Polarized superfluidity in the attractive Hubbard model with population imbalance

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We study a two-component Fermi system with attractive interactions and different populations of the two species in a cubic lattice. For an intermediate coupling we find a uniformly polarized superfluid which is stable down to very low temperatures. The momentum distribution of this phase closely resembles that of the Sarma phase, characterized by two Fermi surfaces. This phase is shown to be stabilized by a potential energy gain, as in a BCS superfluid, in contrast to the unpolarized BEC which is stabilized by kinetic energy. We present general arguments suggesting that preformed pairs in the unpolarized superfluid favor the stabilization of a polarized superfluid phase.

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The study of superfluid phases is a fundamental issue in condensed matter physics. It has received a revived interest with the experimental realization of cold atomic systems that allow to probe such phases with a remarkable controllability.1–3 It is for instance possible to address a large range of interaction strengths or to control the population imbalance between atoms in different hyperfine states. For fermionic fluids composed of two species, the latter parameter, which introduces a mismatch in the Fermi surfaces, raises exciting questions about the stability of the conventional superfluid phase and the possible generation of more exotic ones. Indeed, in the absence of imbalance, a weak attractive interaction between the fermionic species stabilizes a Bardeen-Cooper-Schrieffer (BCS) ground state, with a pairing between species of opposite momentum near their common Fermi surface. When the interaction is strong, the fermions pair in real space, and superfluidity is associated with the Bose-Einstein condensation (BEC) of pairs. The BEC-BCS crossover has been studied intensively both experimentally4–6 and theoretically7–10.

The situation is far less clear when a population imbalance introduces a mismatch between the Fermi surfaces. At small imbalance, the species are expected to still form a standard BCS or BEC state. At larger imbalance, either superfluidity disappears in favor of a polarized normal fluid or more exotic forms of pairing occur. One candidate is the Fulde-Ferrell-Larkin-Ovchinnikov state11–14 in which Cooper pairs appear at a non-zero total momentum. At zero temperature, two other possible phases that exhibit both a non-zero superfluid order parameter and a finite polarization have been proposed: the Sarma (or breached-pair BP2) phase15,16 and the BP1 phase17–19. At weak-coupling, the Sarma phase is unstable unless specific types of interactions are considered.20 The BP1 has been proposed as a stable ground state deep in the BEC regime of trapped fermionic gases, where the system is described by a Bose-Fermi mixture. While both of these phases are polarized superfluids with gapless excitations, their nature is different: the Sarma phase has two Fermi surfaces while the BP1 phase has a single Fermi surface for the unpaired fermions. These non-standard phases are in general unstable at weak coupling, resulting in phase separation between an unpolarized superfluid and a polarized normal fluid formed by the excess fermions, an effect which has been observed experimentally.21–23 At zero temperature T = 0, the Sarma and BP1 phases are signaled by a non-zero superfluid order parameter together with a finite polarization. When T > 0, this criterion is no longer valid because a standard BCS or BEC state also acquires a small polarization coming from thermally excited quasiparticles.

In this paper, we focus on polarized superfluid phases (pSF) in a three-dimensional cubic lattice. We study their nature at weak and intermediate coupling as a function of the temperature, treating the effect of correlations beyond static mean field. Our main result is that, at intermediate coupling, a pSF phase can be stabilized down to very low temperatures, with properties which are clearly associated with the Sarma phase. The mechanism responsible for this stabilization is the reduction of the polarizability of the normal fluid due to the existence of preformed pairs. We will show that this phase is profoundly different from the unpolarized BEC superfluid which holds at the same coupling strength in the absence of imbalance.

We start with some energetic considerations, which clarify the general conditions under which a pSF phase can be stable at T = 0. In order to control the imbalance between the populations of the two species, we introduce a chemical potential difference (or effective ‘magnetic field’) $h \equiv (\mu_1 - \mu_2)/2$ between them. In Fig. 1 we show two typical behaviors of the energy in different phases as a function of the magnetic field. In both cases, a small magnetic field h is expelled from the unpolarized superfluid, and the energy is independent of h. This unpolarized superfluid is locally stable up to a critical value...
$h_c$. For $h > h_c$ the magnetic field breaks the pairs, leading to the disappearance of this solution. On the other hand, the energy of the polarized normal state is a decreasing function of $h$: its derivative $p \equiv -\partial E/\partial h > 0$ is the polarization (population imbalance) and its curvature $\chi \equiv -\partial^2 E/\partial h^2 - \partial p/\partial h$ defines the polarizability of the normal fluid.

In general the pSF phase can bridge between these two solutions. The way in which this connection occurs depends on the two key parameters $h_c$ and $\chi$. When $h_c$ and $\chi$ are large, we anticipate the situation in Fig. 1a. In this case, the pSF branch is expected not to be stable, and the system undergoes a first-order transition as a function of $h$. When $h_c$ and $\chi$ are small, we expect the situation in Fig. 1b. In this case, the pSF branch is stable.

In order to explore the validity of these qualitative arguments we study an attractive Hubbard model at half-filling, on a three-dimensional cubic lattice with nearest-neighbor hopping:

$$\mathcal{H} = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) - U \sum_i n_i \mu_i - \mu \sum_i n_i \sigma$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (destroys) a fermion of species $\sigma$ on the site $i$, $n_i = c_{i\sigma}^\dagger c_{i\sigma}$ is the number operator, $t$ is the hopping amplitude and $U > 0$ is the Hubbard on-site attraction. When the total number of fermions is identical to the number of lattice sites (half-filling) $\mu_1 = -U/2 + h$ and $\mu_1 = -U/2 - h$. In the following, all energies will be expressed in units of the half-bandwidth $D = 6t = 1$. We analyze the model within dynamical mean-field theory (DMFT) [24], which realizes a quantum (dynamical) mean field of the lattice model in terms of a single correlated site embedded in a self-consistent bath. This correlated local problem is then solved using continuous-time quantum Monte Carlo (CTQMC) [23]. Contrary to static mean-field approximations, whose validity is expected to be limited to weak interactions, DMFT allows to study all the interaction regimes [24]. We compare the DMFT results with simpler static mean-field calculations, namely with a standard BCS mean field and a more accurate ‘BCS-Stoner’ mean field [13, 26], which introduces a mean-field decoupling of the interaction both in the particle-particle channel (as in BCS) and in the particle-hole channel (as in Stoner theory) in order to compute both the superfluid order parameter and the polarization self-consistently.

We first consider a rather weak coupling $U = 0.5$. The phase diagram obtained by using the BCS, BCS-Stoner and DMFT approaches is presented in Fig. 2. For large $p$ or at high $T$ the stable phase is the polarized normal fluid. As $T$ is decreased the system enters

![FIG. 1: (Color online) Sketches of the energy $E$ vs $h$, for the normal state, the unpolarized superfluid (SF) and the pSF phase. Two situations can appear as function of the external parameters (e.g. the interaction strength). Left panel (a): the pSF branch is unstable and the system undergoes a phase separation. Right panel (b): the pSF branch is stable.](image1)

![FIG. 2: (Color online) Lower panel (e): Phase diagram in the $T - p$ plane at weak coupling $U = 0.5$ (lower panel) obtained using DMFT, BCS and BCS-Stoner mean-field. $T_{SF}$ and $p_c$ are defined in the text. pSF, PS and N label polarized superfluid, phase separation and normal phase, resp. The results are plotted against $p/(p_cD_{pSF})$ to allow for a comparison in relative units. Upper panels (a-b): free-energy vs. $h$ below and above the critical temperature $T_c$. Middle panels (c-d): momentum distribution $n(k)$ at three points (A), (B), (C) indicated on the free-energy curves of panel (a).](image2)
a pSF phase which exhibits both a non-zero superfluid order parameter $\Delta = (U/N) \langle \sum_i c_i^\dagger c_i \rangle$ and a finite polarization. When $T$ is further lowered, the pSF phase becomes unstable towards a phase separation between a thermally excited BCS superfluid and a polarized normal fluid. While the overall phase diagram is the same in all approaches in relative units (defined below), the BCS mean-field underestimates the extent of the pSF phase with respect to DMFT, mainly because it overestimates $\chi$ in the normal state. This effect is substantially reduced by the BCS-Stoner mean-field, in which the population imbalance is determined self-consistently. This leads to a lower $\chi$, which extends the stability of the pSF phase and improves the agreement with DMFT. Note that, for each approach, the temperature is normalized by $T_{SF}$, the superfluid critical temperature at $h = 0$. The polarization is normalized by $p_c/p_{c,DMFT}$, where $p_c$ is the polarization of the normal phase at $T = 0$, $h = h_c$, and $p_{c,DMFT}$ is the value of $p_c$ obtained with DMFT. The values of $T_{SF}$ and $p_c$ are overestimated in static mean-field approximations, making a comparison in relative units more appropriate. In these units, the BCS-Stoner phase diagram is seen to be in good agreement with the DMFT result in this weak-coupling regime.

Let us now discuss the nature of these phases. The BCS-Stoner mean-field calculation shows that in the phase-separated region, with $T < T_c$, the free-energy as a function of $h$ has three branches (Fig. 2a) as in the scenario of Fig. 1h. If $T$ is small, the properties of the three branches are directly linked to their $T = 0$ counterparts. One branch corresponds to the BCS superfluid with thermal excitations. It has a small polarization that comes from thermally excited Bogoliubov quasiparticles in a small momentum-range around the Fermi momentum $k_F$ of the unpolarized state. As a consequence, the density $n(k)$ deviates from the standard BCS distribution around $k_F$ over a range of order $T/k_F$ (see A in Fig. 2c). This branch is connected to the unstable thermally excited Sarma phase. In contrast to the BCS state, the Sarma phase has two Fermi surfaces at $T = 0$, which are individually broadened when $T > 0$. This is clearly visible in $n(k)$ (see B in Fig. 2b) which displays two humps associated with each Fermi momentum, with a separation set by the polarization instead of the thermal broadening.

As the temperature $T$ is increased, the unstable branch becomes smaller and eventually disappears at $T = T_c$. For $T > T_c$, the pSF phase is stable and the free-energy has the behavior shown in Fig. 2b, with only two solutions. Because $T_c$ is rather large, there is no clear distinction between the thermally excited BCS and the Sarma phases: as $h$ is increased along the superfluid branch a crossover takes place between the BCS regime and the Sarma regime. However, because $T$ is large, no particular structure appears in the density $n(k)$, even close to the normal phase (see C in Fig. 2c). Therefore, at weak coupling, the stable pSF phase has essentially a thermal nature and its properties cannot be linked to the physics of the Sarma phase.

We now turn to an intermediate coupling $U = 2.5$, where for identical populations the superfluid state is on the BEC side of the BCS/BEC crossover [27, 28, 29]. In this regime, the static mean-field approximations are not expected to be accurate and we only describe our DMFT results. As is clear from Fig. 3e, the interaction strongly increases the stability region of the pSF phase compared to the small $U$ case: it exists for a larger range of polarization (up to $p \lesssim 16%$ instead of $p \lesssim 3%$ for $U = 0.5$) and is stable down to the lowest temperature we could investigate with DMFT ($T/T_{SF} = 0.049$). From our present CTQMC solutions of DMFT, we cannot determine whether a phase separation eventually appears at lower temperatures, as in the weak coupling regime, but extrapolations of our numerical data are consistent with a stable pSF phase down to $T = 0$.

In Fig. 3a–d we plot the superfluid order parameter $\Delta$ and the polarization as a function of $h$ for different temperatures. At high temperatures, the polarization gradually increases with $h$ and the pSF phase smoothly connects to the normal phase. As the temperature is decreased, two regimes appear in the pSF phase, even though there is no phase transition between them. At small $h \lesssim 0.75$, the polarization is very small and can be traced back to thermal excitations in the BEC state.
Around $h \sim 0.75$ a stable branch connects to the normal phase. The polarization in this branch is too large to originate from thermal fluctuations and it has a different nature. Indeed, the density $n(k)$ in this region (Inset in Fig. 3b) displays two humps, just like in the weak-coupling Sarma phase (Fig. 2). This is very different from what is expected at low temperature in a standard thermally excited superfluid where $n(k)$ is broadened around $k_F$ over a small range $\sim T/v_F$. The two humps also indicate that the underlying $T = 0$ phase has two Fermi surfaces, unlike the BP1 phase proposed deep in the BCS regime of trapped fermionic gases. This shows that at intermediate couplings on a lattice, it is not possible to reduce the problem to a simple Bose-Fermi mixture.

Hence, our results show that a larger coupling stabilizes a region which displays properties very similar to the Sarma phase discussed at weak coupling, in agreement with the qualitative energetic arguments that a reduced polarizability and preformed pairs help stabilizing the pSF phase at low temperatures. This is actually confirmed by a direct computation of the energetic balance underlying this stabilization. The total internal energy and the kinetic energy of each phase are displayed in Figs. 3a-b as a function of $h$, for $U = 2.5$ and $T = 0.148 T_{SF}$. For this very low temperature, the entropy term can be neglected and we consider the energy instead of the free-energy. The total energy curve nicely follows the second scenario described above (Fig. 1b). A stable pSF phase bridges between the flat energy of the unpolarized superfluid and the energy curve of the polarized normal fluid. The total energy branch corresponding to the normal phase is seen to have a reduced curvature in comparison to weaker couplings, indicating a small $\chi$ of the normal fluid (within DMFT, this branch has actually vanishing polarization up to a field $h \sim 0.4$). These effects strongly favor the stability of the pSF phase.

The energetic balance of the transition to the pSF state is particularly interesting. In the absence of imbalance it has been shown that for $U = 2.5$ the system is in the BEC regime and the superfluid state is stabilized by a gain in kinetic energy [27, 28, 29], in contrast with the BCS state. The total energy curve of this branch is broadened around $k_F$ over a small range $\sim T/v_F$. The two humps also indicate that the underlying $T = 0$ phase has two Fermi surfaces, unlike the BP1 phase proposed deep in the BCS regime of trapped fermionic gases.

In conclusion, general arguments based on energy considerations suggest that a polarized superfluid phase can be stabilized by the formation of preformed pairs with a reduced polarizability on the BEC side of the BCS-BEC crossover. We have substantiated these arguments with a DMFT solution of the half-filled attractive Hubbard model on the cubic lattice, which demonstrates the stabilization of a pSF phase down to very low temperatures for an intermediate coupling $U/(6t) = 2.5$. The nature of this phase is closely connected to the physics of the Sarma’s (BP2) phase that has been previously discussed at weak coupling by static mean-field theory, but is usually unstable in this regime. We have shown that the stabilized pSF phase is clearly distinct from a BP1 phase and from a standard thermally excited superfluid state. Finally, while the BEC superfluid (in contrast to the weak-coupling BCS one) is stabilized by a gain in kinetic energy, the pSF-phase condensation energy corresponds to a potential energy gain in comparison to the polarized normal fluid.

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