BEC-BCS crossover in “magnetized” Feshbach-resonantly paired superfluids

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We map out the detuning-magnetization phase diagram for a “magnetized” (unequal number of atoms in two pairing hyperfine states) gas of fermionic atoms interacting via an s-wave Feshbach resonance (FR). The phase diagram is dominated by coexistence of a magnetized normal gas and a singlet paired superfluid with the latter exhibiting a BCS-Bose Einstein condensate crossover with reduced FR detuning. On the BCS side of strongly overlapping Cooper pairs, a sliver of finite-momentum paired Fulde-Ferrell-Larkin-Ovchinnikov magnetized phase intervenes between the phase separated and normal states. In contrast, for large negative detuning a uniform, polarized superfluid, that is a coherent mixture of singlet Bose-Einstein-condensed molecules and fully magnetized single-species Fermi-sea, is a stable ground state.

Recent experimental realizations of paired superfluidity in trapped fermionic atoms interacting via a Feshbach resonance (FR) [1, 2] have opened a new chapter of many-body atomic physics. Almost exclusively, the focus has been on equal mixtures of two hyperfine states exhibiting pseudo-spin singlet superfluidity that can be tuned from the momentum-pairing BCS regime of strongly overlapping Cooper pairs (for large positive detuning) to the coordinate-space pairing Bose-Einstein condensate (BEC) regime of dilute molecules (for negative detuning) [3].

In contrast, s-wave pairing for unequal numbers of atoms in the two pairing hyperfine states has received virtually no experimental attention and only some recent theoretical activity [4-11]. Associating the two pairing hyperfine states with up (↑) and down (↓) pseudo-spin σ, the density difference δn = n↑ - n↓ is isomorphic to “magnetization” m ≡ δn and the corresponding chemical potential difference δµ = µ↑ - µ↓ to a purely Zeeman field h ≡ δµ/2.

This subject dates back to the work of Fulde and Ferrell (FF) [11] and Larkin and Ovchinnikov (LO) [11] who proposed that, in the presence of a Zeeman field, an s-wave BCS superconductor is unstable to magnetized pairing at a finite momentum Q ≈ kF↑ - kF↓ with kFσ the Fermi wavevector of fermion σ. This FFLO state, which remains elusive in condensed matter systems where it is obscured by orbital and disorder effects, spontaneously breaks rotational and translational symmetry and emerges as a compromise between competing singlet pairing and Pauli paramagnetism.

Thus atomic fermion gases (where the above deleterious effects are absent), tuned near an s-wave FR, are promising ideal systems for a realization of the FFLO and related finite-magnetization paired states, that can be studied throughout the full BCS-BCS crossover.

In this Letter, we map out the detuning-magnetization phase diagram (Fig. 1) of such paired superfluids. We find that for positive detuning δ and arbitrarily small m, the system phase-separates into a magnetized normal gas (N) and a singlet-paired BCS superfluid that exhibits a BCS-BEC crossover with reduced δ. The FFLO state intervenes in a sliver on the boundary between this coexistence region and the N state. For large negative detuning a uniform magnetized superfluid (SF_D), that is a coherent mixture of singlet Bose-condensed molecules and fully magnetized single-species Fermi-sea is a stable ground state. Our predictions of these states and transitions between them are testable via thermodynamics (qualitatively modified by gapless atomic excitations inside the SF_D and FFLO states), sound propagation (with zeroth sound velocity vanishing at the SF_D-N transition), and

![FIG. 1: (Color Online) Detuning, δ - population difference, m/n = (n↑ - n↓)/(n↑ + n↓) phase diagram (for coupling γ = 0.1) in (a) displaying “normal” (N), magnetized superfluid (SF_D), FFLO (thick red line) and SF-N coexistence states, (b) showing the FFLO wavevector Q(δ) along the FFLO-N phase boundary, and (c) zoom-in on the FFLO state, stable only for δ > δ_c ≈ 2.2kF. To the right of the dashed lines in (a) and (c), the SF-N coexistence undergoes a transition to SF-FFLO coexistence.](image-url)
time of flight imaging (displaying density discontinuity and striking Bragg peaks associated with the finite momentum pairing in the FFLO state).

We now sketch the analysis that led to these results. A gas of fermionic atoms, $\tilde{a}_{k\sigma}$, resonantly interacting through a diatomic (closed-channel) molecule, $\tilde{b}_q$, is described by a two-channel Hamiltonian $H$:

$$H = \sum_{k,\sigma} (\epsilon_k - \mu) \tilde{a}_{k\sigma}^\dagger \tilde{a}_{k\sigma} + \sum_{q} \left( \frac{\epsilon_q}{2} + \delta_0 - 2\mu \right) \tilde{b}_q^\dagger \tilde{b}_q + g \sum_{k, q} \left( \tilde{b}_q^\dagger \tilde{a}_{k+\frac{1}{2}} \tilde{a}_{-k+\frac{1}{2}} + h.c. \right),$$  (1)

where $\epsilon_k \equiv k^2/2m_a$, $\mu_{\uparrow,\downarrow} = \mu + \delta$ are the chemical potentials to impose atom number in hyperfine states $\uparrow, \downarrow$, or the total atom density $n = n_{\uparrow} + n_{\downarrow} + 2 \sum_q (\tilde{b}_q^\dagger \tilde{b}_q)$ (imposed by $\mu$, with $n_{\sigma} = \sum_{q,\sigma} (\tilde{a}_{k\sigma}^\dagger \tilde{a}_{k\sigma})$) and density difference (magnetization) $m = n_{\uparrow} - n_{\downarrow} \equiv \delta_0$ (imposed by $h$). Here, $\delta_0$ is the bare FR detuning, $h$ is the FR coupling determining the resonance width and the system volume is unity.

For a narrow FR (small $h$), $g$ can be accurately analyzed by treating $\tilde{b}_q$ as a single-momentum $\tilde{b}_q$ c-number mode ($\tilde{b}_q \equiv b_q \hat{\delta}_{q,Q}$) with corrections small in powers of $\gamma \equiv \gamma_0 = g^2N(\epsilon_F)/\epsilon_F$, the ratio of the FR width to Fermi energy, with $N(\epsilon_F) = m_a^{3/2}/\sqrt{\pi}\epsilon_F^{1/2} \equiv c/\sqrt{\epsilon_F}$ the density of states at the Fermi energy $\epsilon_F = k_F^2/2m$ set by the total atom density $n = 4\pi\epsilon_F^3/2$. To lowest order in $\gamma$, standard Bogoliubov analysis gives the ground-state energy ($\hbar = 1$):

$$E_G = \langle H \rangle = \left( \frac{\epsilon_Q}{2} + \delta_0 - 2\mu \right) \frac{\Delta_Q^2}{\gamma^2} - \sum_k (E_k - \epsilon_k) + \sum_k \left[ E_{k\uparrow} \Theta(-E_{k\uparrow}) + E_{k\downarrow} \Theta(-E_{k\downarrow}) \right],$$  (2)

where $E_{k\sigma} = E_k \mp \hbar k \cdot Q/2m_a$ is the excitation spectrum for a hyperfine state $\sigma$, with “gap” $\Delta_Q \equiv gb_Q$ and $E_k \equiv (\epsilon_k^2 + \Delta_Q^2)^{1/2}$, $\epsilon_k \equiv \frac{k^2}{2m_a} - \mu + Q^2/8m_a$, and $\Theta(x)$ the Heaviside step function. The corresponding ground state is of the BCS form, but with pairing limited to momenta $k$ satisfying $E_{k\sigma} > 0$.

The phase diagram is determined by minimizing $E_G$ over $Q$ and $\Delta_Q \neq 0$ at fixed average total density $n$, population difference $m$, and physical detuning $\delta = \delta_0 - \gamma^2 \sum_k 1/2\epsilon_k$ (determined by the 2-body scattering amplitude). The competing ground states are: (i) a normal Fermi gas (N) with $\Delta_Q = 0$, (ii) a non-“magnetically” fully paired BCS-BEC superfluid (SF) with $\Delta_Q \neq 0$, $Q = 0$, and $m = 0$, (iii) a magnetized partially paired superfluid (SF$_M$) with $\Delta_Q \neq 0$, $Q = 0$, and $m \neq 0$, and (iv) a magnetized, finite-momentum paired superfluid (FFLO) with $\Delta_Q \neq 0$, $Q \neq 0$, and $m \neq 0$. Anticipating the existence of first-order transitions, across which $m, n$ are discontinuous, in order to guarantee a solution everywhere it is essential to also include phase-separated states where two of above pure states coexist as a mixture in fractions $1 - x$ and $x$ to be determined.

The computation of the ground-state energy is simplified by noting that $E_G(h) = E_G(0) - \int_0^h m(h')dh'$, where $E_G(0)$ is the well-studied fully-paired $h = 0$ energy and $m(h) = -\partial E_G/\partial h$ is the atom species imbalance number. We compute $E_G$ by first neglecting the FFLO state (i.e., $Q = 0$), which, as we shall show, is only stable for a narrow window of parameters (see Fig. 1). Then,

$$m(h) = \frac{2}{3} e\Theta(h - \Delta) \left[ \mu + \sqrt{h^2 - \Delta^2} \right]^{3/2} - \left( \mu - \sqrt{h^2 - \Delta^2} \right)^{3/2} \Theta(\mu - \sqrt{h^2 - \Delta^2}).$$  (3)

For positive detuning $\delta \gg \epsilon_F \gamma^{1/2}$, appropriate in the BCS and throughout most of the crossover regimes, $\Delta \ll \mu$ and the density of states inside $E_G(0)$ can be well approximated by a constant $N(\mu)$, giving:

$$E_G^+ \approx \frac{1}{g^2} (\delta - 2\mu) \Delta^2 + N(\mu) \left[ -\frac{1}{2} \Delta^2 + 2 \Delta^2 \log \left( \frac{\Delta}{8\epsilon_0^2 - \mu} \right) \right] - 8N(\mu)/15 - \int_0^h m(h')dh'.$$  (4)

For small $h \ll \mu$ the species imbalance contribution to $E_G$ is well approximated by $\int_0^h m(h')dh' \approx N(\mu)\Theta(h - \Delta) \left[ h/\sqrt{h^2 - \Delta^2} - \Delta \cosh^{-1}(h/\Delta) \right]$. For $0 < h < \Delta_{BCS}/2$, $E_G$ exhibits a single minimum at a standard ($h = 0$) BCS value $\Delta_{BCS} = 8\epsilon_0^2 - \mu \epsilon_F^{-1}(\delta - 2\mu)/(\epsilon_F \mu)^{1/2}$ and a maximum at $\Delta = 0$. For a higher Zeeman field $\Delta_{BCS}/2 < h < \Delta_{BCS}/\sqrt{2}$, the normal state at $\Delta = 0$ becomes a local minimum separated from the $h$-independent global minimum at $\Delta_{BCS}$ by a maximum at $\Delta_{BCS} = \sqrt{2}/2\Delta_{BCS} - 1$.

For $h > \Delta_{BCS}/\sqrt{2}$ the minimum at $\Delta = 0$ lowers below that of the BCS state. For a fixed $\mu$, this predicts a first-order SF-N transition at $h_c(\mu, \delta)$, with asymptotic form in the narrow FR limit given by:

$$h_c(\mu, \delta) \approx a_1 \mu e^{-a_2^2(\delta - 2\mu)/\sqrt{\epsilon_F}},$$  (5)

where $a_{1,2} = 8\epsilon_0^{-2}/\sqrt{2}, 1$ ($20\epsilon_0^{-5} e^{-8/5}, 4/5$), for $\mu / \delta \ll 1$. The transition is accompanied by a jump in atom density from $n(\mu, \delta) \approx \frac{4}{9} N(\mu)(\mu + 2g^2\Delta_{BCS}^2)$ down to $n(\mu, \delta) \approx \frac{4}{9} N(\mu)(\mu + \delta)^2 \Theta(\mu - h_c) \approx n(S, \delta)(\mu, \delta) \approx \frac{1}{2} e^2 E_c(1 - \gamma(\mu)/8)$, a jump in specics imbalance from 0 to $m \approx 2N(\mu)h_c$, as well as other standard thermodynamic singularities.

In a more experimentally relevant ensemble of fixed total atom number $n = -\partial E_G/\partial \mu$, for $h_c1 \equiv h_c(\mu(\mu), \delta) < h < h_c2 \equiv h_c(\mu(\mu), \delta)$ neither SF nor N states can satisfy the atom number constraint while remaining a ground state; $\mu(S,N)$ are SF and N chemical potentials at density $n$, Zeeman field $h$ and detuning $\delta$, obtained by solving $n = n(S,N)(\mu(S,N))$ above.
For a narrow FR, $\gamma \ll 1$, we find

$$h_{c1}(\delta, n) \approx \begin{cases} \frac{1}{\sqrt{2}} \Delta_F(\delta) e^{-\frac{(\Delta_F(\delta))^2}{2}}, & \text{for } \delta \gg 2\epsilon_F, \\ \frac{1}{2} g \left[ n - \frac{\epsilon}{2}(\delta/2)^{3/2} \right]^{1/2}, & \text{for } \delta \ll 2\epsilon_F, \end{cases}$$

$$h_{c2}(\delta, n) \approx \begin{cases} \frac{1}{\sqrt{2}} \Delta_F(\delta) e^{-\frac{(\Delta_F(\delta))^2}{2}}, & \text{for } \delta \gg 2\epsilon_F, \\ \frac{1}{h(N)(\delta/2, n)}, & \text{for } \delta \ll 2\epsilon_F, \end{cases}$$

where $\Delta_F \equiv \Delta_{BCS}(\delta, \epsilon_F)$ and $h(N)(\delta/2, n)$ is the solution of $n = n(N)(\delta/2, h(N))$. Hence for $h_{c1} < h < h_{c2}$ the gas phase separates into SF and N rich regions in $1 - x(h, \delta)$ and $x(h, \delta)$ proportions, determined by the atom number constraint $\bar{x}n(N) + (1 - x)n(S) = n$. In above $n(S)(\mu_c, \delta) > n > n(N)(\mu_c, \delta)$ are the SF and N state densities computed along the critical chemical potential $\mu_c(h, \delta)$ determined by Eq. (5) with limiting values $\mu_c(h_{c1,2}, \delta) = \mu^{S,N}(n, \delta)$. The fraction of the N state admixture is then given by $x(h, \delta) = \left( n(S)(\mu_c, \delta) - n \right) \left[ n(S)(\mu_c, \delta) - n(N)(\mu_c, \delta) \right]^{-1}$ ranging between 0 and 1 for $h_{c1} < h < h_{c2}$ spanning the coexistence region.

A single-valued relation between the magnetization (species imbalance) $m(h, \delta) = \frac{1}{2} \xi \left[ (\mu_c(h, \delta) + h)^{3/2} - (\mu_c(h, \delta) - h)^{3/2} \right] \Theta(\mu_c - h)$ and Zeeman field $h$ in the normal paramagnetic state allows us to reexpress above predictions in terms of the species imbalance number $M = mn$, that is, the quantity (rather than $h$) that we anticipate to be kept fixed in atomic gas experiments. As illustrated in Fig. 1 in a phase diagram expressed in terms of $\mu$ and $\gamma$ for a fixed atom density $n$ the fully-paired SF state is confined to the detuning axis ($m = 0$) and the boundary between the coexistence region and the N state is given by $m_{c2}(n, \delta) = m(h_{c2}, \delta)$.

We now turn to the negative detuning (BEC) regime. Although $E_G$, Eq. (2) and the phase diagram that follows from it can be accurately computed numerically (Fig. 1), considerable insight can be gained by analytical analysis. This is particularly simple in the $\gamma \rightarrow 0$ limit in which $E_G \approx (2\epsilon - 2\mu) \delta^2 + c\mu^2 \pi^2 \int \left( \frac{\Delta}{|\mu|} \right)^2 + \frac{1}{2} \left( \frac{\Delta}{|\mu|} \right)^4 - \frac{5}{16} \left( \frac{\Delta}{|\mu|} \right)^6 + \frac{105}{16} \left( \frac{\Delta}{|\mu|} \right)^8 - \int_0^1 m(h') dh'$. Its minimization together with the atom number constraint fixes $\mu \approx \delta/2 + O(\gamma)$ and leads to the phase diagram in Fig. 1. We find that above expressions for $h_{m}(\delta)$ and $h_{c2}(\delta)$ receive only small $O(\gamma)$ correction for $\delta < -\gamma^{1/2}\epsilon_F$. Hence in contrast to the BCS side, where the system undergoes phase separation for an arbitrary small $m \neq 0$, on the BEC side the transition at $h_{c1}(\delta)$ is into a uniform magnetized superfluid (SF$_M$) that persists over a finite range of $m$ and is a coherent superposition of a singlet molecular condensate and fully spin-polarized Fermi gas. The sequence SF$\rightarrow$SF$_M\rightarrow$N of continuous transitions remains unchanged for $\delta < \delta_c \approx -10.66\epsilon_F$. However, for a finite $\gamma$ and $\delta_c \approx -10.66\epsilon_F < \delta < -\gamma^{1/2}\epsilon_F$ a secondary local (N state) minimum develops at $\Delta = 0$ leading to a 1st-order SF$_M \rightarrow$N transition at $h_{c1}(\delta) \approx -0.66\epsilon_F < h_{c2}(\delta)$, preempting a continuous one at $h_{c2}(\delta)$. For a fixed atom density $n$ and $h_{c1}(\delta) < h < h_{c2}(\delta)$ the gas phase-separates into coexisting SF$_M$ and N states.

This $h_{c1}(\delta)$ boundary (equivalent to $m_{c1}(\delta) \equiv m(h_{c1}(\delta), \delta/2) \approx 0.029n/|\epsilon_F|^{3/2}$) is accurately (to $O(\gamma^2)$) computed inside the BCS and crossover regimes.

For a narrow FR $E_G^- (\Delta, \mu, \delta, h)$ can be accurately computed analytically giving

$$E_G^- \approx \frac{1}{g^2} \delta^2 - 2\mu \delta^2 + c\mu^2 \pi^2 \left( \frac{\Delta}{|\mu|} \right)^2 + \frac{1}{2} \left( \frac{\Delta}{|\mu|} \right)^4 - \frac{5}{16} \left( \frac{\Delta}{|\mu|} \right)^6 + \frac{105}{16} \left( \frac{\Delta}{|\mu|} \right)^8 - \int_0^1 m(h') dh'. \quad (8)$$

FIG. 2: Bogoliubov sound speed $u$ in the BEC regime as a function of species imbalance $m$ for $\delta = -2\epsilon_F$, vanishing at boundary of the SF$_M$ with the SF $- N$ coexistence region.
is illustrated in Fig. [2] and given by (with $\hat{\delta} \equiv \delta/\epsilon_F$)
\[
 u \approx u_0 \sqrt{1 - m/n} \sqrt{F\left(1 + \frac{2^{5/3}}{\epsilon_F} \left(\frac{m}{n}\right)^{2/3}\right)},
\]
with $F(x) \equiv 1 - \frac{2}{x} \left[\sqrt{x - 1}(x + 2) + x^2 \tan^{-1}\sqrt{x - 1}\right]$ and $u_0 = \frac{2^{3/2} \epsilon_F^{3/2}}{8\sqrt{3} |\delta|^{3/4}}$ the sound velocity at $m = 0$.

We now turn to the FFLO state. Because $Q \neq 0$ pairing is driven by the mismatch of the up $\uparrow$ and down $\downarrow$ Fermi surfaces, with $Q \approx h_F - k_F$, it is clear that the FFLO state can only be stable at large positive detuning. Computing $E_G^\uparrow$ for $Q \neq 0$ at leading order in $\Delta_Q \ll \mu$ (using dimensionless quantities $\Delta_Q \equiv \Delta_Q/\epsilon_F$, $\mu \equiv \mu/\epsilon_F$ $\hat{h} \equiv h/\epsilon_F$, $Q = Q\sqrt{\mu}/k_F$, and $\epsilon_G \equiv E_G/\epsilon_F^{5/2}$), we find:
\[
\epsilon_G \approx -\frac{8}{15} \mu^{5/2} + \frac{\hat{h}^2}{2\gamma} + \sqrt{\mu} \left[\Delta_Q^2 - \hat{h}^2\right]
\]
\[
+ \frac{\Delta^2_{BCS}}{2} \ln \frac{4(\hat{h} + Q)(\hat{h} - Q)}{2} + \frac{\Delta^2_{BCS}}{2Q} \ln \frac{\hat{h} + Q}{Q - \hat{h}} + \frac{\Delta^2_{BCS}}{8}
\]
\[
\frac{\Delta^2_{BCS}}{Q^2 - h^2}.
\]

At fixed $\mu$, for a given $\hat{\delta}$ and $\hat{h}$, the ground state is determined by minimizing $\epsilon_G(\Delta_Q, Q)$ over $\Delta_Q$ (the gap equation) and $Q$ (equivalent to vanishing of the ground state momentum). For $\delta \gtrsim 2\epsilon_F$ we find a 1st-order SF-FFLO (preempting SF-N) transition approximately at $h_{c1}(\delta, \mu)$, Eq. [6]. At fixed atom number, for $h > h_c$, the gas phase separates into coexisting SF and FFLO states, approximately bounded above by $h_{c2}(\delta)$, computed for $Q = 0$ above. At slightly higher field, $h_{cFLO}(\delta)$, we find that the FFLO state undergoes a continuous transition (that on general grounds we expect to be driven 1st-order by fluctuations) into the N state. Numerical solution of the gap, number and momentum equations yields $h_{FLO}(\delta)$ (and thus $m_{FLO}$) via Eq. [3], plotted in Fig.1 that interpolates between 0.7544$\xi_\rho(\delta)$ for large $\delta$ (in agreement with FF [10] and $h_{c1}(\delta, n)$ for $\delta \rightarrow \delta_s$, with the crossing point $\delta_s \approx 2\epsilon_F$. This microscopically calculated value of $\delta^* \gtrsim 0$ contrasts with the conclusion of Ref. [8], the latter based on a purely qualitative discussion, that has little quantitative predictive power, e.g., in determining the precise location of phases.

In free expansion experiments, the FFLO state, most easily observed with a trap having a typical size that is large compared to $Q^{-1}$, should exhibit a BEC peak (observed by its projection onto the molecular condensate) shifted by $\hbar Q t / m_a$ (time expansion) corresponding to the finite momentum $hQ(\delta)$ (Fig.1b) of its condensate, and a (spontaneous) Bragg lattice of peaks in the more-likely case of multiple-$Q$ pairing. The anisotropy of the FFLO pairing should also be reflected in “noise” experiments sensitive to angle-dependence of pairing correlations across the Fermi surface. Our predictions of gapless atomic excitations in the SF$_M$ and FFLO states, as well as the vanishing of the molecular scattering length $a_m$ and of the 0th sound velocity $u$ at the SF$_M$-N phase boundary should be observable through Bragg spectroscopy and reflected in thermodynamics (e.g., heat capacity that is power-law in $T$). We also expect standard thermodynamic anomalies across phase transitions in $\xi$ (a), and phase separation accompanied by density discontinuity and local density variation with detuning and atom imbalance across the coexistence region.

Finally, because a gas trapped in a smooth potential $V(r)$ is well-characterized by a local chemical potential $\mu(r) = \mu - V(r)$ (the Thomas-Fermi approximation), our fixed $\mu$ analysis is directly experimentally relevant. For negative detuning and finite species imbalance we predict SF state in the cloud’s core of radius $r_0(\delta)$, with density discontinuity to the outer-shell N state, with $r_0(\delta)$ determined by $\mu(r_0) = \mu_c(\delta, \mu)$ (see center inset of Fig.1a). We expect that this shell structure should be readily observable, particularly if different hyperfine states and closed and open channels can be imaged independently. Details of these experimental predictions will be presented in a forthcoming publication [15].

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