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Exotic phase separation and phase diagrams of a Fermi-Fermi mixture in a trap at finite temperature

Jibiao Wang, Hao Guo, and Qijin Chen

1Department of Physics and Zhejiang Institute of Modern Physics, Zhejiang University, Hangzhou, Zhejiang 310027, China
2Department of Physics, Southeast University, Nanjing 211189, China
3Department of Physics, University of Hong Kong, Hong Kong, China

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The pairing and superfluid phenomena in a two-component Fermi gas can be strongly affected by the population and mass imbalances. Here we present phase diagrams of an atomic Fermi-Fermi mixture as they undergo BCS–Bose–Einstein condensation (BEC) crossover using a pairing fluctuation theory. We focus on the finite temperature and trap effects, with an emphasis on the mixture of $^6\text{Li}$ and $^{40}\text{K}$. We show that there exist exotic types of phase separation in the (near)-BEC regime, associated with a pseudogap effect. Moreover, in the BCS and unitary regimes, the spatial density and gap profiles exhibit sandwichlike shell structures with superfluid or pseudogapped normal state in the middle shell. Such a sandwichlike shell structure appears when the mass imbalance increases beyond a certain threshold. Our result is relevant to future experiments on the $^6\text{Li}$-$^{40}\text{K}$ and other possible Fermi-Fermi mixtures.

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Ultracold Fermi gases provide an excellent model system for studying condensed matter physics, e.g., the pseudogap phenomena in high-$T_c$ superconductivity [1], owing to various experimentally tunable parameters. Using a Feshbach resonance, a population balanced two-component Fermi gas of equal mass exhibits a perfect crossover from a BCS type of superfluidity to Bose–Einstein condensation (BEC) [2,3]. There have been a great deal of experimental and theoretical studies on equal-mass systems with and without population imbalance [4,5]. In particular, population imbalance adds a new dimension to the phase diagrams, leading to phase separation [6]. Sarma superfluid [7], and possibly Fulde–Ferrell-Larkin-Ovchinnikov (FFLO) states [8]. Mass imbalance, e.g., pairing of different mass atoms, will further enrich the physics, e.g., leading to significant trimer correlations under certain conditions [9], and thus make the subject very complex. Indeed, there have been worldwide efforts on the study of Fermi-Fermi mixtures of different species. Over the past several years, Feshbach resonances between different species of fermionic atoms, e.g., $^6\text{Li}$ and $^{40}\text{K}$, have been found and studied [10–12], although it remains to achieve superfluidity experimentally. There have been some theoretical studies in this aspect, e.g., on the strong attraction limit at zero temperature $T$ [13], few-body physics [14], the polaron physics [15], as well as thermodynamics of a high $T$ normal mixture [16]. There have also been studies on phase diagrams, which, however, are mostly restricted to zero temperature using a mean-field theory either in a homogeneous Fermi gas [17,18] or in a trap [19–21]. Recently, Guo et al. [22] as well as Stoof and co-workers [23] studied the mass imbalanced Fermi gases at finite temperatures. Due to technical complexity, this study was restricted to homogeneous cases. In order to address various experiments, which are always done at finite $T$ and in a trap, it is important to take into account the trap and finite $T$ effects simultaneously.

In this Rapid Communication, we consider a two-species Fermi-Fermi mixture with a short-range s-wave pairing interaction in a three-dimensional (3D) isotropic harmonic trap at finite temperature. We emphasize on the interplay between the finite $T$ and trap effects while the mass ratio $m_1/m_2$ and population imbalance (or “spin polarization”) $p = (N_1 - N_2)/(N_1 + N_2)$ (as well as the ratio $\omega_1/\omega_2$) between the trapping frequencies are varied within a pairing fluctuation theory [25], where spin index $\sigma = \uparrow, \downarrow$ refers to the heavy and light species, respectively. In order to address experiments, we pay special attention to the $^6\text{Li}$-$^{40}\text{K}$ mixture, while our result as a function of mass ratio covers other possible mixtures such as $^6\text{Li}$-$^{173}\text{Yb}$ and $^{171}\text{Yb}$-$^{173}\text{Yb}$. One special feature of our theory is the emergence of widespread pseudogap phenomena [26–28] at finite $T$. The analogous pseudogap phenomena are of central importance in the field of high-$T_c$ superconductivity [1]. For high enough mass imbalance, we find that, in the $T$-$p$ phase diagrams, three-shell sandwichlike spatial structures occupy a large region both at unitarity and in the BCS regime, including sandwiched phase separated superfluid, sandwiched Sarma superfluid, and sandwiched polarized pseudogap states with increasing $T$. In the BEC regime, there are exotic “inverted” phase separations with a normal Fermi gas core in the trap center surrounded by paired (superfluid or pseudogap) states in the outer shell. Our result provides important predictions for future experiments.

Except for slightly different notations, our formalism is a combination of that used in Refs. [22,29], where a single-channel Hamiltonian is used to describe the Fermi gas, with a local density approximation (LDA) for addressing the trap inhomogeneity. The bare fermion Green’s function is given by $G_{\sigma}(K) = i\omega_n - \xi_{\sigma K}$, with dispersion $\xi_{\sigma K} \equiv \xi_{\sigma K} - \mu_\sigma = K^2/2m_\sigma - \mu_\sigma$, chemical potential $\mu_\sigma$, and fermionic Matsubara frequency $\omega_n$. Here again, we take $\hbar = k_B = 1$ and use the four-vector notation, e.g., $K \equiv (\omega_n, k)$, $\sum_K \equiv T \sum_n \sum_k$, etc. The self-energy $\Sigma_{\sigma}(K) = \Sigma_{\sigma c}(K) + \Sigma_{\sigma p}(K)$ contains two parts, where the condensate contribution $\Sigma_{\sigma c}(K) = -\Delta_{\sigma}^2 G_{\sigma 0}(\bar{K})$ vanishes above $T_c$ (with $\bar{\sigma} = -\sigma$), and the finite momentum pair contribution

Corresponding author: qchen@zju.edu.cn
we impose a cutoff where

\[ \Sigma_{g\sigma}(K) = \sum_{Q} t_{pg}(Q) G_{\sigma\sigma}(Q - K) \]

persists down to \( T = 0 \). The \( T \)-matrix \( t_{pg}(Q) = g/[1 + g\chi(Q)] \) represents an infinite series of particle-particle scattering processes, with a short-range interaction strength \( g < 0 \) and the pair susceptibility \( \chi(Q) = \sum_{K,\sigma} G_{\sigma\sigma}(Q - K) G_{\sigma\sigma}(K)/2 \).

For \( T \leq T_c \), we have \( \Sigma_{g\sigma}(K) = \sum_{Q} t_{pg}(Q) G_{\sigma\sigma}(K) + \delta \Sigma_{\sigma} = -\Delta_{qg} G_{\sigma\sigma}(K) + \delta \Sigma_{\sigma} \), which defines a pseudogap \( \Delta_{pq} \) within \( \Delta_{qg} = -\sum_{Q} t_{pg}(Q) \).

Ignoring the less important incoherent term \( \delta \Sigma_{\sigma} \), we obtain \( \Sigma_{\sigma}(K) = -\Delta_{qg} G_{\sigma\sigma}(K) \) in the simple BCS form, where \( \Delta^2 = \Delta_{sc}^2 + \Delta_{pq}^2 \). Therefore, the full Green's function is given by

\[ G_{\sigma}(E) = \frac{u_k^2}{i\omega_n - E_{k\sigma}} + \frac{v_k^2}{i\omega_n + E_{k\sigma}}, \]

where \( u_k^2 = (1 + \xi_k/E_k)/2 \), \( v_k^2 = (1 - \xi_k/E_k)/2 \), \( E_k = \sqrt{\xi_k^2 + \Delta^2} \), and \( E_{k\sigma} = E_k + \delta_{\sigma0} \xi_k = (\delta_{k\sigma} + \xi_k)/2 \). With \( n_s = \sum_k G_{\sigma}(E) \), the number equations read

\[ n = \sum_k \left[ \left( 1 - \frac{\xi_k}{E_k} \right) + 2f(E_{k\uparrow}) \frac{\xi_k}{E_k} \right], \]

where the average Fermi function \( f(x) \equiv \frac{1}{e^{x/T} + 1} \).

At \( T \leq T_c \), the Thouless criterion leads to the gap equation

\[ g^{-1} + \chi(0) = 0. \]

For \( T > T_c \), it is amended by \( g^{-1} + \chi(0) = Z\mu_p \), where the effective pair chemical potential \( \mu_p \) and the coefficient \( Z \) can be determined from the Taylor expansion of the inverse \( T \)-matrix \( t_{pg}(Q) = Z(i\Omega - \delta_{qg}) \), where \( \delta_{qg} = g^2/2M^* \). The pair mass. Thus the gap equation reads

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\[ n_s = \sum_{k} \left[ (1 - \xi_k/E_k) + 2f(E_{k\uparrow}) \frac{\xi_k}{E_k} \right]. \]
disappear, similar to the Sarma state found in Ref. [29]. Correspondingly, the sandwiched PS phase becomes a sandwiched Sarma phase. As seen from Figs. 2(b) and 2(e), $\Delta$, $\Delta_c$, and $n_1$ vanish continuously at the outer interface. The difference between $\Delta$ and $\Delta_c$ defines the presence of the pseudogap.

At higher $T$, the superfluidity disappears so that the Sarma phase becomes a polarized pseudogap (PG) phase with $\Delta_{PG} \neq 0$ in the inner core. Similarly, the sandwiched Sarma phase evolves into a sandwiched PG phase. Representative density and gap profiles are shown in Figs. 2(a) and 2(d). Finally, at very high $T$ we have a normal phase. Note that in Fig. 1 the dashed line separating the normal and the (sandwiched) PG phases indicates a crossover rather than a phase transition.

Figure 3 presents the phase diagrams at (a) $1/k_F a = -0.5$ and (b) 0.5, similar to Fig. 1, but in the (near-)BCS and (near-)BEC regimes, respectively. For the BCS case, except for the high-$T$ normal phase, the phase diagram is essentially occupied by three-shell structures. The middle shell is an unpolarized BCS superfluid at the lowest $T$, Sarma superfluid at intermediate $T$, and a polarized PG state at slightly higher $T$. As shown in Figs. 4(a) and 4(b), in the sandwiched PS phase, the outer shell is a normal mixture, surrounded by light atoms alone at the trap edge. This is different from the sandwiched PS at unitarity [Fig. 2(f)], where the outer shell contains no normal mixture at $T = 0$. In comparison with the unitary case, one can see that the decreased pairing strength squeezes out the PS phase completely. The temperature evolution of the various phases is similar to their unitary counterparts, except that the sandwiched PG phase now occupies a very slim region, reflecting a much weaker pseudogap effect in the BCS regime.

The phase diagram for the BEC case in Fig. 3(b) is rather different. First, for $p < 0$, where the light species dominates, a Sarma superfluid phase occurs at low $T$. Indeed, polarized superfluid becomes stable in the BEC regime [6,30]. As $T$ increases, $\Delta_c$ vanishes and the system evolves into a polarized pseudogap state. The large area of the “PG” phase indicates greatly enhanced pseudogap effects in the BEC regime. On the other hand, for (roughly) $p > 0$, we have an “inverted” phase separated superfluid state at low $T$, labeled as “PS-SF,” where a normal gas core of the heavy species is surrounded by a shell of unpolarized superfluid. This should be contrasted with the PS phase in the unitary case [Fig. 2(e)], where the normal Fermi gas is outside the superfluid core.

![Figure 2](image1.png)  
**FIG. 2.** (Color online) Representative density (main panels) and gap (insets) profiles for $p = -0.85$ and 0.25 at unitarity: (a)–(c) $T/T_F = 0.2, 0.1, 0.02$; (d)–(f) $T/T_F = 0.15, 0.05, 0.01$, corresponding to each phase in Fig. 1. In (c) and (f), essentially $6\text{Li}$ (black solid) and order parameter $\Delta_{SC}$ (blue dashed lines). Here $n_s$ is in units of $n_F = k_F^2/3\pi^2$.

![Figure 3](image2.png)  
**FIG. 3.** (Color online) Phase diagram of $^6\text{Li}^{40}\text{K}$ as in Fig. 1 but for (a) $1/k_F a = -0.5$ and (b) 0.5. Here “PS-SF” and “PS-PG” represent phase-separated superfluid and phase-separated pseudogap phases, respectively, with a normal gas core surrounded by an outer shell of superfluid or pseudogapped normal mixture.

![Figure 4](image3.png)  
**FIG. 4.** (Color online) Typical density and gap profiles for BCS (left column, $1/k_F a = -0.5$) and BEC (right column, $1/k_F a = 0.5$) regimes. The convention is the same as in Fig. 2. Panels (a) and (b) are for $p < 0.25$ at $T = 0.01T_F \approx 0$, corresponding to the sandwiched PS phase in Fig. 3(a). Panels (c) and (d) plot the density and gap (insets) distributions for $p = 0.25$ at $T = 0.2T_F$ and 0.1$T_F$, representing the PS-PG and PS-SF phases in Fig. 3(b), respectively.
As $T$ increases, a phase-separated pseudogap state (labeled “PS-PG”) appears, where pseudogap exists in the polarized outer shell but without superfluidity. This is an exotic new phase in that in a homogeneous system the evolution with increasing $T$ from a pseudogap state to the unpaired normal state is a crossover rather than a phase transition. It is only for energetic reasons that at the same intermediate $T$ in the presence of trap inhomogeneity does such phase separation occur in real space. Across the phase boundaries between the Sarma and PS-SF and between PG and PS-PG phases, the densities undergo dramatic restructuring. Typical density and pairing strength increases from unitarity, the outer shell of the heavy species becomes close to $\omega_{T}/\omega_{1}$, pairing is always easier at $\omega_{T}/\omega_{1}$ or both, since $R_{TF}^{P}$ depends on the product $m_{σ}ω_{σ}$. As shown in the inset, the threshold $m_{σ}ω_{σ}$ for the three-shell structure to occur is roughly doubled when $\omega_{T}/\omega_{1}$ is reduced by 1/2. While the difference between different $\omega_{T}/\omega_{1}$ is mainly quantitative, for the $\delta$-Li-$\delta$K mixture, a three-shell structure appears in the main figure, while only a regular Sarma phase shows up in the inset.

Finally, the neglected incoherent part of the self-energy $\deltaΣ_{\sigma}$ may induce polarons in the mixed normal states, which, however, is unimportant for the present study. Following common practice $[2,3,25,31–35]$, we have also dropped the particle-hole channel contributions $[36]$, which can be roughly approximated by a shift in $1/k_{F}a$ $[37,38]$. These approximations are expected to influence the phase boundaries only quantitatively. In addition, the FPLO states, which appear to be of less interest in a 3D equal-mass Fermi gas $[39–42]$, will be investigated in a future work.

We end by noting that the widespread pseudogap phenomena, which are unique to our theory, and the prediction of exotic phases, e.g., the phase-separated pseudogap phase, can be tested using vortex measurements $[43]$ and rf spectroscopy $[27,44]$, etc. Comparison with concrete experiments using detailed parameters such as $N_{σ}$, $ω_{σ}$ will be possible when such experiments become available in the (near) future.

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EXOTIC PHASE SEPARATION AND PHASE DIAGRAMS OF . . .


[42] We note that the supersolid phase discussed in Ref. [23] is just the LO state.
