Deformed Fermi surfaces in ultracold Fermi gases

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The superfluid transition in an ultracold two-component atomic Fermi gas is analyzed in the case where the two components have different densities. We describe a superfluid state which spontaneously breaks the rotational-symmetry by deforming the Fermi surfaces of both species into ellipsoidal form. At relatively large hyperfine-spin asymmetries, this deformation is shown to help the appearance of pairing, which in the rotationally-symmetric (BCS) case would be forbidden by Pauli blocking. The prospects for experimental detection of such a deformed Fermi surface phase are discussed.

The present capabilities of cooling of atomic ensembles allow for reasonable expectations to observe a superfluid transition in ultracold fermionic systems, in direct analogy to the BCS superconductivity [1]. The temperatures achieved in recent experiments on fermionic atoms [2] are a fraction (∼ 0.1 – 0.3) of the Fermi temperature, i.e. atoms in a trap are in the quantum degenerate regime and, therefore, attractive two-body forces are expected to drive the Cooper instability. The strength of the two-body interactions can be tuned using a Feshbach resonance by varying the external magnetic field [3], thus the entire range from weak to strong couplings can be probed. In the crossover region the Feshbach resonance may strongly enhance the pairing interaction and give rise to high temperature superfluidity [4]. Recent experiments have probed the condensation of fermionic pairs above the Feshbach resonance, where the system does not support a genuine two-body bound state [3, 5, 6, 7]. Whether the observed correlated pairs are, in fact, weakly bound and spatially extended Cooper pairs, is not clear yet; however the measured collective modes of 6Li atoms under these conditions are consistent with the superfluid hydrodynamics of a Fermi gas and provide evidence for superfluidity in a resonantly interacting Fermi gas [7].

The very low temperatures (in the nanokelvin range) and densities reached in the experiments considerably reduce the contribution from \( L \neq 0 \) orbital angular momentum waves to atomic collisions. Therefore, s-wave collisions, which can be characterized by the scattering length \( a \), are the most relevant for the description of these systems. As usual, we take \( a < 0 \) to indicate an attractive interaction between the atoms. Since Pauli’s exclusion principle forbids s-wave interaction between indistinguishable fermions the pairing should appear between fermionic atoms belonging to different hyperfine states. Such systems, where two hyperfine levels are populated, have been created and studied experimentally with 6Li and 40K atoms [3, 5, 6, 7]. The BCS theory predicts a suppression of the pairing correlations when the Fermi energies, or equivalently, the densities of the two hyperfine states \( |1 \rangle \) and \( |2 \rangle \) are different. In the low density limit \( k_F|a| \ll 1 \) (\( k_F \) is the Fermi-momentum) the value of the critical density asymmetry \( \alpha = (\rho_1 - \rho_2)/(\rho_1 + \rho_2) \), where \( \rho_{1,2} \) are the densities of hyperfine states \( |1 \rangle \) and \( |2 \rangle \), for which the superfluidity vanishes can be deduced analytically [8]. The dependence of the pairing gap \( \Delta \) at the Fermi surface on the total density \( \rho = \rho_1 + \rho_2 = k_F^3/(3\pi^2) \) and the density asymmetry \( \alpha \) is described by

\[
\frac{\Delta(\alpha)}{\Delta_0} = \sqrt{1 - \frac{4\mu}{3\Delta_0^2} \alpha}, \tag{1}
\]

where \( \Delta_0 \approx 8e^{-2} \mu \exp[-\pi/(2k_F|a|)] \ll 1 \) is the gap in the symmetric matter and \( \mu \) is the chemical potential. Therefore the gap disappears for asymmetries \( \alpha > \alpha_{\text{max}} = 3\Delta_0/(4\mu) \), which in this limit is a very small number. For example, for the pairing of 6Li atoms in the states \( |1 \rangle = |F = 3/2, m_F = 3/2 \rangle \) and \( |2 \rangle = |3/2, 1/2 \rangle \), for which the triplet scattering length is \( a = -2160a_B \) (where \( a_B \) is the Bohr radius), and at the density \( \rho = 3.8 \times 10^{12} \text{ cm}^{-3} \) (corresponding to \( k_F|a| = 0.55 \)) the maximum asymmetry at which BCS pairing is possible is only \( \alpha_{\text{max}} = 0.07 \).

The purpose of this work is to demonstrate that the superfluid state in ultracold atomic gases can persist for density asymmetries \( \alpha > \alpha_{\text{max}} \), and can be enhanced in a range of \( \alpha < \alpha_{\text{max}} \) due to spontaneous deformation of the Fermi spheres of two-hyperfine states in the momentum space. It has been shown earlier (in other contexts) that the deformation of the Fermi surfaces of asymmetric two-component superconductors into ellipsoidal form leads to a novel ground state with deformed Fermi surfaces; the associated superconducting phase breaks global rotational symmetry of the space from O(3) down to O(2) [9]. The deformed Fermi surface superfluid (DFS) phase belongs to the class of the superconducting states with broken space symmetries, an example of which is the Larkin-Ovchinnikov-Fulde-Ferrell (LOFF) phase [10]; which has been studied in ultracold atomic gases in Ref. 11. The
underlying principle that makes these phases favorable is the compensation in the increase in the kinetic energy of the superconducting phase by the gain in the (negative) condensation energy due to a rearrangement of quasiparticle distributions. In the LOFF phase the compensation is achieved by sampling Cooper pairs with finite total center-of-mass momentum; in the DFS phase the same is achieved by a deformation of Fermi surfaces at zero total momentum of the pairs. Formally, these phases correspond to the first and second order expansion of the quasiparticle spectrum with respect to the angle formed by the particle momentum and the axis of spontaneous symmetry breaking.

Consider a uniform gas of Fermi atoms with two hyperfine states, which we assign labels 1 and 2 (these states equivalently can be thought of as pseudospins ↑ and ↓.) The model Hamiltonian that describes our system is

$$\hat{H} = \sum_{p,\sigma} \epsilon_p \hat{a}^\dagger_{p\sigma} \hat{a}^{\vphantom{\dagger}}_{p\sigma} - g \sum_{pp'vv'} \hat{a}^\dagger_{p',1} \hat{a}^\dagger_{-p',2} \hat{a}^{\vphantom{\dagger}}_{-p,2} \hat{a}^{\vphantom{\dagger}}_{p,1}, \quad (2)$$

where $\hat{a}^\dagger_{p\sigma}$ and $\hat{a}_{p\sigma}$ are the creation and annihilation operators of a state with momentum $p$, pseudospin $\sigma (= 1, 2)$ and energy $\epsilon_p = p^2/2m$, where $m$ is the atom bare mass (here and below we set the volume $V = 1$). The two-body coupling constant is determined by the $s$-wave scattering length $a < 0$ as $g = 4\pi\hbar^2|a|/m$. In the following we will work in a scheme where the particle number conservation is explicitly implemented by fixing their densities

$$\rho_{1(2)} = \sum_p \hat{a}^\dagger_{p\sigma,1} \hat{a}^{\vphantom{\dagger}}_{p\sigma,1} = \hat{a}^\dagger_{p,1(2)} \hat{a}^{\vphantom{\dagger}}_{p,1(2)} \quad \text{(or equivalently the total density $\rho$ and the asymmetry parameter $\alpha$) by adjusting the chemical potentials $\mu_\sigma$ of the hyperfine states.}$$

There is a significant difference between the scheme above and the one where the total chemical potential is fixed and the gap is studied as a function of the difference in the chemical potentials of species; in the latter case double valued solutions appear which are absent in the former case.

The mean-field solutions for the model Hamiltonian can be obtained by diagonalizing the Hamiltonian with the help of the familiar Bogolyubov transformations: $b_{p,1} = u_p \hat{a}^\dagger_{p,1} + v_p \hat{a}^{\vphantom{\dagger}}_{-p,2}$ and $b_{p,2} = u_p \hat{a}^\dagger_{p,2} - v_p \hat{a}^{\vphantom{\dagger}}_{-p,1}$, where $u_p^2 + v_p^2 = 1$. A variational minimization of the energy with respect to the parameter $u_p$ (or $v_p$) leads to the gap equation

$$\Delta = g \int \frac{dp}{(2\pi)^3} u_p v_p \left[1 - f(E_1) - f(E_2)\right], \quad (3)$$

where $f(E) = [1 + \exp(E/T)]^{-1}$ is the Fermi distribution function, $T$ is the temperature. The two branches of quasiparticle spectra are defined as

$$\frac{E_1}{E_2} = \sqrt{\xi_S^2 + \Delta^2} \pm \xi_A, \quad (4)$$

where the symmetrized $\xi_S = \frac{1}{2}(\varepsilon_1 + \varepsilon_2)$ and anti-symmetrized $\xi_A = \frac{1}{2}(\varepsilon_1 - \varepsilon_2)$ spectra are written in terms of the normal state spectra $\varepsilon_\sigma = \epsilon_p - \mu_\sigma$ (we do not distinguish the masses of different hyperfine states) and the transformation parameters are defined as

$$\frac{u_p^2}{v_p^2} = \frac{1}{2} \left(1 \pm \frac{\xi_S}{\sqrt{\xi_S^2 + |\Delta|^2}}\right). \quad (5)$$

The occupation of the states in the superfluid phase are given by

$$n_{p,1(2)} = \left\{u_p^2 f(E_{1(2)}) + v_p^2 [1 - f(E_{2(1)})]\right\}, \quad (6)$$

with the normalization condition

$$\rho_\sigma = \sum_p n_{p,\sigma}. \quad (7)$$

We now turn to the description of the perturbations of the Fermi surfaces from the spherically symmetric form and the study of the stability of these perturbations. The two Fermi surfaces in momentum space are defined by the equations $\varepsilon_\sigma = \epsilon_p - \mu_\sigma = 0$. When the chemical potentials $\mu_\sigma = \beta S_{F,\sigma}/2m$, where $p_{F,\sigma}$ are the Fermi-momenta of the hyperfine states, are isotropic in the momentum space the Fermi surfaces are spherical. Relaxing the latter assumption we expand the quasiparticle spectrum in spherical harmonics $\varepsilon_\sigma = \sum_x \xi_{\sigma x} P_l(x)$, where $x$ is the cosine of the angle formed by the particle momentum and a randomly chosen symmetry breaking axis, $P_l(x)$ are the Legendre polynomials. The $l = 1$ terms break the translational symmetry by shifting the Fermi surfaces without deforming them; these terms are ignored below. Truncating the expansion at the second order ($l = 2$), we rewrite the spectrum in a form equivalent to the above one

$$\varepsilon_\sigma = \epsilon_p - \mu_\sigma \left(1 + \eta_\sigma x^2\right), \quad (8)$$

where the parameters $\eta_\sigma$ describe the quadrupole deformation of the Fermi surfaces. It is convenient to work with the symmetrized and anti-symmetrized combinations $\delta \epsilon = (\eta_1 - \eta_2)/2$ and $\Xi = (\eta_1 + \eta_2)/2$, which we will refer to as ‘relative’ and ‘conformal’ deformations. Our next task is to examine the energy of the superfluid state at finite deformations to assess whether the deformations lower the energy of the system and lead to a new stable ground state. We shall work at fixed temperature and number density of the hyperfine states and will examine the difference between the free-energies of the superfluid state with deformations and the undeformed normal state. We shall assume that the conformal deformation is absent $\Xi = 0$ and look for a minimum of this difference with respect to a single parameter $\delta \epsilon$. The situation is similar to the description of the LOFF phase where one allows for the normal state spectrum to have a finite momentum $P$ and seeks the minimum of the appropriate thermodynamical potential as a function of $P$.

The free-energy of the superfluid phase is defined as

$$F_S = E_{\text{kin}} + E_{\text{pot}} - TS_S, \quad (9)$$
where the first two terms comprise the internal energy which is the statistical average of the Hamiltonian $H$ and $S_S$ is the superfluid entropy, defined by the well-known combinatorial expression. In our model the sum of the kinetic and potential energies is

$$E_{\text{kin}} + E_{\text{pot}} = \sum_p \epsilon_p \left( n_{p,1} + n_{p,2} \right) - \frac{\Lambda^2}{g}. \quad (10)$$

The free-energy of the undeformed normal state follows by setting in the above expressions $\Delta = 0 = \delta \epsilon$. Because of the contact form of the interaction the gap equation and the superfluid kinetic energy need a regularization. The regularized gap equation is

$$1 = \frac{g}{2(2\pi)^2} \int_0^\Lambda dp^2 \int_{-1}^{1} dx \left( \frac{1 - f(E_1) - f(E_2)}{\sqrt{\xi_S^2 + \Delta^2}} - \frac{\gamma}{\epsilon_p} \right), \quad (11)$$

where the case $\gamma = 1$ and $\Lambda \to \infty$ corresponds the common practice of regularization [1], which combines the gap equation with the $T$-matrix equation in the free space. The case $\gamma = 0$ and finite $\Lambda$ corresponds to the cut-off regularization of the original gap equation. The term $E_{\text{kin}}$ is regularized by a cut-off $\Lambda$, which is deduced from the requirement that both regularization schemes give the same result for the gap.

Eq. (11) was solved numerically with the constraint (7) for various values of the dimensionless parameter $k_Fa$ at density $\rho = 3.8 \times 10^{12}$ cm$^{-3}$ and temperature $T = 10$ nK. This density corresponds to $k_F \approx 4.8 \times 10^4$ cm$^{-1}$ and Fermi-temperature $T_F = 942$ nK. The triplet scattering length in vacuum for $^6$Li atoms in the hyperfine states $|1\rangle = |F = 3/2, m_F = 3/2\rangle$ and $|2\rangle = |3/2, 1/2\rangle$ is $a = -2160 a_B$, but as already pointed out can be easily manipulated using Feshbach resonances. Figure 1 displays the dependence of the pairing gap and the free-energy difference $\Delta F = F_S - F_N$ on the relative deformation for several density asymmetries and zero conformal deformation. We restrict the density asymmetry to positive values, i.e. assume $\rho_1 > \rho_2$; positive values of $\delta \epsilon$ correspond to a prolate (cigar-like) deformation of the majority and oblate (pancake-like) deformation of the minority population’s Fermi-spheres; for negative $\delta \epsilon$ the reversed is true. When there are no deformations, the antisymmetric part of the quasiparticle spectrum $\xi_A$, acts in the gap equation (10) to reduce the phase space coherence between the quasiparticles that pair; (when $\xi_A = 0$ the BCS limit is recovered with equal occupations for both particles and perfectly matching Fermi surfaces). This blocking effect is responsible for the reduction of the gap with increasing asymmetry and its disappearance above $\alpha \approx 0.07$ [see Eq. (1)]. Allowing for deformations introduces a modulation of $\xi_A$ with the cosine of the polar angle $x$ (in the frame where the $z$ axis is along the symmetry breaking axis), which acts to restore the phase space coherence for some values of $x$ at the cost of even lesser coherence for the remainder values. The result, seen in Figure 1, is the increase of the gap for finite deformations. At extreme large asymmetries the re-entrance effect sets in: the gap exists only for the deformed state, with lower and upper critical deformations marking the pairing regions. These features are seen for both the positive and negative values of $\delta \epsilon$, but are more pronounced for $\delta \epsilon > 0$; (quite generally our equations are not symmetric under the interchange of the sign of deformation, except when $\alpha = 0$). The free-energy difference $\Delta F$ mimics basically the gap function due to the contribution from the potential energy; note that the critical values of deformations at which $\Delta F$ vanishes do not coincide with those for the gap due to the positive contribution of the kinetic energy difference. The same calculations as above were carried out for larger couplings $k_Fa = 1$ and $k_Fa = 2$ with qualitatively similar results; the gaps found in the symmetric case are 1.93 and 3.75 nK, respectively, the reentrance effect is observed in each case for asymmetries around 0.18 and 0.3 and the pairing disappears above the asymmetries 0.22 and 0.43. Figure 2 compares the quasiparticle spectra $E_1$ and $E_2$ for combinations of $\alpha$ and $\delta \epsilon$. An important feature of the asymmetric ($\alpha \neq 0, \delta \epsilon = 0$) spectrum is its gapless nature, i.e. the existence of nodes for one (or both) branches of the spectra (c.f. with the gapped BCS spectrum also shown in Fig. 2). The spectra of the DFS phase cover the range bounded by the curves with $x = 0$ and $x = 1$. We conclude that the spectrum of deformed superfluid states is likewise gapless for a range of the an-
system was in the deformed superfluid state one would detect a mean momentum of particles of type 1 (majority) in the direction of symmetry breaking by about 20% larger than that of particles of type 2 (minority) in the same direction. Therefore, the presence of anisotropy in the detected momentum distributions is an evidence for a deformed superfluid state being the ground state of the system, as deformation alone (i.e., without pairing) would not lower the energy so as to produce a deformed non-superfluid ground state. The direction of spontaneous symmetry breaking (in \(k\)-space and, therefore, also in real space) is chosen by the system randomly and needs to be located in an experiment to obtain maximum anisotropy.

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FIG. 2: (Color online) The dependence of the quasiparticle spectra of two hyperfine states \(E_1\) and \(E_2\) on the momentum for \(\alpha = 0 = \delta \varepsilon\) (solid line); \(\alpha = 0.05\) and \(\delta \varepsilon = 0\) (dashed lines); \(\alpha = 0.05, \delta \varepsilon = 0.1\), \(x = 0\) (dashed-dotted) and \(x = 1\) (short-dashed lines). The Fermi-momentum \(k_F = 4.8 \times 10^4\) cm\(^{-1}\) is indicated by the vertical line. The remaining parameters are as in Fig. 1.

FIG. 3: (Color online) The dependence of the occupation probabilities of two hyperfine states on the momentum. The Fermi-momentum \(k_F = 4.8 \times 10^4\) cm\(^{-1}\) is indicated by the vertical line. The labeling of the lines is as follows: \(\alpha = 0 = \delta \varepsilon\) (solid line), \(\alpha = 0.05\) and \(\delta \varepsilon = 0\) (dashed lines); \(\alpha = 0.05, \delta \varepsilon = 0.1\), \(x = 0\) (dashed-dotted) and \(x = 1\) (short-dashed lines). The bell-shaped curves show the anisotropy - the difference between the \(x = 1\) and \(x = 0\) occupation numbers - for \(\alpha = 0.05, \delta \varepsilon = 0.1\). The remaining parameters are as in Fig. 1.

angles defined by the variable \(x\). The macroscopic features of the atomic DFS phase, such as responses to the density perturbations or electromagnetic probes, and their thermodynamic functions (heat capacity, etc) would differ from the ordinary BCS phase due to the nodes and anisotropy of their spectrum, as is the case for gapless and/or anisotropic metallic superconductors. Figure 4 shows the occupation numbers in BCS, deformed and/or asymmetric cases; varying the cosine of the polar angle \(x\) covers a range of probabilities which includes the undeformed asymmetric state. The bell-shaped curves show the angular polarization of the occupation numbers defined as \(\delta n_\sigma = |n_\sigma(x = 1) - n_\sigma(x = 0)|\). We observe up to 20% anisotropy in the occupation probabilities of particles along and orthogonal to the symmetry breaking axis.

In closing, we would like to address the issue of an experimental detection of the DFS phase. A direct way to detect the DFS phase is the measurement of the anisotropy in the momentum distribution of the trapped atoms. Such a measurement can be realized by the time-of-flight technique. This method uses the fact that after releasing the trap, the atoms fly out freely and an image of their spatial distribution taken after some time of flight provides information on their momentum distribution when confined inside the trap. Assuming that the...
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