Ground state description of a single vortex in an atomic Fermi gas: From BCS to Bose-Einstein condensation

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We use a Bogoliubov-de Gennes (BdG) formulation to describe a single vortex in a neutral fermionic gas. It is presumed that the attractive pairing interaction can be arbitrarily tuned to exhibit a crossover from BCS to Bose-Einstein condensation. Our starting point is the BCS-Leggett mean field ground state for which a BdG approach is microscopically justified. At strong coupling, we demonstrate that this approach is analytically equivalent to the Gross-Pitaevskii description of vortices in true bosonic systems. We analyze the sizable density depletion found for the unitary regime and relate it to the presence of unoccupied (positive energy) quasi-bound states at the core center.

One of the most exciting developments in atomic and condensed matter physics has been the observation of superfluidity in trapped fermionic systems \[1,2,3,4\]. In these systems, the presence of a Feshbach resonance provides a means of tuning the attractive pairing interaction with applied magnetic field. In this way the system undergoes a continuous evolution from BCS to Bose-Einstein condensed (BEC) superfluidity.

The most conclusive demonstration of the superfluid phase has been the experimental observation of vortices \[5\]. Particularly interesting from a theoretical viewpoint is the way vortices evolve from BCS to BEC. This evolution is associated, not just with a decrease in vortex size but with a complete rearrangement of the fermionic states which make up the core. As a result, there is a continuous evolution of the particle density within a vortex, thereby affecting the visibility of vortices in the laboratory. In this paper we discuss the behavior of a (single) vortex as the system crosses from BCS to BEC. Our work is based on simplest BCS-like ground state first introduced by Leggett \[4\] and Eagles \[7\] to treat BCS-BEC crossover. With this choice of ground state inhomogeneity effects are readily incorporated as in generalized Bogoliubov-de Gennes (BdG) theory. Here we demonstrate analytically that the BdG strong coupling description of the $T = 0$ vortex state coincides with the usual Gross-Pitaevskii (GP) treatment of vortices in bosonic superfluids. A fermionic theory based on BdG is, thus, very inclusive, and within this approach one expects a smooth evolution of vortices from the BCS to BEC limit as the statistics effectively change from fermionic to bosonic.

Previous studies of vortices in these fermionic superfluids addressed the BCS limit at $T = 0$ \[8\] and $T \approx T_c$ \[9\]. There is also work \[10\] on the $T = 0$ strict unitary case where a BdG approach was used with Hartree-Fock contributions included. In the present work, by contrast, we discuss the entire crossover regime and, importantly, present a detailed analysis of the energy and spatial structure within the core and how it evolves from BCS to BEC. A very different path integral approach was introduced in Ref. \[11\] to address vortices with BCS-BEC crossover, but here the authors note that density depletion effects appear to be unphysically large in the BCS regime. Our analytical approach builds heavily on previous work \[12\] which showed a general connection between GP theory and BdG. From this one can conclude that a generalized BCS theory \[6\] treats the bosonic degrees of freedom at the same level as GP theory. Different ground states can be contemplated, (with incomplete condensation, say) but they will not be compatible with BdG theory. In a similar way, once $T \neq 0$ one has to incorporate noncondensed pairs, and associated pseudogap physics \[13\] which are not present in a finite temperature BdG theory.

For the most part, BdG approaches require detailed numerical solution \[8,14,15,16\], so it is particularly useful to have analytical tools in the BEC limit. We present this non-numerical description first. Our general self consistent equations \[17\] are

\[
\begin{pmatrix}
 h - \mu & \Delta^{*}(\mathbf{r}) - \hbar^{*} + \mu \\
 \Delta(\mathbf{r}) & -h^{*} + \mu
\end{pmatrix}
\begin{pmatrix}
 u_n \\
v_n
\end{pmatrix}
= E_n
\begin{pmatrix}
 u_n \\
v_n
\end{pmatrix},
\]

where $h = -\frac{1}{2m} \nabla^2 + V_{ext}(\mathbf{r})$, $\Delta(\mathbf{r})$ is the $T = 0$ gap function which is importantly the same as the $T = 0$ order parameter, $\Delta_{\nu}(\mathbf{r})$, $V_{ext}(\mathbf{r})$ is the external potential associated with the trap, and we choose $\hbar = 1$ with $\int d\mathbf{r}(|u_n|^2 + |v_n|^2) = 1$ for all energy levels $n$. The difference between the present approach and the usual BdG applications of superconductivity is that here the fermionic chemical potential $\mu$ must be self consistently determined, as the attractive coupling constant is varied.

We use a Green’s function formulation \[14\] to write the zero-temperature free energy $E_0 = \langle H - \mu N \rangle$, (where $N$ is the number operator) in the form

\[
E_0 = \int d\mathbf{r} \frac{(|\Delta(\mathbf{r})|^2)}{V} + \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \omega' Tr[i\tau_{3} G(\mathbf{r}, \mathbf{r}', \omega)] \]

Here $\tau_i$ ($i = 1, 2, 3$) are the Pauli matrices. The elements of $\hat{G}$ corresponding to the normal and anomalous channels can be further expressed as coupled integral equations in terms of the...
noninteracting Green’s function \( G_{11}^{(0)} \)

\[
G_{11}(r, r'; \omega) = G_{11}^{(0)}(r, r'; \omega) + \int dr_2 [G_{11}^{(0)}(r, r_2; \omega) \times \Delta(r_2) G_{21}(r_2, r'; \omega)],
\]

where the gap and number equation are given by parametrized in terms of the

\[
\Delta(r) = -V \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G_{21}(r, r; \omega) \quad \text{and} \quad n(r) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \epsilon_0 G_{11}(r, r; \omega).
\]

The coupling constant \(-V < 0\) for the attractive inter-fermion contact interaction is parametrized in terms of the \( s \)-wave scattering length \( a_F \) with \( m/4\pi a_F = -1/V + \sum_r m/k^2 \).

In the strong pairing limit \( a_F \) is small and positive and \( \Delta/|\mu| \) is small. To derive the ground state energy \( E_0 \) from Eq. \( \text{[3]} \), we expand the Green’s function \( G \) in the gap equation in terms \( \text{[12]} \) of \( G_{11}^{(0)} \). Including terms up to fourth order in \( |\Delta| \), it follows that

\[
E_0[\Delta] = \int dr \left\{ \frac{\Delta(r)^2}{V} - a_0(r)|\Delta(r)|^2 + \frac{1}{2} b_0(r)|\nabla \Delta(r)|^2 - \frac{1}{2} c_0(r)|\Delta(r)|^4 \right\}
\]

where \( a_0(r) \approx \frac{1}{V} + \frac{ma_{ec}}{8\pi} |\mu_B - 2V_{ext}(r)| \), \( b_0(r) \approx ma_F/16\pi \), and \( c_0(r) \approx -ma_F^2/16\pi \). Here \( \mu_B = 2\mu + \epsilon_0 \) is the effective “bare” bosonic chemical potential, and \( \epsilon_0 = (ma_F^2)^{-1} \) is the binding energy of the composite boson, with \( |\mu_B| \ll \epsilon_0 \). It is assumed that \( V_{ext} \) is slowly varying \( \text{[12]} \) so that \( G_{11}^{(0)}(r, r'; \omega_0) \approx G_{11}^{(0)}(r-r'; \mu - [V_{ext}(r)+V_{ext}(r')]/2) \). Similarly, \( \Delta(r) \) is assumed to vary slowly on the scale of \( a_F \).

As a consequence of these assumptions, and for the purposes of this paper, (which ultimately focuses on a single vortex), trap effects are not particularly relevant.

It should be stressed that this expansion is similar to Gor’kov’s derivation of Ginzburg-Landau (GL) theory in the BCS limit at \( T \approx T_c \), albeit here we consider strong coupling and \( T = 0 \). In conventional superconductors \( \text{[13]} \), minimizing the energy \( E_0[\Psi] \) with respect to \( \Psi \), one obtains

\[
E_0[\Psi] = -\frac{2\pi a_B}{m_B} \int dr \, |\Psi|^4 + \frac{1}{2m_B} \int dl \, \Psi^* \mathbf{n} \cdot \nabla \Psi |\Psi|^2,
\]

where we have identified the condensate wave function \( \Psi(r) \) as \( \sqrt{m^2 a_F/8\pi} \Delta(r) \) and \( \mathbf{n} \) is the unit vector normal to the surface. The second term is a surface term, which vanishes for an infinite system. In a neutral superfluid, however, the energy has to be calculated within a finite region of radius \( R \) around the vortex core, to avoid divergences, so this surface term cannot be neglected.

Equivalently, the zero-temperature energy can be written in a more conventional form as

\[
E_0[\Psi] = \int dr \left\{ \frac{1}{2m_B} |\nabla \Psi(r)|^2 + 2V_{ext}(r)|\Psi(r)|^2 + \frac{1}{2} U_0|\Psi(r)|^4 - \mu_B|\Psi(r)|^2 \right\},
\]

where \( U_0 = 4\pi a_B/m_B, m_B = 2m \) and \( a_B = 2\alpha_F \) are the mass and the scattering length of the composite boson.

Importantly, this expression has the same form as the \( T = 0 \) energy of a gas of weakly-interacting bosons \( \text{[19]} \) associated with GP theory. It should be noted that here this GP theory is written in terms of the grand canonical representation where the bosonic chemical potential (rather than the number of particles \( N \)) is held fixed. Minimizing the zero-temperature energy \( E_0 \) (via \( \delta E_0/\delta \Psi^* = 0 \)), leads to the well known GP equation:

\[
-\frac{1}{2m_B} \nabla^2 \Psi(r) + 2V_{ext}(r) + U_0|\Psi(r)|^2 \Psi(r) = \mu_B \Psi(r).
\]

We emphasize that this BdG analysis has, in effect, derived GP theory from a fermionic starting point. The presence of a Hartree term in the BdG equations will destroy the simple analytic arguments presented here. Nevertheless, a Hartree contribution for the composite bosons is found here of the form \( U_0 \Psi^2 \Psi \rightarrow U_B n_B \Psi \), (where \( n_B \) is the density of bosons). This is, of course, unrelated to the Hartree term of the original fermions, which is absent in Eq. \( \text{[1]} \), as is consistent with the usual BCS-Leggett mean field theory \( \text{[6]} \). The inclusion of Hartree terms \( \text{[3]} \) in the vortex problem has been accounted for in the literature, at weak \( \text{[8]} \) and strict unitary coupling \( \text{[10]} \), but they do not appear to lead to important differences.

Expanding the zero-temperature energy \( E_0 \) to next order in \( \Delta \), a term \( \int dr d\omega d\xi d\omega \Delta(r)^6 \) with \( d_0(r) \approx -5m^2 a_F^6/256\pi \) appears in. This term contributes a term \( g_3|\Psi(r)|^4 \Psi(r) \) with \( g_3 = -15\pi^2 a_F^2/4m_B \) in Eq. \( \text{[8]} \); it introduces the appropriate analogue in Eq. \( \text{[7]} \) as well. This three-body correction to the usual GP equation \( \text{[g3]} \) \( \text{[12]} \) represents an effective attraction.

In the composite-boson system, it provides a first-step correction of the BEC limit en route to the fermionic or BCS end point.

In the presence of a single vortex, the wave function can be written as \( \Psi(r) = f(r)e^{-i\theta} \). We introduce the BEC correlation length \( \xi_{\text{BEC}} \) in the strong-pairing limit as \( (2m\xi_{\text{BEC}}^2)^{-1} = \mu_B = U_B n_B^2 \), with \( f_0 = f(r \rightarrow \infty) \). We rescale \( r = \xi_{\text{BEC}} \cdot x \) and \( f(r) \rightarrow f_0 \cdot X(x) \) and apply standard boundary conditions \( \text{[19, 20]} \). The results for \( \Psi(r) \) in these units are plotted as the solid lines in Fig. \( \text{[1]} \). As shown in Fig. \( \text{[1]} \), (and consistent with earlier results in the literature \( \text{[13, 20]} \)), the wavefunction rises smoothly from zero at the center of the core to its full magnitude at infinity on a length scale of \( \xi_{\text{BEC}} \).

An important feature of this figure should be noted. In this BEC limit of the BdG equations, the wavefunction is smooth. This behavior, which is in contrast to the BCS limit, is a consequence of the absence of localized fermionic bound states in the core region. In the weak coupling limit, as first noted by Caroli et al. \( \text{[21]} \), these bound states are associated with energy eigenvalues \( E_n < \Delta_\infty \). Here \( \Delta_\infty \) is the value of gap function in the bulk, away from the core. The gap \( \Delta(r) \) provides an effective potential well for the quasiparticles around the vortex core. From Eq. \( \text{[1]} \) we have \( E_n \geq -\mu \). Since \( -\mu \gg \Delta_\infty \), these bound states are necessarily absent in the strong pairing limit.

The first appearance of fermionic properties in our
The energy cost per unit length is given by Eq. (7) and the result is plotted in Fig. 1(c). In the BEC case, where there is complete depletion, the energy cost of a single vortex can also be calculated from the wave function as \( E \propto \ln(D_G R/\xi_{BEC}) \), where \( D_G = 1.48 \). The three panels in Fig. 1(c) present results for BEC, within the core region.

The energy cost of a single vortex can also be calculated from the ansatz \( E \propto -g_3 \left( \frac{\Psi^2}{n} \right) \), where \( g_3 \) is the three-body \( g_3 \)-term in the GP equation and the corresponding term in the zero-temperature energy \( E_0 \). The effects of this addition are plotted as dashed lines in Fig. 1(c) for rescaled \( g_3' = -g_3 f_0^2 / U_0 = 0.1 \). This \( g_3 \) contribution represents an attractive interaction, and, as shown in the figure, leads to a slight increase in the core size.

To understand the details of the core structure we turn now to numerical solutions of the BdG equation. We build on our analytical analysis at strong coupling to provide a check for our numerical algorithms. Here the physical coupling strength is controlled by the parameter \( 1/k_F a \). We have verified that changes in our high cutoff energy and associated coupling constant \( V \) do not affect the numerical results. Our numerical method is very similar to that in Ref. [22]. The chemical potential \( \mu \) is approximated by the homogeneous solution, since the vortex core only occupies a small portion of the entire system. Here we begin with a study of the localized (fermionic) density of states (LDOS), \( N(E, r) \), within the core region. There is considerable interest in the literature in the behavior of the LDOS for high \( T_c \) as well as low \( T_c \) superconductors [3], since this quantity is accessible through scanning tunneling microscopy measurements. \( N(E, r) \) is given by \( \sum_n [u_n^2 \delta(E - E_n) + v_n^2 \delta(E + E_n)] \). We ignore, for numerical simplicity, dependencies of the wave functions on the cylindrical variable \( z \), since these do not lead to qualitative effects. Integrating \( N(E, r) \) over \( E \leq 0 \) reflects the particle density distribution \( n(r) \) inside the core. Thus, this quantity provides a means of understanding the density depletion, or lack thereof, inside the core. It is essential for arriving at a deeper understanding of the core region and structure.

In Fig. 2, we plot \( N(E, r) \) inside the core, as a function of energy \( E \) for \( r = 0 \) and \( r = 25/k_F \). The dashed line in Fig. 2(a) (BCS, \( k_F a = -1 \)) represents \( n_B(r) \) associated with composite bosons which is simply related to the density of fermions. The density \( n(x) \) is plotted in Fig. 1(b), normalized at the bulk value \( n_\infty \approx n(\infty) \), as a function of \( x \). As expected the particle density is strictly zero at the core center in the BEC limit, where there is complete depletion.

The energy cost per unit length is given by \( E_v = \pi \xi_{BEC}^2 \int_{0}^{R/\xi_{BEC}} \left( \frac{dX}{dx} \right)^2 + \frac{X^2}{2} + \frac{1}{2} (X^2 - 1)^2 \right) \ dx \), where \( R \) is a cutoff needed to regularize a calculation of the vortex core energy. In Fig. 1(c) the solid line indicates \( E_v \) as a function of \( R/\xi_{BEC} \). The shape of the curve at the region \( R/\xi_{BEC} > 2 \) can be fitted to the usual functional form \( E_v \propto \ln(D_G R/\xi_{BEC}) \), where \( D_G = 1.48 \). The dashed line in Fig. 1(c) presents results for \( E_v \) in the presence of the three-body term, where we take \( g_3' = 0.1 \). This correction (red dot-dashed curve) lowers the vortex energy, as shown in the figure, and it approaches an asymptote as \( R/\xi_{BEC} \to \infty \).

Figure 1: (a) Numerical solution of GP equation in the BEC limit with \( g_3' = 0.1 \), dashed lines) and without (solid lines) the three-body \( g_3 \)-term, (b) the corresponding normalized particle density \( n(x)/n_\infty \) as a function of \( x \), and (c) the zero-temperature vortex energy cost \( E_v \) as a function of \( R/\xi_{BEC} \). In (c), the difference is shown as the red dot-dashed curve. Here \( n_\infty \equiv n(\infty) \).

Figure 2: Local fermionic density of states \( N(E, r) \) as function of \( E \) for BCS (\( k_F a \approx -1 \)), unitary and BEC (\( k_F a \approx 1 \)) cases, at the center \( r = 0 \) (black dashed curves) and radius \( r = 25/k_F \) (red solid curves) of the vortex core. The bulk value of the gap \( \Delta \) is 0.21, 0.68, 1.3\( E_F \), respectively. In the BEC case, \( \mu \approx -0.8E_F \). Here \( E_F \) is the noninteracting Fermi energy at the trap center.

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$k_F a = -1$, unitary and BEC ($k_F a = 1$). Rather than showing results for the strict BCS and BEC regimes, these plots represent a physically accessible range of magnetic fields. Because $N(E, r)$ is a fundamentally fermionic quantity, this information is lost from the analytical analysis which leads to a Gross-Pitaevskii transcription of the BEC limit. In the BCS case, the $r = 0$ peak at $E = 0$ reflects a bound fermionic state. This state together with the continuum of scattering states is responsible for the fact that there is no core density depletion. For the unitary regime, the lower energy peak in Fig. 2 arises from scattering states and appears at energies near the bulk gap $\Delta_\infty$. This quasi-bound state has energy close to the scattering state continuum and is reflected in the LDOS by a slight movement of the BCS central peak to the right. The energy integral of this feature is important in determining the finite particle density $n(r)$ at the core center. The peak at positive energy is a reflection of a quasi-bound state. This unoccupied quasi-bound state effectively depletes the spectral weight for $E < 0$, and therefore leads to the density depletion within the core. By the BEC limit all remnants of fermionic states have disappeared, until one provides energy large enough to break the pairs. It can be seen from the figure that in all three cases at sufficiently large distances from the core center the fermionic density of states assumes the bulk value.

In Fig. 3 we plot the position dependent order parameter $\Delta(r)$ along with the particle density distribution $n(r)$ for the unitary and BCS ($k_F a = -1$) cases shown in the previous figure. This BCS-like case still has a reasonably large bulk gap, so there a non-negligible depletion at the core. This is in contrast to arbitrarily weak coupling, where the depletion vanishes. The small $r$ oscillations shown here in both $\Delta(r)$ and $n(r)$ reflect the presence of a true bound state, as in earlier work [8]. The oscillations at large $r$ are an effect of the finite system size.

Importantly, in the unitary case, the particle density at the core center is substantially lower than in the BCS case. This is a consequence of the reduced spectral weight seen in the lower peak in the middle panel of Fig. 2. Our results are within 20% of those obtained in Ref. [10]. In this earlier work a Hartree-Fock correction was applied to the BdG equations which was argued to be the source of the density depletion. Here, we interpret this depletion differently as associated with the behavior of the core excitation spectra in conjunction with the reduced chemical potential ($\mu < E_F$).

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**Note** After this work was complete we learned of a related calculation by Machida and Koyama (Phys. Rev. Lett. 94, 140401 (2005)) which attributed the density depletion within the vortex core at unitarity to closed-channel bosons.

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