Asymmetric Two-Component Fermion Systems in Strong Coupling

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We study the phase structure of a dilute two-component Fermi system with attractive interactions as a function of the coupling and a finite number asymmetry or polarization. In weak coupling, a number asymmetry results in phase separation. A mixed phase containing symmetric superfluid matter and an asymmetric normal phase is favored. For strong coupling we show that the stress on the superfluid phase to accommodate a number asymmetry increases. Near the infinite-scattering length, we calculate the single-particle excitation spectrum and the ground-state energy. A picture of weakly interacting quasiparticles emerges for modest polarizations. In this regime a homogeneous phase with a finite population of quasiparticle states characterized by a gapless spectrum is favored over the phase separated state. These states may be realized in cold atom experiments.

Recent experiments on cooled Fermi atoms [1–4] and theoretical developments in dense QCD [5] have motivated renewed theoretical interest in Fermion superfluids. In Fermi systems it is well known that attractive interactions destabilize the Fermi surface. This instability is resolved by the BCS mechanism characterized by pairing between spin-up and spin-down particles with opposite momenta on the Fermi surface. The system exhibits superfluid properties and has a gap in the excitation spectrum. Measurements have been performed probing the equation of state (EOS) [2] and the pairing gap [3,4] in the strongly interacting regime. Quantum Monte Carlo (QMC) methods have also been employed to examine these properties [6–9].

These studies have primarily addressed the unpolarized system. In contrast, the ground-state properties of an asymmetric two-component system remain unclear as several competing states have been proposed. These include: a gapless superfluid [10–14], a mixed phase consisting of BCS and normal components [15], and the Larkin, Ovchinnikov, Ferrel, and Fulde (LOFF) phase where the order parameter acquires a spatial variation [16,17] which, in three dimensions, may manifest as the crystalline state [18]. The competition between these states is especially relevant to understanding the phase structure of dense quark matter [5]. In this Letter we address several issues relating to the ground state of an asymmetric two-component Fermi system in the strong-coupling regime. Using both mean-field theory and QMC we find that in strong coupling and at finite polarization the stress on the BCS state to accommodate the number asymmetry increases. In the intriguing strong-coupling regime near $k_F a = \infty$, a superfluid state with nontrivial gapless excitations may be favored. We also find that these quasiparticles are weakly interacting.

Two-component Fermi system.—We consider a system consisting of nonrelativistic spin-up and spin-down

Fermions at finite polarization. A short-range potential (range range $\ll$ interparticle distance) between spin-up and spin-down particles characterizes the interaction. The interaction between spin-up particles (or spin-down particles) is considered to be negligible compared to the interaction between up and down spins. We study both weak coupling and strong-coupling limits to explore the phase structure from the BCS-like regime characterized by pairing at the Fermi surface to the Bose Einstein condensate regime characterized by bound bosonic states.

The Hamiltonian (grand canonical) is given by

$$H = \sum_{k,s=\uparrow,\downarrow} \left(\frac{k^2}{2m} - \mu_s \right) a_s^\dagger a_s + g \sum_{k,p,q} a_{k+q\uparrow}^\dagger a_{p-q\downarrow}^\dagger a_{k\uparrow} a_{p\downarrow},$$

where g is the effective four-fermion interaction whose strength at low energy is determined by the two-body scattering length a. For the two-component system, the spin-up and spin-down chemical potential may be written as $\mu_\uparrow = \mu + \delta\mu$ and $\mu_\downarrow = \mu - \delta\mu$, respectively. The density $n = n_\uparrow + n_\downarrow$ determines μ and the polarization density $\delta n = n_\uparrow - n_\downarrow$ determines $\delta\mu$. In trapped atom experiments this regime can be accessed by adjusting the population of the two species.

Initially, we consider a Fermi system in the "universal" regime characterized by an infinite-scattering length. When $a = \infty$, the interaction does not present a dimensionful scale. Consequently, the energy density, pressure, and chemical potential of the unpolarized system are related to that of the Fermi gas (FG) by the relation $\epsilon(a = \infty) = \xi \epsilon_{FG}$, $P(a = \infty) = \xi P_{FG}$, and $\mu = \xi k_F^2/2m$, respectively. Quantum Monte Carlo studies in small systems with 12–20 particles have determined this numerical coefficient to be $\xi = 0.44(2)$ [7]. The system also exhibits a gap in the excitation spectrum; numerical studies indicate that the gap $\Delta = 0.95(5)E_{FG} = \beta\mu$ with $\beta \approx 1.4$. Below we present new calculations for larger system sizes, which

are useful to more fully explore the dispersion of the single-particle excitations. For these larger systems we find $\xi = 0.42(1)$ and $\Delta = 0.84(5)E_{FG}$. We note that the value for ξ is in agreement with experimental studies described in Ref. [2].

Our primary interest here is the spin-polarized system. Earlier work by Bedaque, Caldas, and Rupak based on BCS mean-field theory showed that a finite polarization would lead to phase separation [15]. A heterogeneous mixed phase consisting of an unpolarized superfluid state coexisting with a partially polarized Fermi gas state was shown to have lower free energy than the homogeneous gapless superfluid phase (also called the breached-pair phase) suggested earlier by Liu and Wilczek [12]. More recently, Forbes, Gubankova, Liu, and Wilczek [19] have shown that the this phase may be stabilized by finite-range interactions and different masses for the two species. Here, though, we consider the equal mass case with short-range interactions, examining the phase structure at stronger coupling.

Normal-superfluid mixed phase.—Polarizing the superfluid state is disfavored due to the presence of a gap in its excitation spectrum A heterogeneous state containing normal and superfluid phases provides an alternate route to accommodate a finite polarization. Here the excess spin-up particles could reside in the normal phase.

Phase coexistence is possible between states separated by a first order transition if at fixed chemical potential they can have the same pressure. Hence we require

$$P_{\text{Superfluid}}(\mu, \delta\mu) = P_{\text{Normal}}(\mu, \delta\mu). \qquad (1)$$

Pressure equilibrium uniquely determines $\delta\mu$ for a given μ. We emphasize that at fixed μ, $\delta\mu$ in the mixed phase does not change with polarization—it is driven to lie exactly at the first order transition point satisfying Eq. (1). An increase in net polarization is accommodated by an increase in the volume fraction of the normal phase.

We observe that $\delta\mu$ is the energy required to introduce a spin-up particle into the normal component of the mixed phase and Δ is the corresponding energy in the superfluid component (where the energy is measured with respect to the chemical potential μ). In the weak coupling BCS regime, the mixed phase is characterized by $\delta\mu/\Delta = 1/\sqrt{2}$ and the BCS state remains unpolarized. When $\delta\mu \geq \Delta$ the BCS state will acquire a finite polarization resulting in gapless excitations in its spectrum. Otherwise, a finite polarization will result in phase separation [15,20]. Thus, at infinitesimal polarization, $\delta\mu - \Delta$ is the energy difference per unit polarization between the homogeneous gapless phase and the mixed state. These observations motivate us to examine how the ratio $\delta\mu/\Delta$ changes with coupling strength.

We first analyze the situation at $k_F a = \infty$. Using the EOS results of Ref. [7] and conditions of Gibbs equilibrium [Eq. (1)] we find that the ratio

$$\frac{\delta\mu}{\Delta} = \frac{1}{\beta}\left(\frac{2^{2/5}}{\xi^{3/5}} - 1\right). \qquad (2)$$

Substituting the QMC results for ξ and β, we find that $\delta\mu/\Delta = 1.00(5)$. This suggests that the BCS state is close to the polarization threshold; and that by tuning the coupling strength cold-atom experiments in traps containing two-Fermion species should be able to explore the large $\delta\mu/\Delta$ regime. Further, we find that $\delta\mu \gtrsim \mu$—indicating that the polarization in the normal phase is maximal. It is intriguing that we find $\Delta \simeq \delta\mu$ at $k_F a = \infty$.

The gap increases with coupling but $\delta\mu$ increases at a faster rate. The increase in $\delta\mu$ is driven by the pressure equilibrium condition. This trend can be demonstrated by using mean-field theory in the weak coupling regime where $\Delta(k_F a) = 8\mu \exp[-2 + (\pi/2\sqrt{2}k_F a)]$. Earlier studies of the mixed phase ignored the leading order $k_F a$ corrections to the pressure and chemical potential [15]. However, including these corrections is straightforward [21]. We find the pressure in the normal and BCS state is given by

$$P_{\text{Normal}} = \frac{k_{F\uparrow}^5}{30\pi^2 m} + \frac{k_{F\downarrow}^5}{30\pi^2 m} + \frac{a}{9\pi^3 m}k_{F\uparrow}^3 k_{F\downarrow}^3, \qquad (3)$$

$$P_{\text{BCS}} = \frac{k_F^5}{15\pi^2 m} + \frac{a}{9\pi^3 m}k_F^6 + P_\Delta, \qquad (4)$$

respectively, where $P_\Delta = mk_F\Delta^2/(4\pi^2)$ is the pairing contribution to the pressure. The chemical potentials also receive corrections at order $k_F a$. In the normal phase $\mu_{\uparrow(\downarrow)} = k_{F\uparrow(\downarrow)}^2/2m + (4\pi a/m)k_{F\downarrow(\uparrow)}^3/(6\pi^2)$.

Gibbs equilibrium condition determines the variation of $\delta\mu$ as a function of $1/k_F a$ at fixed μ. While we expect the mean-field result to be valid only for small coupling, the results which are shown in Fig. 1 show the expected trend—an increase in $\delta\mu/\Delta$ with increasing coupling. The QMC result at the universal point $k_F a = \infty$ confirms
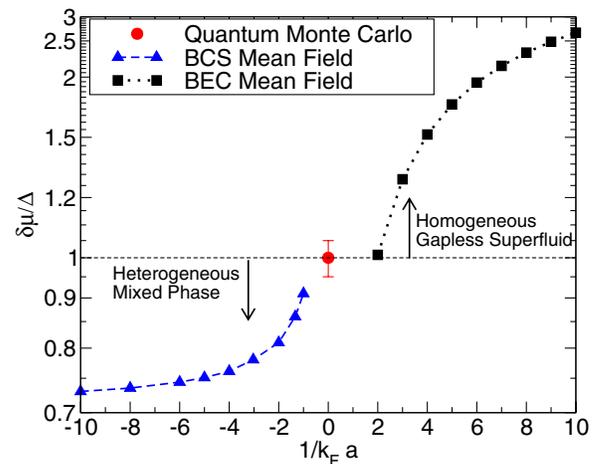
FIG. 1 (color online). Variation of $\delta\mu/\Delta$ with increasing coupling.

this increase. The behavior in the extreme BEC limit is also shown. In this region, we may use mean-field theory to calculate the self energy of a spin-up Fermion in the BEC phase. This is given by $\Delta_{\mathrm{BEC}} = 4\pi a_{\mathrm{BF}} n_B / \tilde{m}$, where $a_{\mathrm{BF}} \simeq 1.2a$ is the Fermion-Boson scattering length [22], n_B is the Boson density and $\tilde{m}$ is the reduced mass of the Fermion-Boson system. The Boson-Boson scattering length is also known and is given by $a_{\mathrm{BB}} \simeq 0.6a$ [22]. We use this to calculate the pressure of the BEC at leading order in the $n_B^{1/3} a_{\mathrm{BB}}$ expansion [21]. Pressure and chemical equilibrium then uniquely determine the chemical potential of spin-up Fermions in the Fermi gas phase. In agreement with earlier work by Viverit, Pethick, and Smith [23], we find that the homogeneous BEC phase easily accommodates a finite polarization in the dilute regime—as evidenced by $\delta\mu / \Delta_{\mathrm{BEC}} \gg 1$.

Quasiparticle dispersion and polarized superfluid state.—In addition to calculating the paired ground-state energy and the superfluid gap, we have performed QMC calculations of the homogeneous superfluid phase to examine the quasiparticle dispersion as a function of momentum. In addition, we have calculated the ground-state energy of systems at finite polarization to examine the interaction between these quasiparticles and determine if the gapless phase can support a macroscopic polarization. The methods used are identical to those employed earlier and the same (finite-range) cosh potential was used [6,7]. As before, we expect the small but finite-range of the potential to have a small effect upon the ground-state energy and the gap. Here we employ somewhat larger system sizes, however, ranging from 54–66 particles rather than the earlier studies from 12 to 20 particles. The larger system sizes allow for a somewhat finer momentum grid which is useful for examining the dispersion.

For the dispersion calculations, we place an unpaired spin in a state of definite momenta $k = (n_x, n_y, n_z)2\pi/L$, where L is the (cubic) box length and the n_i are integers describing the momenta in each coordinate. The BCS plus unpaired particle wave function can be calculated efficiently as a determinant [6]. As for the unpolarized system, we employ the fixed-node algorithm to avoid the fermion sign problem. This yields an upper bound to the energy for this system, the parameters in the BCS pair function $\phi(r_{ij})$ are (approximately) optimized to yield the best fixed-node energy. We include Jastrow correlations between antiparallel and parallel spins in the trial wave function to minimize the statistical errors [9]. These do not affect the energy, however, as they do not change the nodal surfaces where $\Psi_T = 0$.

The quasiparticle spectrum at $k_F a = \infty$ is displayed in Fig. 2. The BCS prediction at $k_F a = \infty$ is shown for comparison. The QMC points are calculated by computing $E_k(N + 1) - [E_0(N) + E_0(N + 2)]/2$ at constant density, where $E_k(N + 1)$ is the energy of the state of momentum k with 1 unpaired and N paired particles. The E_0 are the ground states of the N and $N + 2$ particle systems.
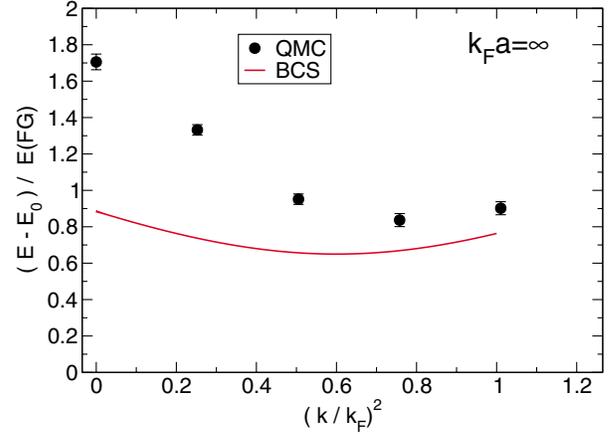
FIG. 2 (color online). The quasiparticle spectrum above the superfluid phase at $k_F a = \infty$. For reference, the quasiparticle spectrum in BCS theory for $k_F a = \infty$ is also shown.

Note that the minimum is at a momentum significantly less than the Fermi momentum. For larger coupling, the minimum in the dispersion will continue to trend towards lower momenta. This is apparent in the figure from the two sets of QMC results. From the QMC calculations we extract $\xi = 0.42(1)$ and a gap of $0.84(4)E_{\mathrm{FG}}$, or $\beta = 1.2$, somewhat smaller than earlier results.

In order to understand if the BCS phase can support a finite polarization, it is important to also study the interaction between the (polarized) quasiparticles. We have used QMC techniques to search for the ground-state energy as a function of polarization. The lowest variational energy in each case is found by filling the states at the minima of the quasiparticle spectra.

The results are shown in Fig. 3. These results demonstrate that the quasiparticles at small polarization are nearly noninteracting. This would be expected at small polarizations since the pair size is expected to be of the order of the interparticle separation. The solid points are the QMC
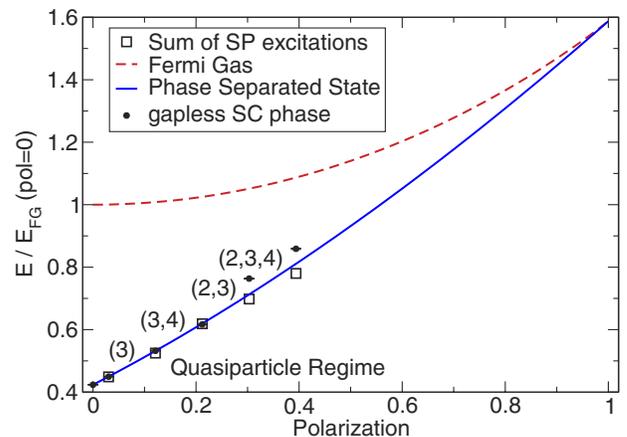
FIG. 3 (color online). Ground-state energy vs polarization at fixed density and $a = \infty$.

calculations with finite polarization. The integers next to these solid points indicate the momentum shells n^2, where $k^2 = n^2(2\pi/L)^2 = (n_x^2 + n_y^2 + n_z^2)(2\pi/L)^2$, filled in the trial wave function. Calculations were performed for 66 particles at various polarizations.

The open symbols represent the sum of single-particle energies obtained from the single-particle dispersion calculations of Fig. 2. At small polarizations this is nearly degenerate with the full calculation. The solid line in the figure is the energy of a phase separated unpolarized paired phase and a fully polarized Fermi gas.

The calculations indicate that the mixed and homogeneous phases are essentially degenerate at $k_F a = \infty$. Our calculations reproduce momentum distributions similar to those proposed for the gapless SC state, the states near the minimum of the dispersion are nearly fully occupied for one species, and nearly unoccupied for the other.

For larger couplings ($k_F a > 0$) at small polarizations, a transition to the homogeneous phase is expected to occur at some point from examining the behavior at very large couplings. Here the system can be thought of as a dilute mixed Fermi-Bose system where the bosons are tightly bound pairs of Fermions. The zero-temperature phase diagram of such mixtures has been investigated by Viverit, Pethick, and Smith [23]. They find that at small fermion densities the system is homogeneous, while at larger densities it phase separates into either a pure fermion plus mixed or pure fermion plus pure boson phase.

The results shown in Fig. 3 are qualitatively similar. Beyond a certain value of polarization, around 0.3 in the figure, the homogeneous system is clearly higher in energy than a phase separated state consisting of an unpolarized BCS plus fully polarized fermions. In this regime it appears that the BCS component would continue to support a smaller polarization.

Conclusions.—From our calculations it appears that at couplings near and beyond $k_F a = \infty$ a homogeneous superfluid state with finite polarization and nontrivial gapless excitations may be accessible experimentally. We also find that at low polarization, the polarization is carried by quasiparticles that are nearly noninteracting and occupy momenta below k_F. In cold-atom experiments we expect the trap potential to favor the phase separated state, while finite-range effects, which are expected to suppress the gap, and surface energy cost may help stabilize the homogeneous phase relative to the phase separated state. A naive interpretation of our results would indicate that a gapless superfluid exists only at very strong coupling where $\Delta/\mu \gtrsim 1$. However, in more complex systems such as dense quark matter, charge neutrality imposed by long-range forces plays an important role in this phase competition [13,14,24]. We also note that we have not analyzed other exotic possibilities such as the LOFF state which may

be relevant. We are planning on examining such possibilities in future calculations, and also examining systems at large polarizations.

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