 Introduction

1.1 The unitary regime

Pauli’s exclusion principle imposes that the many-particles wave function of a system of fermions must be antisymmetric \[1\]. If the fermions were non-interacting this would imply that the \( N \) particles should occupy \( N \) different states. Even for interacting fermions at very low temperature, far below the Fermi temperature

\[ T_F = \frac{\hbar^2}{2mk_b}(3\pi^2n)^{2/3} \]  \hspace{1cm}(1)

(where \( m \) is the mass of the fermions, \( k_b \) the Boltzmann constant and \( n \) the density of fermions), the effects of quantum statistic are not negligible, as happens for the electrons in metals.

When the density of the two spin components are equal, and when the gas is dilute, i.e. the range of inter-atomic potential is much smaller than the interparticle distance, the interaction effects are described by only one parameter: the s-wave scattering length \( a_s \) \[2\]. The sign of \( a_s \) determines the character of the gas. If \( a_s < 0 \) the gas exhibits superfluidity at sufficiently low temperature, according to the theory of Bardeen, Cooper and Schrieffer, developed to explain superconductivity of electrons in metals at very low temperatures \[3\]. The main physical feature of the BCS regime is the formation of bound states, the Cooper pairs in \( k \)-space, characterized by a small binding energy. Instead if \( a_s > 0 \), under the same hypothesis of a dilute gas (|\( a_s k_F | \ll 1 \) and low temperature, bound dimers of fermions of different spin are formed in real space and consequently, being these dimers of spin 0, the system is transformed in a bosonic gas. In this situation the gas behaves as a Bose-Einstein condensate (BEC regime).

Physicists have found a way to use the phenomenon of Fano-Feshbach resonances to change the value and the sign of the scattering length, simply by tuning an external magnetic field. Near one such these resonance \( a_s \) changes as a function of the external field \( B \), according to

\[ a_s = a_{bg} \left( 1 - \frac{\Delta B}{B - B_0} \right), \]  \hspace{1cm}(2)

where \( a_{bg} \) is the background scattering length away from the resonance and \( \Delta B \) is the width of the resonance.

When \( B \simeq B_0 \) the scattering length diverges so that the gas display a very peculiar character, being at the same time dilute and strongly interacting. In this
regime all scales associated with interactions disappear from the problem and the
energy of the system is expected to be proportional to that of a non interacting
fermions system. This regime, placed in between the BCE and BCS regimes, is
called the \textit{unitary regime}.

\subsection*{1.2 The choice of the functional}

It has been suggested that the unitary Fermi gas at zero temperature can be
described approximately by the density functional theory (DFT). Different theo-
retical groups have proposed various density functionals. For example Bulgac and
Yu introduce a superfluid DFT based on a Bogoliubov-de Gennes approach to
superfluid fermions \cite{bulgac}. We follow Salasnich and Toigo \cite{salasnich} and adopte a functional
written only in terms of the fermions number density $n$ and its derivatives with
respect to position, the \textit{extended Thomas-Fermi functional} (ETF). The total en-
ergy in the ETF contains a term proportional to the kinetic energy of a uniform
non interacting gas of fermions, plus a term containing a gradient correction of
the form $\lambda \hbar^2/(8m)(\nabla n/n)^2$.

The main advantage of taking such a functional is the fact that, as it depends
only on a single function of the coordinates, there is no limitation in the number of
particles $N$ which it can treat. Other functionals, which take into account single-
particle states require self-consistent calculations whose numerical load increases
with $N$.

By fitting the Monte Carlo total energy data obtained recently \cite{monte-carlo}, we de-
terminate the optimal value of the two parameters which determine the ETF func-
tional: $\xi$, the scaling factor of the self-interaction term, and $\lambda$, the scaling factor
of the gradient term. In doing this we regard $\xi$ and $\lambda$ as free parameters.
2 The extended Thomas-Fermi model

For simplicity we take an even number of particles, in order to avoid in the functional the even/odd correction term accounting for the presence of an unpaired particle, and assume that the Fermi gas is confined in a spherically symmetric harmonic potential,

$$U(r) = \frac{1}{2}m\omega^2 r^2. \quad (3)$$

The TF energy functional is

$$E_{TF} = \int d^3r \, n(r) \left[ \epsilon(n(r)) + U(r) \right], \quad (4)$$

where \(\epsilon(n)\) is the energy per particle of a uniform Fermi gas with density \(n(r)\). The normalization condition is

$$N = \int d^3r \, n(r). \quad (5)$$

To find the ground state density profile of the system we have to minimize the functional \((4)\).

As said in the previous section in the unitary regime, because the scattering length diverges, no characteristic length is set by the interaction. The only length appearing in the functional is the average distance between particles, which is proportional to \(n^{-1/3}\). The energy per particle of the Fermi gas depends on \(n\), \(\hbar\) and \(m\), the mass of fermions. It is usually written as

$$\epsilon(n) = \xi \frac{3}{5} \frac{\hbar^2}{2m} \left( \frac{3\pi^2 n}{2} \right)^{2/3} = \xi \frac{3}{5} \epsilon_F, \quad (6)$$

where \(\xi\) is one of the two universal parameters we want to determine and \(\epsilon_F\) is the Fermi energy of a uniform non interacting fermionic gas of density \(n\) at zero temperature.

In order to take into account some of the effects of to the spatial variation of density, the TF functional has to be extended. As in Ref. [5], we add a correction term of the form

$$\lambda \frac{\hbar^2}{8m} \left( \frac{\nabla n}{n} \right)^2, \quad (7)$$

where \(\lambda\) is the second universal parameter we want to determine. This term may be considered as the first term in a gradient expansion.

The functional \((4)\) is then extended to

$$E_{ETF} = \int d^3r \, n(r) \left[ \epsilon_g(n(r), \nabla n(r)) + U(r) \right], \quad (8)$$
where
\[ \epsilon_g(n(r), \nabla n(r)) = \epsilon(n) + \lambda \frac{\hbar^2}{8m} \left( \frac{\nabla n}{n} \right)^2 \] (9)
is the energy per particle including the gradient correction.

By minimizing the functional (8) with the constraint (5) we derive the equation obeyed by the ground state density:
\[
\left[ -\lambda \frac{\hbar^2}{2m} \nabla^2 + \mu(n(r)) + U(r) \right] \sqrt{n(r)} = \bar{\mu} \sqrt{n(r)},
\] (10)
where \( \mu(n(r)) = \frac{\partial \epsilon(n(r))}{\partial n} \) is the bulk chemical potential of the non-uniform system and \( \bar{\mu} \) is the Lagrange multiplier fixed by the normalization (5). This is a nonlinear Schrödinger equation (NLSE) where \( \sqrt{n(r)} \) is the amplitude of the wave function \( \psi(r) \).
3 Technical implementation

3.1 Imaginary time propagation

To solve the time-independent NLSE (10) we use the imaginary time propagation (ITP) method [7]. This consists in taking the corresponding Schrödinger time-dependent equation

\[
-\frac{i\hbar}{2m} \nabla^2 + \mu(n(r)) + U(r) \psi(r,t) = i\hbar \frac{\partial \psi(r,t)}{\partial t} \tag{11}
\]

and integrating it in imaginary time \( \tau = it \). The formal solution of this equation could be written as

\[
\psi(r,\tau) = \psi(r,0)e^{-H\tau/\hbar} = a_0 \psi_0(r,0)e^{-E_0\tau/\hbar} + a_1 \psi_1(r,0)e^{-E_1\tau/\hbar} + \ldots \tag{12}
\]

where \( \psi_i \) and \( E_i \) are respectively the eigenstates and the eigenvalue of the Hamiltonian and

\[
a_i = \int d^3r \psi^*(r,0)\psi_i(r,0). \tag{13}
\]

Thus, by integrating Eq. (11) for a sufficiently large imaginary time, we obtain the ground state wave function, because exited components are exponentially filtered out. Note that as the Hamiltonian is time-dependent (through the density itself), Eqs. (12) and (13) have only an heuristic meaning.

3.2 The Crank-Nicolson method

We have integrated Eq. (11) using the Crank-Nicolson method, which is a finite difference method used to solve partial differential equations. This method is based on central difference in space, plus the trapezoidal rule in time. We assume the following convention: we use the apex and the subscript to indicate time and space intervals respectively, which the discretized wave function refers to. The Crank-Nicolson discretization of equation (11) is

\[
-h \frac{\psi_i^{n+1} - \psi_i^n}{\Delta t} = \frac{1}{2} \left( H_i(\psi_i^{n+1}) + H_i(\psi_i^n) \right) \tag{14}
\]

where

\[
H_i(\psi_i) = -\frac{\hbar^2}{2m} \left( \psi_{i+1} - 2\psi_i + \psi_{i-1} \right) + \frac{\psi_{i+1} - \psi_{i-1}}{\Delta r} + \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3} \psi_i^{7/3} + \frac{1}{2} m\omega^2 r_i^2 \psi_i. \tag{15}
\]
By moving the terms \( \psi^{n+1}_i, \psi^n_i \) and \( \psi^{n+1}_i \) to the left hand side of Eq. (15), and assuming for simplicity that \( \hbar, m \) and \( \omega \) are of unitary value, the system to solve is

\[
\psi^{n+1}_i + \frac{\Delta t}{2} \left[ -\frac{\lambda}{2} \left( \frac{\psi^{n+1}_{i+1} - 2\psi^{n+1}_i + \psi^{n+1}_{i-1}}{\Delta r^2} + \frac{\psi^n_{i+1} - \psi^n_{i-1}}{r_i \Delta r} \right) \right] + \varepsilon \sqrt{N} (3\pi^2 n)^{2/3} (\psi^{n+1}_i)^{7/3} + \frac{1}{2} \frac{E^2}{r_i \Delta r} \psi^n_i = \psi^n_i - \frac{\Delta t}{2} \left[ -\frac{\lambda}{2} \left( \frac{\psi^n_{i+1} - 2\psi^n_i + \psi^n_{i-1}}{\Delta r^2} + \frac{\psi^n_{i+1} - \psi^n_{i-1}}{r_i \Delta r} \right) \right] + \varepsilon \sqrt{N} (3\pi^2 n)^{2/3} (\psi^n_i)^{7/3} + \frac{1}{2} \frac{E^2}{r_i \Delta r} \psi^n_i \]

Its linear part in \( \psi^n_i \) may be written in a matrix form as

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\psi^n_i \\
\psi^n_{i+1} \end{bmatrix} = \begin{bmatrix}
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\]

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\begin{bmatrix}
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\vdots \\
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\psi^{n+1}_{i+1} \\
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\psi^n_i \\
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\psi^n_{i+1} \end{bmatrix} = \begin{bmatrix}
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\]

It is easy to see that both matrices are tridiagonal, so it is convenient to use specific algorithms to treat them, which have the advantage to require \( O(N) \) operations instead of \( O(N^3) \) for complete matrices. At each time step the nonlinear term is added to both matrices and the system is solved by solving a linear system of equations. We take for initial wave function a Gaussian or, when available, a ground state wave function computed for similar values of the parameters \( \xi, \lambda \) and the number of particles \( N \). To use a \( \psi \) averaged over the time step in the nonlinear term, and not evaluated at the beginning of the step, we use a predictor-corrector scheme, as done in [S]. This means that each integration step is done twice using at first \( \psi(r, t) \), obtaining \( \tilde{\psi}(r, t + \delta t) \) and then \( \frac{1}{2} [\psi(r, t) + \tilde{\psi}(r, t + \delta t)] \).

We have take significant care to the choice of the size of the spatial and temporal intervals. Indeed too large intervals may have negative effect on the precision of results, but on the other hand too small intervals require a large number of steps and consequently a pointless growth of the computation time. We have adopted this strategy: to check the variation of the total energy and of the values of the wave functions after widening the temporal and spatial intervals.
We have seen for example that in the passage from 0.001 to 0.01 natural units $\omega^{-1}$ of the time intervals the ground state energy changes of the order of $10^{-6}$, while from to 0.01 to 0.05 it becomes ten times larger, indicating poor convergence. Eventually we have settled for a time step of 0.005. We do not fix the total number of time steps but we let the integration continue until the discrepancy between the energy of two successive steps is smaller than $10^{-10}$ natural units $\hbar\omega$. For the radial discretization, we have first fixed the upper limit of integration to 4 natural units $a_h = \sqrt{\hbar/(m\omega)}$, by checking that the wave function $|\psi|$ is smaller than $10^{-5}$ natural units $a_h^{-3/2}$ at a distance of 1 from the boundary for every reasonable value of the parameters. We have fixed the radial and temporal intervals width at 0.008 and 0.01 respectively.

### 3.3 The downhill simplex method

We have fitted the Monte Carlo data of [6] by minimizing the function

$$
\chi^2(\xi, \lambda) = \sum_N \left( \frac{GSE(\xi, \lambda N) - GSE_{MC}(N)}{\delta GSE_{MC}(N)} \right)^2
$$

(18)

where $GSE(\xi, \lambda N)$ are the ground state energies we have computed, $GSE_{MC}(N)$ are MC total energy data and $\delta GSE_{MC}(N)$ the statistical MC error bars on each of them. To minimize the function $\chi^2(\xi, \lambda)$ we used the downhill simplex method, which is not very efficient in terms of the number of function evaluations but has the advantage of requiring only evaluations of $\chi^2$ and not its derivatives [9]. The method is based on deformations of simplex, which is a special polytope of $d+1$ vertices in $d$ dimensions (in our case a triangle as the number of parameters is $d = 2$). Given an initial simplex, in each step the algorithm can (i) replace one of the points reflecting the simplex with respect to the others points or (ii) expand or contract the simplex, depending on the evaluations of the function at its vertices.
4 Results

4.1 Fit of Monte Carlo energies

Before doing the minimization of function (18) it is useful to evaluate it on a grid of 30 x 30 points in order to have evidence of the existence of a minimum and information on its eventual location. We see in Fig. 1 that the function has a rotated paraboloid form. Along the bottom of the rather flat valley $\chi^2$ varies of the order of unit from its minimum, while perpendicularly from the valley, the variation is much more important.

Using the downhill simplex method explained above we have obtained as best fit $\xi = 0.469$ and $\lambda = 0.082$. Figure 2 locates this minimum in the $(\xi, \lambda)$ plane where also a few contour lines of $\chi^2$ are drawn. A second arrow indicates the position of the estimate of Salasnich and Toigo in Ref. [5], namely $\xi = 0.455$
The discrepancy $\chi^2(\xi, \lambda)$ represented in the plane $(\xi, \lambda)$ by means of contour lines (at 50, 100, 200, 400, 1000, 2000). The two arrows indicate the position of our best fit point, where $\chi^2(0.469, 0.082) = 41.97$ and that of parameters of Ref. [5], where $\chi^2(0.455, 0.13) = 281.76$.

and $\lambda = 0.13$. Table I reports the fitted MC ground-state energies [6], and those computed by using ETF theory based on the parameter values obtained by Salasnich and those obtained by our best fit. Figure 3 compares the ETF energies per particle computed with our best fit values of the parameters and the MC data indicated with their error bars. We see that compatibility of the fit does not deteriorate as $N$ increases. Figure 4 reports the curves of ETF energies per particle for varied value of $\xi$. The valley of Fig. 1 has a linear slope, so that it is possible to obtain a relation between the value of one parameter and the value of the other that gives the best fit. The relation is $\lambda = 1.027 - 2.014\xi$. 
<table>
<thead>
<tr>
<th>$N$</th>
<th>MC data</th>
<th>ETF (parameters as in [5])</th>
<th>ETF (best fit parameters)</th>
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<td>30</td>
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<td>70.51</td>
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</tr>
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</table>

Table 1: Total ground-state energies of droplets of fermions trapped in a spherical harmonic trap computed according to different approximations.
4.2 Ground states density profiles

In the present section we compare the ETF ground-state wave functions with those obtained by the authors of Ref. [6] with MC simulations. In Figs. 5, 6, 7, 8 we compare the MC density profiles of Ref. [6], those reported in Ref. [4] with a superfluid local density approximation (SLDA) theory, and those computed with ETF theory using the estimate of Ref. [5] and our best fit results, for a few sizes of the cluster. We see clearly that for small $N$ ETF profiles are quite different from the MC one and that the SLDA profile is closer to it. This is not surprising, since for small $N$ one does expect important shell effects. For larger $N$ the discrepancy between the profiles tends to decrease, thus for $N = 20$ the SLDA theory show no significant advantage. It would be interesting to have MC data for a Fermi droplet with $N$ of the order of hundreds to check the validity of the ETF approximation which should become even better for $N$ of such magnitude.

It is useful to check how the ETF ground state density profiles change when the values of the two parameters $\xi$ and $\lambda$ are moved away from their optimal value. We do this by computing the density profiles keeping fixed one parameter
Figure 4: Same as Fig. 3 including ETF energies per particle computed for varied value of $\xi$ and $\lambda = 0.082$ (best fit).
Figure 5: Ground-state density profiles for $N = 4$.

Figure 6: Ground-state density profiles for $N = 8$. 
Figure 7: Ground-state density profiles for $N = 14$.

Figure 8: Ground-state density profiles for $N = 20$. 
and let the other one change. We do this for a small $N = 8$ and for a larger $N = 50$.

It is clear from Figs. 9 and 10 that increasing the value of $\xi$ the density profile broadens. This behaviour is independent of the number of fermions. Figure 11 shows that the value of the coefficient $\lambda$ of the gradient correction affects the density profile of the fermionic gas mainly in the way it approaches its boundary. A small value of $\lambda$ yields the TF approximation, with a sharp boundary of the droplet. The larger the value of $\lambda$ the slower the density goes to zero.
Figure 10: Same as Fig. 9 but for 50 fermions.

Figure 11: Ground-state density profiles of a gas of 8 fermions for varied $\lambda$, and fixed $\xi = 0.469$. Inset: a blowup of the boundary region.
References


