Suppression of Superfluidity upon Overflow of Trapped Fermions. Quantal and Thomas-Fermi Studies

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Abstract. Two issues will be discussed in this contribution: (i) the generic fact that if a fermionic superfluid in the BCS regime overflows from a narrow container into a much wider one, pairing is much suppressed at the overflow point. Two examples pertinent to the physics of the outer crust of neutron stars and superfluid fermionic atoms in traps will be presented. (ii) A novel Thomas-Fermi approach to inhomogeneous superfluid Fermi-systems is presented and shown that it works well in cases where the local density approximation breaks down.

1. Introduction

Superfluid fermions in finite systems can exist in traps of cold atoms, in nuclear systems, in small metallic clusters, etc. An interesting question arises what happens to the superfluid if its Fermi level reaches the edge of a finite container, i.e. either the fluid overflows into the continuum or it pours into another container of much larger dimension. A trapping potential of this type has experimentally already been generated for the study of cold bosonic atoms [1]. It should also be possible to use it for fermionic atoms [2].

In the inner crust of neutron stars, there also may occur the situation where coexists a superfluid neutron gas of variable density in between the lattice of (superfluid) nuclei [3, 4]. This situation often is mimicked by a Wigner-Seitz cell, where the single particle (self-consistent) potential has a pocket, representing the nucleus, embedded in a large container. Of course, finite nuclei at the neutron drip line also constitute cases of this category but, as we will see, the situation there is not so clear due to strong shell effects. Still other systems may exist with similar situations.

The purpose of this work is to study superfluidity of fermions at the overflow (drip) in the BCS regime. Since the quantal solution of BCS equations in geometries with rapidly varying single particle potentials with a large number of particles is numerically difficult, we will present, as a second objective of this work, a Thomas-Fermi (TF) approach to inhomogeneous superfluidity which shows good performance in situations where the local density approximation (LDA) fails.
For our study we first will consider a schematic model of slab geometry with a transverse potential of large extension $L$ possessing at the origin a ‘pocket’ of variable depth and size $R$ much smaller than the outer container. Schematically such a potential is shown in Fig. 1. This slab configuration may roughly mock up one sheet of a so-called Lasagne configuration in the inner crust of neutron stars [5]. We, therefore, will use nuclear dimensions for the slab model but they can easily be replaced by dimensions relevant for other systems. Our model and the ensuing generalisations treated below, therefore, are believed to be generic. We will study the slab configuration also because the quantal solution of the gap equation is evaluated relatively directly and the quality of the TF approach can thus be established. Once this is achieved, we also will go over to other geometrical configurations. We, for instance, will treat a second potential, shown below in Fig. 4, left panel, with spherical symmetry, a kind of which, as already mentioned, has been used for bosonic atoms in [1].

2. The formalism
Let us start out with writing down the usual BCS equations in three dimensions.

$$\Delta_\nu = -\sum_{\nu'} V_{\nu,\nu'} \frac{\Delta_{\nu'}}{2\sqrt{(\varepsilon_{\nu'} - \mu)^2 + \Delta_{\nu'}^2}}, \quad (1)$$

where the $\varepsilon_{\nu'}$’s are the single particle energies and $\mu$ the chemical potential which can be used to fix the particle number $N = \sum_\nu n_\nu$ with

$$n_\nu = \frac{1}{2} \left[ 1 - \frac{\varepsilon_\nu - \mu}{\sqrt{(\varepsilon_\nu - \mu)^2 + \Delta_\nu^2}} \right]. \quad (2)$$

The wave functions and eigenenergies of a box as shown in Fig. 1a with a potential-hole are given in [6]. For pairing, we use a contact force with a cut off $\Lambda$, to make things simple. The single particle states in a slab configuration then become $|\nu\rangle = |n, p\rangle$ where $n$ are the discrete quantum numbers in transverse direction and $p$ the momentum quantum numbers in slab direction. Integrating over momenta in slab direction the above gap equation

$$\Delta_n = -\sum_{n'} \int \frac{d^2 p}{(2\pi\hbar)^2} V_{nn'} \Theta(\Lambda - \varepsilon_{n'} - \varepsilon_p) \frac{\Delta_{n'}}{2E_{n'}(p)}, \quad (3)$$
with \( E_n(p) = \sqrt{(\varepsilon_n + \varepsilon_p - \mu)^2 + \Delta_n^2} \) the quasiparticle energy, \( \Theta(x) \) the step function, and \( \varepsilon_n, \varepsilon_p \) being the discrete single particle energies in transverse direction and kinetic energies in slab direction, respectively. After performing the integral, one arrives at the following gap equation

\[
\Delta_n = -\sum_{n'} \Theta(\Lambda - \varepsilon_{n'}) V_{nn'} K_{n'}. \quad (4)
\]

The pairing tensor in equation (4) is then given by

\[
K_n = \frac{m}{4\pi \hbar^2} \Delta_n \ln \frac{\Lambda - \mu + \sqrt{(\Lambda - \mu)^2 + \Delta_n^2}}{\varepsilon_n - \mu + \sqrt{(\varepsilon_n - \mu)^2 + \Delta_n^2}} \quad (5)
\]

where \( m \) is the particle mass and the indices \( n \) stand for the level quantum numbers in the confining potential of Fig. 1a. The matrix elements \( V_{nn'} = -g \int_{-L}^{+L} |\varphi_n(z)|^2 |\varphi_{n'}(z)|^2 dz \) of the contact force \(-g\delta(r-r')\) can be evaluated straightforwardly from the wave functions \( \varphi_n(z) \) given in [6].

For an example we take as cut off \( \Lambda = 50 \, \text{MeV} \) counted from the edge of the pocket potential whose depth be \( V_0 = -40 \, \text{MeV} \). Its extension ranges from \(-R\) to \(+R\) with \( R = 10 \, \text{fm} \). The wide potential with infinite walls has extension from \(-L\) to \(+L\) with \( L = 100 \, \text{fm} \). For the coupling strength we take \( g = 150 \, \text{MeV fm}^3 \). The numerical values for \( \Lambda \) and \( g \) yield maximum gap values around 1 MeV, typical for nuclear systems.

Before we show the results, let us explain our Thomas-Fermi (TF) approach for this problem. In the weak coupling regime, we have \( \Delta/\mu << 1 \). In this case the canonical basis can be replaced by the Hartree-Fock or mean-field one:

\[
H|n\rangle = \varepsilon_n|n\rangle. \quad (6)
\]

At equilibrium and for time reversal invariant systems canonical conjugation and time reversal operation are related by

\[
(r|\bar{n}) = \langle n|r \rangle \Rightarrow (r_1 r_2|n\bar{n}) = \langle r_1 |\hat{\rho}_{n}|r_2 \rangle, \quad (7)
\]

with \( \hat{\rho}_n = |n\rangle \langle n| \). For the pairing matrix element, we, therefore, can write
\begin{equation}
V_{nn'} = \langle n \bar{n} | v | n' \bar{n}' \rangle = \int \langle \mathbf{r}_2 | \tilde{\rho}_n | \mathbf{r}_1 \rangle \langle \mathbf{r}_1' \mathbf{r}_2' | v | \mathbf{r}_1' | \tilde{\rho}_{n'} | \mathbf{r}_2' \rangle d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_1' d\mathbf{r}_2'.
\end{equation}

The Schroedinger equation (6) can be written in terms of \( \tilde{\rho}_n \) as
\begin{equation}
(H - \epsilon_n) \tilde{\rho}_n = 0.
\end{equation}

Taking the Wigner transform of this latter equation, we obtain in the \( h \to 0 \) limit the following c-number equation: \((H_{cl} - \epsilon)f_c(\mathbf{R}, \mathbf{p}) = 0\). The solution of this equation in the sense of distribution theory is with \( x\delta(x) = 0 \) given by
\begin{equation}
f_E(\mathbf{R}, \mathbf{p}) = \frac{1}{g^{TF}(E)} \delta(E - H_{cl}) + O(h^2).
\end{equation}

with
\begin{equation}
H_{cl} = \frac{p^2}{2m^2(\mathbf{R})} + V(\mathbf{R}) \quad \text{and} \quad g^{TF}(E) = \frac{1}{(2\pi \hbar)^3} \int d\mathbf{R} dp \delta(E - H_{cl}).
\end{equation}

Equation (10) means that the phase space distribution corresponding to a state \( |n \rangle \) at high energy is concentrated around the classical energy shell what, indeed, is a well known fact.

The TF version of the gap equation (4) then reads
\begin{equation}
\Delta(E) = - \int_{V_0} A dE' g(E') V(E, E') K(E') \tag{12}
\end{equation}

with \( K(E) \) an obvious generalisation of \( K_n \). The matrix elements \( V(E, E') \) can be evaluated in replacing \( |\varphi_n(z)|^2 \) by [7]
\begin{equation}
\rho^{TF}_E(z) = \int \frac{dp}{2\pi \hbar} f_E(z, p) = \frac{1}{g^{TF}(E)} \frac{1}{2\pi} \left( \frac{2m}{\hbar^2} \right)^{1/2} [E - V(z)]^{-1/2},
\end{equation}

which is the on-shell TF density in transverse direction (please note that we are in a 1D case here, contrary to what is treated above where it is 3D). As the reader will easily realise, the way of proceeding is very different from usual LDA where the finite size dependence is put into the (local) chemical potential, \( \mu(z) = \mu - V(z) \), whereas here it is put into the matrix elements of the pairing force.

3. Results

We are now in a position to solve the quantal and TF gap equations for the above mentioned parameter values of our model. The result for the gap at the chemical potential \( \mu \) is shown in Fig. 2 as a function of \( \mu \). We start with \( \mu \) from the bottom of the pocket well, i.e. with zero density. We then increase \( \mu \), i.e. the density. We see that once the fill up of the pocket reaches its top, the values of the gap sharply drop and practically reach zero. In the continuum the gaps slowly rise again. We see that quantal and TF values are in close agreement.

Before we come to an explanation of the drop of the gaps at overflow (drip), let us study the gaps as a function of position in transverse direction: \( \Delta(z) = -gK(z) \) with \( K(z) = \sum N_n |\varphi_n(z)|^2 \). Semiclassically, this expression becomes:
\begin{equation}
K(z) = \int_{V_0} A dE g^{TF}(E) K(E) \rho^{TF}_E(z). \tag{14}
\end{equation}

In Fig. 3, left panel, we show the gap profiles for three values of \( \mu \): \( \mu = 40, 0.5, \) and -5 MeV. We see that quantal and TF results agree, up to shell fluctuations, very well. We also show the
Figure 3. (Coloronline) Left panel: Position dependence of the gap in the slab geometry for different values of the chemical potential. Quantal, TF, and LDA results are shown. Notice that $\Delta$ for $\mu = 0.5$ and $-5.0$ MeV is practically zero in the gas region. Right panel: Comparison of quantal (dots) and TF (broken lines) values of the pairing tensor $K$.

Figure 4. (Coloronline) Average TF gaps at the Fermi energy as a function of the chemical potential (right panel) for the potential shown in the left panel. In the completely filled optical trap ($\mu = U$) we accommodate $10^5$ atoms in each spin state. The total number of atoms in the trap with $\mu/\hbar\omega_{opt}=40, 80$ and $120$ are indicated in the upper horizontal axis.

LDA results. They can be as wrong as by 50 percent. For other choices of system parameters the LDA error may even be worse. This stems from the fact that in TF (and, of course, also quantally), there is coupling between inside and outside the pocket, i.e. the Cooper pair wave function extends into both regions what tends to equilibrate the values of the gaps. In LDA the contrast is much too strong. The drop of the gaps when crossing the threshold can be explained by the fact that the single particle states are strongly delocalised in the outer container and, thus, their contribution to the pairing matrix element $V_{n,n'}$ becomes very small. In right panel of Fig. 3, we show the quantal and TF pairing tensors, $K_n$ and $K(E)$, defined in (4), (5), and (12), respectively. We emphasize the close agreement between quantal and TF results.

Having gained faith into our TF approach, we now can explore other geometries and other systems, which are more difficult for quantal solutions. In Fig. 4 we show the result for $\Delta$ in the spherical double harmonic oscillator potential which may be realised with cold fermionic atoms.
to study the overflow situation. A zero range force with strength $g=-1.0$ and cut off $\Lambda=164.34$ (in the corresponding optical trap units with $\omega_{\text{opt}} = 2\pi \times 1000$ Hz taken from [2]) is used. We see that the result is qualitatively similar to the slab case, though in this spherical geometry the dip does not quite reach zero and also is shifted slightly to an energy above the break of the potential. Note that this depends strongly on the choice of the ratio $\omega_{\text{mag}}/\omega_{\text{opt}}$ as it can be seen in the figure. Also the gap starts to decrease towards the minimum quite early. This is contrary to what happens in the slab case where the change is very abrupt, the reason probably lying in the spherical symmetry of the considered system. It could be interesting to see whether our prediction can be verified experimentally. We should emphasise that the spherical case has been chosen here for convenience. Nothing essential will, however, change with other geometries, like they are more often realised for trapping potentials with cold atoms.

Let us now make a more realistic study of Wigner-Seitz (WS) cells including electrons in $\beta$ equilibrium to simulate the inner crust of neutron stars [5]. The mean-field, as explained in [11],

Figure 5. (Coloronline) Binding energies per particle as a function of average density in a Wigner-Seitz cell. Red dots indicate quantal Skyrme HF calculations by Negele-Vautherin and black dots correspond to semiclassical results with the variational Wigner-Kirkwood (VWK) method and the Gogny D1S force.

Figure 6. (Coloronline) Left panel: Radial dependence of the TF gap in the considered WS cells. The end points indicate the radius of the WS cells. Right panel: Comparison between TF and LDA gaps as a function of the position in a WS cell containing a single $^{500}_{40}$Zr nucleus.
is computed selfconsistently using the BCP energy density functional [10] together with the TF approach.

The semiclassical description of the WS cells including pairing correlations at TF level is obtained from this mean-field using the finite range part of the Gogny D1S force [12] in the pairing channel [13]. It must be pointed out that the total energy per baryon obtained with our TF approach is in very good agreement with the old quantal calculation of Negele and Vautherin [14], as it is explicitly discussed in Ref.[11] and again shown here in Fig. 5. In the left panel of Fig. 6, we display the radial dependences of the gaps in some selected Wigner-Seitz cells. It is seen that when the gap is small outside the region of the nucleus, then the gap also is small inside the nucleus. This stems from the very large coherence length where one neutron of a Cooper pair can be in the huge volume of the gas and the other inside the small volume of the nucleus. In this way the gas imprints its behavior for the gap also inside the nucleus. Such a conclusion was also given in a quantal Hartree-Fock-Bogoliubov (HFB) calculation by Grasso et al. in [15] what shows that the here employed BCS approximation apparently yields very similar answers as a full HFB calculation for WS cells [3, 16]. Finally, in the right panel of Fig. 6, we show a comparison of LDA and present TF results for the gaps in a particular WS cell. We see a huge difference in the surface region of the nucleus. This simply stems from the fact that in this case of the $^{500}_{40}$Zr nucleus in the WS cell the gap is very small and, therefore, the coherence length very large invalidating LDA. A study with examples a little less unfavorable for LDA is given in [17]. We also show in Fig. 7 the gaps for several WS cells including some which correspond to the outer crust where all neutrons are bound. Again we see that the gap practically vanishes at zero chemical potential when the neutrons start to drip.

For isolated nuclei at the neutron drip the difference between HFB and BCS approaches may be more significant. Also strong shell fluctuations surely play an important role. Somewhat conflicting results in this respect exist in the literature. In ref [18] very similar results to ours are found for $S$-wave pairing, see Fig. 8. On the other hand in [19] the gap seems to rise towards the drip before it bends down. Similar results have recently been found in [20]. However, very small Oxygen isotopes have been considered in [19] and [20] where shell fluctuations may be dominant. The HFB calculation of Hamamoto has recently been repeated and extended passing from negative chemical potentials to positive ones and it was found that the $S$-wave gap of Fig. 8 clearly continues down to zero, touching zero at a slightly positive value of $\mu$ [21]. In explaining why in other works the gap is rising towards the drip, one has to keep in mind that an average gap should be calculated with the pairing tensor and not with the density matrix. The latter picks up the gaps at all energies which may not be small at all, even though the gap at the Fermi level is very small, see Fig. 2. On the other hand, an average with the pairing tensor only picks up the gaps around the Fermi level. It also is intuitively clear that for other than $S$-wave (i.e. $l > 0$) gaps the situation will be different, see Fig. 8 and [18]. This is due to resonant states below the centrifugal barrier with wave function concentrated on the domain of the nucleus. In situations where the resonant states are sufficiently close to the Fermi level, so that they can contribute to pairing, $l > 0$ gaps will exist also at positive energies. This remark also holds for spherical nuclei in WS cells, since, as we have seen, the gas couples very little with states belonging to the nucleus. Therefore, our results of above for nuclei in WS cells are only valid for $S$-wave pairing or for cases where the resonance states under the centrifugal barrier are almost not contributing to pairing. For deformed nuclei, the situation of resonant states in the continuum is less clear and depends on the magnitude of the deformation. For one dimensional systems, as the slab considered above, the situation will be like with $S$-waves, since in 1D there is no centrifugal barrier.
4. Summary

Summarizing, we have studied superfluid fermions in a large container, either external (cold atoms) or created self consistently (nuclei) for situations where the top of the fluid reaches the edge of a small pocket located at the origin of the wide confining potential. The gap drops to zero at the edge before rising again when the density fills up the outer container. This at first somewhat surprising phenomenon can be explained quite straightforwardly. Such situations, as already mentioned, can exist in cold atoms and nuclei in the inner crust of neutron stars, two examples treated here with their specific form of containers. For small systems, like isolated nuclei at the neutron drip, the situation may be blurred by shell effects.

As an important second aspect of this work, we showed that a novel Thomas-Fermi approach to inhomogeneous situations can cope with situations where LDA fails. This means that our TF approach is free of the restrictive condition, prevailing for LDA, that the Cooper pair coherence
length must be shorter than a typical length $l$ (the oscillator length in the case of a harmonic container) over which the mean field varies appreciably. On the contrary, our TF theory has the usual TF validity criterion, namely that local wavelengths must be shorter than $l$.

The accuracy of our TF approach opens wide perspectives for a treatment of inhomogeneous superfluid Fermi-systems with a great number of particles not accessible for a quantal solution of the BCS (HFB) equations. Such systems may be cold atoms in deformed containers (eventually reaching millions of particles), superfluid-normal fluid (SN) interfaces, vortex profiles, etc. As a matter of fact, as is well known [9], the TF approach becomes the more accurate, the larger the system. Thus the TF approximation is complementary to the quantal one in the sense that the former works where the latter is difficult or even impossible to be obtained numerically.

Part of this work has in the meantime been published in [22].

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