Breakdown of the Thomas-Fermi approximation for polarized Fermi gases

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We use Bogoliubov de-Gennes theory to show that the commonly used Thomas-Fermi approximation (TFA) can fail in describing polarized unitary gases in anisotropic harmonic traps. We find a magnetized superfluid region inside the trap, with order parameter oscillations, even though there is no such stable bulk phase. This leads to magnetization profiles that deviate from contours of constant potential energy. We determine how this violation scales with trap anisotropy and number of particles, and show that we are able to account for important differences between the MIT and Rice experiments.

The study of strongly interacting Fermi systems using ultracold atomic gases has attracted interest across the physics community. The phenomena observed in these dilute gases are expected to shed light on systems as diverse as high Tc superconductors, quark-gluon plasmas and quantum chromodynamics. The great virtue of atomic gases is the tunability of interactions using a Feshbach resonance so that the entire BCS to BEC crossover can be studied, with the most strongly interacting, unitary regime in-between these two limits. A series of beautiful experiments have probed condensation of fermionic pairs, pairing gaps, quantized vortices and the thermodynamics of the crossover. A particularly exciting new direction is the study of partially polarized gases with an imbalance in the number of up and down ‘spin’ fermions.

An important aspect of cold atom experiments is the presence of a harmonic trap. A “local density” or Thomas-Fermi approximation (TFA) has usually been adequate to take this into account. The TFA asserts that the properties at point $r$ in a ‘slowly varying’ potential are the same as those of the uniform gas at a chemical potential $\mu_r(r) = \mu_0 - V(r)$ with $\sigma = \uparrow$, $\downarrow$. This leads to the simple result that the spatial dependence of any observable must follow contours of constant trapping potential, which is directly testable for the densities $n_\sigma(r)$.

The two experiments on polarized, unitary Fermi gases find rather different results with respect to the TFA. The MIT group, with a large number of atoms $N = 10^7$ and a small trap anisotropy $1/\alpha = \omega_r/\omega_z \approx 5$, finds that the densities follow contours of $V(r)$. On the other hand, the Rice group, with smaller $N = 10^5$ and larger anisotropy $1/\alpha \approx 50$ observes gross violations of the equipotential contour condition for the densities.

Motivated by this, we have investigated the validity of the TFA using $T = 0$ Bogoliubov-deGennes (BdG) calculations and scaling arguments for the unitary gas in anisotropic, three dimensional traps with polarization up to 40%. Our main results are:

1. The TFA is always violated in a trap in so far as the spatial variation of the order parameter is concerned. Between the unpolarized superfluid at the center and the fully polarized normal gas at the edges of the trap, there is an intermediate region which is a magnetized superfluid with an FFLO-like oscillation of the order parameter. We emphasize that there is no corresponding stable phase for the uniform system.

2. We find that the size of the magnetized superfluid region depends on both polarization and anisotropy and can be much larger than $k_F^{-1}$ for large anisotropy.

3. The violation of the equipotential contour criterion for the magnetization $m(r) = n_\uparrow(r) - n_\downarrow(r)$ increases with increasing anisotropy $1/\alpha$, but decreases with increasing total number of particles $N = N_\uparrow + N_\downarrow$.

4. We derive a simple condition for the consistency of the TFA: $\delta \mu / \omega_r = (N\alpha)^{1/3} f(P) \gg 1$, where $f$ is a function of the polarization $P = (N_\uparrow - N_\downarrow) / N$. We use this $(N\alpha)^{1/3}$ scaling of $\delta \mu / \omega_r$ to get a better understanding of the $N$ and $\alpha$ dependences of our BdG results.

5. We are thus able to account for the differences between the MIT and Rice experiments with respect to the question of when the magnetization should or should not follow contours of constant potential at $T = 0$.

6. A general implication of our results is that the TFA based on the bulk phase diagram must be used with caution to describe a system in a trap when there are several competing phases.

**Bogoliubov-deGennes equations:** Our approach to the problem of strongly interacting, polarized Fermi gases in anisotropic traps is to solve the Bogoliubov-deGennes (BdG) equations. This is the simplest approach which goes beyond the TFA and is a generalization of the BCS-Leggett mean field theory for a spatially inhomogeneous gas. This method has been applied to the study of vortices in the strongly interacting regime, as well as the study of polarized gases in isotropic traps. For a single-channel description valid for the experimentally-relevant wide resonance, the Hamiltonian density for the polarized gas is

$$H(r) = \sum_\sigma \langle \Psi_\sigma | (H_0(r) - \mu_\sigma) \Psi_\sigma | r \rangle - g \langle \Psi_\uparrow | \Psi_\downarrow \Psi_\downarrow \Psi_\uparrow | r \rangle,$$

where $H_0 = -\nabla^2 / 2m + V(r)$, $m$ is the fermion mass and we set $\hbar = 1$. The trapping potential is $V(r) = \frac{1}{2} m \omega_0^2 (r^2 + \alpha^2 z^2)$, where we use cylindrical coordinates.
The wavefunctions in terms of the eigenfunctions of the BdG equations \[ H^{(\ell)} = \begin{pmatrix} T^{(\ell)} & \Delta^{(\ell)} \\ \Delta^{(\ell)} & -T^{(\ell)} \end{pmatrix}, \] where $T_{nn''pp'} = \epsilon_{np} \delta_{nn''} \delta_{pp'}$ and
\[
\Delta^{(\ell)}_{nn''pp'} = \int_0^\infty r^2 dr \int_{-\infty}^\infty dz f_{p\ell}(r) f_{p'\ell}(r) g_n(z) g_{n'}(z) \Delta(r, z)
\]
Since $\Delta(r, z) = \Delta(r, -z)$, the only non-zero matrix elements of $\Delta_{nn''pp'}$ correspond to even $n + n'$.

The mean field state is found through the solution of the BdG equations \[ \text{BdG equations} \ [15] \]

The solution of these equations is simplified if we express
\[
\Delta^{(\ell)} = \frac{\epsilon_q}{2} \int_0^\infty r^2 dr \int_{-\infty}^\infty dz f_{p\ell}(r) f_{p'\ell}(r) g_n(z) g_{n'}(z) \Delta(r, z)
\]

We now discuss the self-consistent solution of the BdG equations as a function of total $N = N_1 + N_1$, polarization $P = (N_1 - N_1)/N$ and trap anisotropy $1/\alpha$ at unitarity ($a_s = \infty$). We have extensively studied the problem for $N$ up to 2500 particles, $0 \leq P \leq 0.4$ and $\alpha = 1, 1/2, 1/4$. In Fig. 1(A) we plot the majority ($n_1$) and minority ($n_1$) densities along the $z$ axis for a representative data set ($\alpha = 1/4$, $N = 865$ and polarization $P = 30\%$). In Fig. 1(B) we plot the corresponding magnetization $m(r) = n_1 - n_1$ together with the local order parameter $\Delta(r)$. In both panels the solid lines are BdG results, while dashed lines are TFA predictions (using the bulk phase diagram \[12\] as input).

Both the BdG and TFA results show an unpolarized superfluid at the center of the trap and a fully polarized normal gas at the edge. There is a marked decrease in the BdG central density relative to TFA, with a redistribution of minority atoms to an intermediate region. The main difference between BdG and TFA is precisely in this intermediate region. Within the TFA there is a discontinuous jump in the order parameter which is smoothed out in the BdG solution since this lowers the gradient energy. What is perhaps unexpected is that the decaying BdG order parameter exhibits oscillations, similar to those expected in a putative FLL phase \[12\] with a period roughly consistent with $2\pi/(k_F - k_F)$ (where $k_F$ are the local Fermi wavevectors). Irrespective of the importance (or otherwise) of the limited number of rather small amplitude oscillations, it is unambiguous that this intermediate region is a magnetized superfluid: it has both a non-vanishing superfluid order parameter and a non-zero magnetization.

We note that the magnetized region that we see is completely different from a partially polarized normal region. The latter, though barely visible, is present in the TFA results of Fig. 1(A) and derives from the partially polarized normal phase which exists for a small range of $\mu/h$ in

\[
\Delta(n) = g \sum_{E_i > \mu} u_i(r)v_i^*(r), \]
\[
m(r) = \sum_{0 < E_i < \mu} (|u_i(r)|^2 + |v_i(r)|^2), \]
\[
n(r) = m(r) + \sum_{E_i > \mu} 2|v_i(r)|^2. \]

These equations are solved self-consistently for $\Delta(r), \mu$ and $h$ using the constraints that the total number of particles is $N = \int d^3r n(r)$ and the polarization $P = \int d^3r m(r)$.

The solution of these equations is simplified if we expand the wavefunctions in terms of the eigenfunctions of the diagonal piece $H_0(r) - \mu$. Measuring lengths in units of the radial harmonic oscillator length $a_0 = 1/\sqrt{\omega_0}$ and energies in units of $\omega_0$, these functions are $\phi_{np} = f_{p\ell}(r) \exp(i\theta) g_n(z)/\sqrt{2\pi}$, where the radial and axial functions are related to associated Laguerre and Hermite polynomials, $f_{p\ell}(r) = \sqrt{p!/(p+\ell)!} e^{-r^2/2\ell} r^\ell L_p^\ell(r^2)$ and $g_n(z) = \sqrt{\alpha/(2^n \sqrt{\pi n!})} e^{-z^2/2} H_n(\sqrt{\alpha} z)$, respectively. The corresponding eigenvalue is $\epsilon_{np} = (2p + \ell + 1) + \alpha(n + 1/2) - \mu$. The BdG Hamiltonian is block-diagonal in $\ell$ due to axial symmetry. For a given $\ell$ we need to diagonalize

\[
\Delta^{(\ell)} = \frac{\epsilon_q}{2} \int_0^\infty r^2 dr \int_{-\infty}^\infty dz f_{p\ell}(r) f_{p'\ell}(r) g_n(z) g_{n'}(z) \Delta(r, z)
\]
The trapping potential has $\alpha$. Such a partially polarized normal region, which is also seen prominently in phenomenological implementations of the TFA [17], is never observed in our BdG calculations with $P \leq 40\%$.

The existence of a magnetized superfluid region implies the breakdown of TFA. There is no such phase for a uniform gas in the thermodynamic limit at unitarity and this region is stabilized only by the presence of a trap. Earlier BdG studies in isotropic traps [11] already found this region is stabilized only by the presence of a trap.

For the spherical case ($\alpha = 1$) the equipotential contour condition must be satisfied by symmetry, despite the violation of TFA in the order parameter. As the anisotropy $\alpha^{-1}$ increases we see that the magnetization gets more concentrated along the wings. Moreover, the boundary between the magnetized and unmagnetized regions near the $z = 0$ plane becomes straighter, yielding a magnetization “hole” that becomes more rectangular. This is very similar to the observed profiles in the Rice experiments [9].

To understand why the MIT results look so different, we must study the dependence on the total number of particles, for a fixed trap anisotropy and polarization. In Fig. 3 we plot the results for (from top to bottom) $N = 865$, 1538, and 2307 particles in a trap with $\alpha = 1/2$ and $P = 30\%$. For the smallest $N$ the magnetization is localized along the axis, and is seen to spread out toward the radial direction with increasing $N$. The largest $N$ results show a rather elliptical magnetization density indicating that the magnetization begins to follow the equipotential contours as $N$ increases.

**Scaling with $N$ and $\alpha$:** We next present a simple argument for the consistency of the TFA which will allow us to see better how our results scale with $N$ and $\alpha$. In a polarized Fermi gas the conditions for the consistency of the TFA are $\mu_{e}/\omega_{0} \gg 1$ and $\delta \mu/\omega_{0} \gg 1$. The last inequality is the one that is most easily violated when $P$ is not close to 1.

We emphasize that, despite an apparently widespread feeling to the contrary, the size of the intermediate region is also quite large in the experiments. This size can be determined from the separation between the point at which $n_{f}$ and $n_{1}$ first deviate from each other to the point where $n_{1}$ vanishes. Even the MIT data, which shows little evidence for breakdown of TFA, has an intermediate region of $\simeq 10 \mu m$ along the radial direction, a significant fraction of the unpolarized core radius; see Fig. 5(b) of ref. [8]. In the Rice data the intermediate region is $\simeq 100 \mu m$ along the axial direction. This is two-orders of magnitude larger than $k_{F}^{-1}$ and a significant fraction of the superfluid core size; see Fig. 3(b) of ref. [9].

**Equipotential contours:** At present there are no direct experimental probes of the magnetized superfluid region. Thus we must look for signatures of the breakdown of TFA in the testable question of whether the densities follow contours of constant potential.

We first show how the equipotential contour condition is progressively violated as a function of increasing trap anisotropy $1/\alpha$. In the top panel of Fig. 2 we plot the magnetization $m(r, z)$ for $N = 865$ particles with $P = 30\%$ polarization and $\alpha = 1, 1/2, 1/4$. In the lower panel we show the corresponding plots of the column-integrated magnetization, which is simpler to measure in experiments, and is given by $m_{col}(y, z) = \int_{-\infty}^{\infty} dx m(\sqrt{x^2 + y^2}, z)$. For the spherical case ($\alpha = 1$) the equipotential contour condition must be satisfied by symmetry, despite the violation of TFA in the order parameter. As the anisotropy $\alpha^{-1}$ increases we see that the magnetization gets more concentrated along the wings. Moreover, the boundary between the magnetized and unmagnetized regions near the $z = 0$ plane becomes straighter, yielding a magnetization “hole” that becomes more rectangular. This is very similar to the observed profiles in the Rice experiments [9].
to unity. We start with the TFA densities obtained from the mean-field phase diagram at unitarity \[10\]. By spatially integrating these density profiles we find \(N_{\uparrow}\) and \(N_{\downarrow}\) in terms of \(\delta \mu / \omega_0\) and the average \(\mu\). Inverting these relations we can show that \(\delta \mu / \omega_0 = (N \alpha)^{1/3} f(P) \[20\]. Here \(f(P)\) is a monotonically increasing function of \(P\) which goes like \(P^{2/5}\) for \(P \ll 1\) and is of order unity for the \(P\) values of interest.

We have checked that our BdG results for \(\delta \mu / \omega_0\) are consistent with the \((N \alpha)^{1/3}\) scaling, even though the values are smaller than the TFA estimates. If the condition \(\delta \mu / \omega_0 \gg 1\) is violated the TFA will breakdown. How this breakdown manifests itself in the size of the magnetized superfluid and in the violation of the equipotential contour criterion depends strongly on the anisotropy \(1 / \alpha\), as seen above. For a given \((N \alpha)^{1/3}\) these violations are more pronounced for larger \(1 / \alpha\).

The Rice experiments with \((N \alpha)^{1/3} \approx 10\) and a large anisotropy show a significant violation of the equipotential contour criterion, consistent with our findings. On the other hand, we also understand why the MIT experiments, with \((N \alpha)^{1/3} \approx 100\) and a small anisotropy, find that this criterion is obeyed.

In summary, we have shown using BdG equations for the unitary, polarized Fermi gas that the often used TFA breaks down with the appearance of an intermediate magnetized superfluid region. The deviations from TFA are more pronounced with increasing trap asymmetry, both in terms of the size of the intermediate region and in the violations of the equipotential contour criterion. These violations become less important for large particle numbers and more spherical traps, in a way that is consistent with current experimental results. Important questions for future work are inclusion of finite temperature effects, ways to probe the intermediate magnetized superfluid region, and understanding the nature of the ground state at large polarization.

FIG. 3: Magnetization profiles as a function of total \(N\) (from top to bottom: 865, 1538 and 2307) at a fixed trap anisotropy \((\alpha = 1/2)\) and \(P = 30\%\).

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