Phase diagram of the rotating two-component Fermi gas including vortices

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We determine the conditions under which superfluidity with and without quantized vortices appears in a weakly interacting two-component atomic Fermi gas that is trapped in a rotating cylindrical symmetric harmonic potential. We compute the phase diagram as a function of rotation frequency, scattering length, temperature, total number of trapped atoms, and population imbalance.

Introduction. Superfluids are fluids that can flow with hardly any friction. If a superfluid is put into a rotating container, vortices carrying quantized circulation can be formed. These vortices are the hallmark of superfluidity and have been observed experimentally in Helium-4, in atomic Bose-Einstein condensates and in a two-component atomic Fermi gas made out of $^6$Li atoms [1, 2].

In this Letter we will focus on vortex formation in an equilibrated weakly interacting two-component Fermi gas that is trapped in a rotating cylindrical symmetric harmonic potential. The two components of this gas consist of atoms in different hyperfine states, and will be labeled by $↑, ↓$. We will consider a situation in which both components have equal mass $M$. In experiment, one can vary the strength of the interaction between the components using the Feshbach resonance. Furthermore one can control the rotation frequency $\Omega$, temperature $T$, total number of atoms, and the relative difference between the number of atoms in each component $P$ (population imbalance) [1, 2]. When the interaction is tuned to be attractive, the gas is cooled to low enough $T$, and $\Omega$ and $P$ are made small enough, the components will form Cooper pairs resulting in a Bardeen-Cooper-Schrieffer (BCS) superfluid [3].

The aim of this Letter is to determine in which region of the parameter space that is accessible to experiment vortices will be formed. So far only very limited information about this region is available. Only for weak interactions, $T = 0$ and $P = 0$, the lower critical $\Omega$ has been obtained theoretically. This frequency was estimated in [4] using a Ginzburg-Landau approach and computed by the author through solving the Bogoliubov-de Gennes (BdG) equation [5]. Experimentally only the critical $P$ for vortex formation at one specific $\Omega$ has been determined for different scattering lengths in the strongly interacting regime [2].

We will consider the following trapping potential: $U(x) = \frac{1}{2}M\omega^2\rho^2$, where we have introduced cylindrical coordinates, i.e. $x = (\rho \cos \phi, \rho \sin \phi, z)$. We will allow the trap to rotate with constant angular frequency $\Omega$ in the $x$-$y$ plane. This trapping potential implies harmonic confinement with frequency $\omega$ in the $x$-$y$ plane and infinite extension in the $z$-direction. In an experiment this situation can be approached by choosing the trapping frequency in the $z$-direction ($\omega_z$) much smaller than $\omega$. The characteristic length scale of the potential is the harmonic oscillator length $\lambda = \sqrt{\hbar/\mu \omega}$. In the setup of Ref. [2] the radial trapping frequency was taken to be $\omega/(2\pi) = 110$ Hz. In that case $\lambda \sim 3.9 \mu m$ and the characteristic energy scale $\hbar \omega/k_B \sim 5.3 \text{ nK}$. The order parameter for superfluidity is the pairing field $\Delta(x)$. For a single vortex that is located at the center of the trap it has the following form: $\Delta(x) = \Delta(\rho) \exp(ik\phi)$, with $k$ the winding number of the vortex. The $k = 0$ case corresponds to a superfluid without vortices. We will assume that $\Delta(\rho) \in \mathbb{R}$. There is no superfluidity at the core of a vortex, hence $\Delta(\rho = 0) = 0$ for $k \neq 0$. If $\Omega = 0$, $T = 0$, and $P = 0$, the whole system of atoms forms a vortex-free superfluid. In that situation the vortex is metastable. This is because condensation energy is lost near the vortex core, the atoms traveling around the vortex core have an average velocity resulting in a kinetic energy cost, and the system has to expand to compensate for the density depletion at the vortex core. This expansion costs energy because of the attractive interaction.

Starting from a situation in which $\Omega = 0$, let us now imagine increasing $\Omega$. If both $T = 0$ and $P = 0$, the whole system stays superfluid up to a critical frequency $\Omega_c$. Above $\Omega_c$ part of the system will turn into a normal gas due to breaking of Cooper pairs [6]. If either $T \neq 0$ or $P \neq 0$ there are un-paired atoms present for any nonzero $\Omega$. The unpaired atoms are predominantly located in the outer regions of the system. They rotate like a rigid body and acquire therefore rotational energy. A vortex is also a source of rotational energy since it induces angular momentum in the system. If the rotational energy gains overcome the costs, a single vortex will be preferred above a frequency $\Omega_c$. Because of symmetry and energy arguments, this vortex has unit winding number ($k = 1$) and is located at the center of the trap ($\rho = 0$). By further increasing $\Omega$ more vortices can be created resulting in a vortex lattice [7, 8]. At the same time increasing $\Omega$ will shrink the size of the superfluid region [9], while the system as a whole will expand due to the centrifugal force. At some point the superfluid region will be so small that it can only support a single vortex at $\rho = 0$. By further increasing $\Omega$ this vortex will disappear at a upper critical rotation frequency $\Omega_u$. Then at an even larger rotation frequency $\Omega_u$ superfluidity will vanish completely via a second order transition [7]. The upper critical frequency for superfluidity $\Omega_u$ has been computed in Refs. [9, 10] for a balanced gas using the local density approximation (see also [11] for related analyses of the phase boundary of superfluidity). In this Letter we will obtain $\Omega_u$ by solving the BdG equation. Finally, above $\Omega = \omega$ the system will be torn apart.
As pointed out above, the first vortex that appears and the last vortex that disappears when increasing $\Omega$ has $k = 1$ and is located at $\rho = 0$. Moreover, in experiment it has been observed that the number of vortices goes continuously to zero when increasing $P$ at fixed $\Omega$ [2]. Therefore, we can map out the entire region in which one or more vortices are preferred thermodynamically by determining the conditions under which the $k = 1$ situation has lower Helmholtz free energy than the $k = 0$ situation. For studies of real-time dynamics of vortex formation we refer to Refs. [8] [12]. To obtain $\Omega$, we will determine the point at which $\Delta(\rho = 0)$ vanishes for $k = 0$.

Setup. We will now briefly discuss the details of the calculation, a more extensive discussion can be found in our earlier work [5]. To obtain the Helmholtz free energy one needs to compute the pairing field $\Delta(x) = \Delta(\rho) \exp(i_k \phi)$ and the density profiles $\rho_{\uparrow}(x) = \rho_{\uparrow}(\rho)$ for each component separately. For a weakly interacting gas these can be found by solving the BdG equation self-consistently:

\[
\begin{pmatrix}
\mathcal{H}_1(\Omega) - \Delta(x) \\
\Delta^*(x) - \mathcal{H}^*_1(\Omega)
\end{pmatrix}
\begin{pmatrix}
\rho_{\uparrow}(x) \\
\rho_{\downarrow}(x)
\end{pmatrix} = E \begin{pmatrix}
\rho_{\uparrow}(x) \\
\rho_{\downarrow}(x)
\end{pmatrix}.
\]

(1)

Here $\mathcal{H}_1$ contains the single-particle Hamiltonian, the Hartree self-energy, and the chemical potential $\mu_{\uparrow}$. Explicitly, it reads $\mathcal{H}_1(\Omega) = \frac{p^2}{2m} + \frac{1}{2} M \omega^2 \rho^2 - \Omega L_z - \mu_{\uparrow} + g n_{\uparrow}(\rho)$, where the $z$-component of the angular momentum is given by $L_z = -i \hbar \partial / \partial \phi$, and $g = 4 \pi a \hbar^2 / M$ is the coupling constant with $a$ the s-wave scattering length. The wavefunctions $\rho_{\uparrow}(x)$ and $\rho_{\downarrow}(x)$ have to be normalized as $\int d^3 x \left| \rho_{\uparrow}(x) \right|^2 = 1$ and $\int d^3 x \left| \rho_{\downarrow}(x) \right|^2 = 1$. The number densities are given by $n_{\uparrow}(x) = \sum_i f(E_i) |\rho_{\uparrow}(x)|^2$ and $n_{\downarrow}(x) = \sum_i f(-E_i) |\rho_{\downarrow}(x)|^2$, where $f(E) = \exp(\beta E) + 1 \right\}^{-1}$ with $\beta = 1 / (k_B T)$. The pairing field follows from the regular (reg) part of the anomalous propagator in the following way $\Delta(x) = \rho_{\uparrow\downarrow}(x,x) \delta(x)$, with $\rho_{\uparrow\downarrow}(x,x') = \sum_i f(E_i) \rho_{\uparrow}(x) \rho_{\downarrow}(x')$. To obtain this regular part we have used a method [5] based on the procedures discussed in Refs. [13] [14].

We will consider a fixed number of atoms per unit length $\lambda$ in the $z$-direction, and denote this number by $N_{\uparrow\downarrow} = \lambda / L \int d^3 x \rho_{\uparrow\downarrow}(x)$. Here $L$ is the length of the system in the $z$-direction which we will take to be infinite. We will denote $N = N_{\uparrow} + N_{\downarrow}$ for the total number of atoms per unit length. The population imbalance or polarization is defined as $P = (N_{\uparrow} - N_{\downarrow}) / N$. The chemical potentials $\mu_{\uparrow\downarrow}$ will be solved for such that the required $N_{\uparrow\downarrow}$ is obtained.

To solve the BdG equation numerically, we have discretized the radial part of the wavefunctions on a Lagrange mesh [13] based on Maxwell polynomials [5]. Typically we could reach a relative accuracy of order $10^{-3}$ with about 64 to 96 mesh points for $N = 1000$. The angular and $z$-dependence of the wavefunctions were treated exactly. Integration over the $z$-momentum was performed using the adaptive Simpson method. To solve for self-consistency we have used the Newton-Broyden rootfinding method. The full details of our numerical procedure are explained in [5]. Examples of pairing field and density profiles with and without a vortex can be found in Refs. [5] [13] [16] [17]. In particular we have obtained excellent agreement with Ref. [17], in which a vortex profile for an imbalanced gas that is also trapped in a cylindrical symmetric harmonic potential is presented.

Once the pairing field and the density profiles have been obtained, the Helmholtz free energy per unit length (which is ultraviolet finite) can be computed in the following way

\[
F = \frac{\lambda}{L} \sum_i \left\{ \frac{|E_i|}{2} + \frac{1}{\beta} \log \left( 1 + e^{-\beta E_i} \right) \right\} + \mu_{\uparrow} N_{\uparrow} + \mu_{\downarrow} N_{\downarrow}
\]

\[-\frac{1}{L} \int d^3 x \left[ G_{\uparrow\downarrow}(x,x') \Delta(x) + g n_{\uparrow}(x) n_{\downarrow}(x) \right] + \frac{\lambda}{L} \sum_i \epsilon_i,
\]

(2)

where $\epsilon_i$ are the eigenvalues of the Hartree-Fock Hamiltonian $\mathcal{H}_\text{HF} = (\mathcal{H}_1(\Omega = 0) + \mathcal{H}^*_1(\Omega = 0)) / 2$. We have computed $\Delta F = F_{k=0} - F_{k=0}$ for several values of the external parameters and obtained the phase boundary by determining the point at which $\Delta F = 0$. Typically we could locate this boundary with a relative accuracy of about $10^{-2}$ to $10^{-3}$.

Results. We will now present several phase diagrams from which it can be seen for which values of the rotation frequency $\Omega$, scattering length $a$, temperature $T$, total number of atoms per unit length $N$, and imbalance $P$, superfluidity with one or more vortices will be formed (light gray area). Also we will indicate in these phase diagrams when the system exhibits superfluidity without any vortex (dark gray area). As a measure of the interaction strength we will use $1 / (k_B T a)$, where $k_B T a$ denotes the Fermi momentum of the superfluid at $T = 0$, $P = 0$, $\Omega = 0$ and $\rho = 0$.

In Ref. [5], we have computed the critical frequency for unpairing ($\Omega_b$) and the lower critical frequency for vortex formation ($\Omega_c$) as a function of scattering length for $T = 0$, $P = 0$ and $N = 1000$. In Fig. 1 we display the full phase diagram at $T \approx 0$. Here we write $T \approx 0$ to indicate that the vortex phase boundaries and the unpairing transition were computed at $T = 0$ exactly, whereas $\Omega_c$ was computed at $T = 0.01 \hbar \omega$. We have used this very small $T$ to ensure that $\Delta(\rho = 0)$ approaches zero continuously when increasing $\Omega$, so that we could determine $\Omega_c$. Exactly at $T = 0$ $\Delta(\rho = 0)$ does not
seem to vanish when increasing $\Omega$, although it does become very small.

The successive transitions that one encounters when increasing $\Omega$ were already described in the introduction and can be clearly seen in the diagram. The first transition is the unpairing transition occurring at $\Omega = \Omega_0$. It is of second order and turns into a cross-over for $T > 0$. Therefore it is a quantum transition and at $\Omega_0$ the system resides at a quantum critical point. If $|a|$ increases, it will become more difficult to break the Cooper pairs, hence $\Omega_0$ grows in that case. For $|a| \gtrsim 0.085\lambda$ vortices will be formed for $\Omega_i \leq \Omega \leq \Omega_0$. The structure of $\Omega_i$ is a result of the interplay of two effects [5]. The first is that the energy cost of a vortex at $\Omega = 0$ increases when increasing $|a|$. That naturally leads to a larger $\Omega_0$. The second effect is that unpairing becomes easier for smaller $|a|$, hence more rotational energy can be acquired by the $k = 0$ superfluid. This leads to an increase of $\Omega_i$ for weak interactions and is the reason that for small $|a|$ no vortices will be formed for any $\Omega$. The size of the superfluid region shrinks above $\Omega_0$ when increasing $\Omega$. If $|a|$ grows at fixed $\Omega$, it becomes more difficult to destroy superfluidity by rotation. This results in a larger superfluid region, so that a vortex can fit more easily. For these reasons both $\Omega$ and the upper critical frequency for superfluidity $\Omega_i$ grow with increasing $|a|$. The behavior of $\Omega_i$ is qualitatively in agreement with the results of Refs. [9,10].

This phase diagram will be modified quantitatively when changing $N$. However, the qualitative structure will remain the same if $N$ is large enough. To illustrate this, we display in Fig. 2 the phase diagram in the $N$-$\Omega$ plane for two different interaction strengths. A larger $N$ implies a larger system, and hence for a given $\Omega$ the atoms at the boundaries have a larger velocity. This makes pairing more difficult, leading to a smaller $\Omega_0$ as can be seen in Fig. 2. To explain the behavior of $\Omega_i$, we can use that the rotational energy gain of the vortex is proportional to the angular momentum which is proportional to $N$. The energy costs of the vortex grow much slower when increasing $N$. Hence a larger $N$ leads to a smaller $\Omega_i$. Below a certain $N$ no vortices will be formed for any $\Omega$. The upper critical frequencies $\Omega_0$ and $\Omega_i$ increase if $N$ grows.

If $T$ is increased the window in $\Omega$ in which vortices are formed narrows. This can be seen from Fig. 3 in which we display the phase diagram in the $\Omega-T$ plane for $N = 1000$, $P = 0$ and two different scattering lengths. Above a certain $T$, vortices will not be formed for any $\Omega$ while the system is still partly superfluid. It is the easiest to make vortices at intermediate $\Omega$, since in that case the window in $T$ is the largest. This $\Omega-T$ phase diagram is qualitatively very similar to that of a rotating Bose-Einstein condensate [18].

In Fig. 4 we display the phase diagram in the $\Omega-P$ plane for $T = 0$ and two different scattering lengths. The larger the $P$, the narrower the window in $\Omega$ in which vortices are formed becomes. Above a certain $P$ part of the system can still be superfluid, but vortices will not be formed for any $\Omega$.

From Figs. 3 and 4 it can be seen that the critical $T$ and critical $P$ for vortex formation and superfluidity grow when increasing the interaction strength. When $\Omega$ is increased, $\Omega_i$ always decreases. Especially for large interaction strengths $\Omega_0$ and $\Omega_i$ lie very close each other.

In the experiment described in Ref. [2] a strongly interacting two-component Fermi gas made out of $\sim 7 \times 10^6$ atoms was trapped in a cigar-shaped potential with a frequency ratio of $\omega_z/\omega = 23/110$. Using the Thomas-Fermi approximation at $T = 0$ we estimate that in this experiment $N(z = 0) \sim 1 \times 10^4$. The atoms were stirred with a laser at a frequency of $\Omega = (70/110)\omega \approx 0.636\omega$. After stirring, one waited until the system had equilibrated and measured the number of vortices as a function of $P$. In this way an upper critical imbalance for vortex formation ($P_c$) could be determined. Although this situation is not completely equivalent to
our setup it is nevertheless interesting to make a comparison to this experiment. Therefore we display in Fig.5 the phase diagram in the $P$-$T$ plane for $\Omega = 0.636\omega_0$, and $1/(k_Fa) = 1.0$ (left) and $1/(k_Fa) = 0.8$ (right).

In Fig.6 we display the phase diagram in the $N$-$P$ plane for $T = 0$, $\Omega = 0.636\omega_0$ and two different interaction strengths. As expected and seen in experiment, weaker interactions imply a lower $P_c$. In the experiment it was found that $P_c \sim 0.1$ at $1/(k_Fa) = 0.5$ [2]. The values of $P_c$ we have obtained seem to be large compared to this value, because we consider weaker interactions and our $N(z = 0)$ is much smaller. This quantitative difference could have been caused by the different stirring method or by the shape of the trapping potential. Also it could signal that one should take into account beyond the mean field corrections at $1/(k_Fa) = 0.8$.

Conclusions. For the first time we have unveiled the full phase diagram of a trapped, rotating, and weakly-interacting two-component Fermi gas including vortices. We have made detailed predictions for the conditions under which superfluidity with and without vortices is formed as a function of rotation frequency, scattering length, temperature, number of atoms and population imbalance. The phase diagrams we have obtained are quantitatively reliable and are in principle directly comparable to a possible future experimental determination. Our analysis can be extended to more complicated systems, like Fermi gases with $p$-wave pairing, Fermi gases with more than two components, and Fermi gases in which the two components have unequal mass. This will be useful for the experimental search for superfluidity in such systems.

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FIG. 5: Phase diagram: $P$-$T$ plane, for $N = 1000$, $\Omega = 0.636\omega_0$, and $a = -0.13a$. Here $1/(k_Fa) = 0.8$.

FIG. 6: Phase diagrams: $N$-$P$, for $T = 0$, $\Omega = 0.636\omega_0$, and $1/(k_Fa) = 1.0$ (left) and $1/(k_Fa) = 0.8$ (right).

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