Loss-induced phase separation and pairing for 3-species atomic lattice fermions

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We study the physics of a three-component Fermi gas in an optical lattice, in the presence of a strong three-body constraint arising due to three-body loss. Using analytical and numerical techniques, we show that an atomic color superfluid phase is formed in this system and undergoes phase separation between unpaired fermions and superfluid pairs. This phase separation survives well above the critical temperature, giving a clear experimental signature of the three-body constraint.

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The recent realization of multi-component degenerate Fermi mixtures in experiments [1, 2] offers exciting new opportunities to observe physics beyond that conventionally studied for two-component fermions in the solid state. Three-species mixtures can, e.g., give rise to a competition between bound three-body trions and an atomic color superfluid (ACS) phase, where unpaired fermions coexist with superfluid (SF) pairs of different components [3,4]. The current limitation for observing this physics in three-component Lithium gases is the high rate of three-body loss due to a three-body Efimov resonance in this system [1,5]. However, loading the gas into an optical lattice could be used to suppress losses, as a large rate of onsite three-body loss can prevent coherent tunneling processes from populating any site with three particles [5,7], as was demonstrated for the case of two-body losses in Feshbach molecules [8]. For three-body loss, this mechanism would provide an effective three-body hard-core constraint [6,9,10], suppressing the actual loss events.

Here we address the key question of how this loss-induced constraint affects the many-body physics in a lattice in 2D and 3D. We focus on a regime of medium-to-strong attractive interactions with pronounced asymmetries in the interactions between different species, corresponding to the regime of strong losses in current experiments with 6Li [5]. On a lattice, we find that the loss-induced constraint not only inhibits trion formation, but also drives the homogeneous ACS phase towards phase separation of SF pairs and unpaired fermions [Fig. 1]. In contrast to two-species Fermi mixtures with attractive interactions [11], phase separation takes place here even for a number-balanced mixture. Moreover, this separation persists well above the ACS critical temperature, leaving a strong many-body signature of the constraint accessible at current experimental temperatures.

Below we discuss the model and establish a simple analytical picture for the phase separation based on deriving an effective low-energy Hamiltonian at strong-coupling.

\[ H = -J \sum_{\langle i,j \rangle} \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} - \sum_{\sigma,i} \mu_\sigma \hat{n}_{i,\sigma} + \sum_{\sigma<\sigma',i} U_{\sigma,\sigma'} \hat{n}_{i,\sigma} \hat{n}_{i,\sigma'}, \]

where \( \hat{c}_{i,\sigma}^\dagger \) is a fermionic creation operator for an atom on site \( i \) in internal state \( \sigma = 1,2,3 \), \( J \) is the tunnelling amplitude between nearest neighbour sites \( \langle i,j \rangle \), \( U_{\sigma,\sigma'} \) are the pairwise onsite interaction energies, and \( \hat{n}_{i,\sigma} = \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma} \). The chemical potentials \( \mu_\sigma \) fix the filling factors \( n_\sigma \). This model assumes that \( J, U_{\sigma,\sigma'} \ll \nu \), where \( \nu \) is the energy separation to higher Bloch bands. In the presence of strong on-site three-body loss with a rate \( \gamma_3 \), tunnelling processes populating sites with three atoms are suppressed as \( J^2/\gamma_3 \) [9]. We thus obtain a model with an effective three-body constraint, \( \hat{n}_{i,1} \hat{\nu}_{i,2} \hat{\nu}_{i,3} \equiv 0 \), as discussed in Refs. [6,9,10].

Parameters for Lithium – The requirement \( \gamma_3 \gg J \) is fulfilled if we take \( ^6 \text{Li} \) atoms at a magnetic field of...
where the lattice gradient is defined as consequence of a Bose-Fermi mixture, where fast fermions strongly interact with slow bosonic pairs, whose effective hopping parameter is given by $J^F/|U_{1,2}| \approx J/10 \ll J$. The strong (off-site) boson-fermion repulsion $J$ in $H_{BF}$ is a direct consequence of the three-body constraint. This is the term that gives rise to phase separation - however, this scale is of the same order as the fermionic hopping and phase-separation is not generic for Bose-Fermi mixtures [13], so the problem must be treated carefully.

We assess the instability of the homogeneous system against phase separation by studying the compressibility matrix $M_{\sigma'\sigma} = \partial^2 E/\partial n_{\sigma} \partial n_{\sigma'}$, where $n_{\sigma}, n_{\sigma'} = n_3, n_4$ and $E$ is the canonical energy for Eq. (2). For low filling and at mean-field level, we obtain $E(0)(n_3, n_4) \approx \pi^2 W_2 \left(\frac{D}{\sigma^2}\right)^{2/D} \alpha_3^{D+1} + W_2/(4D|U_{1,2}|)n_3^2 + Wm_3n_3$, where $\Omega_D = 2\pi^2/4$ for $D = 2, 3$. Consequently, the system will be stable provided $1 \leq A = \pi^2(D/\Omega_D)^{2/D} D^{-3} W_2^{2/D-4}$. For $n_3 = 1/6$, $A = 0.07(0.11)$ in 3D (2D), and thus the homogeneous system is unstable against phase separation. Note that there is a critical density below which the homogeneous mixture is stable in 3D ($n \approx 10^{-4}$ for this setup). In 1D the system is not expected to phase separate on typical experimental scales, where the constraint helps instead to stabilize the homogeneous ACS phase [10].

Since in strong-coupling $T_c = \mathcal{O}(J^2/|U_{1,2}|) \ll J$ [14], we expect phase separation (with a typical energy scale of the boson-fermion repulsion $J$) to be present well above the critical temperature for the disappearance of the SF phase. Finally, as the fermion-boson interaction is repulsive, the instability will result in spatially separated domains of fermions and bosons in order to minimize the bulk energy, as shown numerically below.

**Numerical approaches** – In order to treat the system quantitatively in a wider range of parameters and go beyond the effective description above, we employ two complementary numerical approaches. Details on both methods are provided in [15].

In 3D, we employ DMFT as a non-perturbative approach where the (quasi-) momentum dependence of the self-energy is neglected, i.e. $\Sigma(k, \omega) = \Sigma(\omega)$ [16]. We generalized DMFT to the case with three species in order to describe ACS and trionic phase, and also investigated the system at finite temperature. As a solver for DMFT, we used Exact Diagonalization [17]. Onsite thermodynamic observables, e.g. densities $n_{\sigma} = \langle \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} \rangle$, double occupancies $d_{\sigma,\sigma'} = \langle \hat{n}_{i\sigma} \hat{n}_{i\sigma'} \rangle$ and the SF order parameter $P = \langle \hat{c}_{i} \hat{c}_{\bar{i}} \rangle$, are estimated directly as averages on the impurity site of the auxiliary Anderson model at self-consistency [16].

The momentum distribution $n_{\sigma}(k)$ and spectral properties are obtained from the normal components of the single-particle Green function $G_{\sigma}(k, i\omega_n)$, which is a natural output in DMFT. Then, $n_{\sigma}(k) = T \sum_{\nu} G_{\sigma}(k, i\omega_n) e^{-\nu\omega_n}$ and the average kinetic energy per lattice site is given by $K = \frac{1}{N} \sum_{k,\sigma} \varepsilon_k n_{\sigma}(k)$, where $N$ is the number of lattice sites. The internal energy per site $E$ is then $E = K + V_{pot}$, where $V_{pot} = \sum_{\sigma<\sigma'} U_{\sigma,\sigma'} d_{\sigma,\sigma'}$ is the mean potential energy per site.

In 2D, we work with a VMC method, based on a strong-coupling expansion of Eq. (2) [15]. We can determine the stability of the ACS phase with respect to trion formation and its instability towards phase separation by comparing trial wavefunctions for the ground
state. For the normal phase we use
\[
|NFF\rangle = \mathcal{P} \prod_{\sigma} \prod_{k,\sigma} \hat{c}^\dagger_{k,\sigma}(0),
\]
where \(\mathcal{P}\) is a fixed number projection, \(\mathcal{P}_3\) is a projector enforcing the three body constraint, and \(\mathcal{J}\) is a Jastrow variational factor that can also include off-site trion correlations. For the homogeneous ACS phase we use
\[
|ACS\rangle = \mathcal{P} \prod_{k} \left[ u_k + v_k \hat{c}^\dagger_{-k,1} \hat{c}^\dagger_{k,2} \right] \prod_{\lambda,\sigma} \hat{c}^\dagger_{\lambda,\sigma}(0),
\]
where \(u_k\) and \(v_k\) are the usual BCS functions.

Since DMFT and VMC work respectively in the grand-canonical and canonical ensemble, they provide us with complementary descriptions of the system. This is particularly relevant in the presence of phase separation.

**Numerical results at** \(T = 0\) — We first treat the strong-coupling regime (\(\lambda = 1\)), and characterize the ground state properties as a function of the overall density \(n\) for fixed interactions. In particular, we establish the instability of the homogeneous ACS phase beyond the range of validity of the effective Hamiltonian approach and characterize quantitatively the equilibrium mixture.

Within DMFT we find no values of the chemical potentials \(\mu_{\sigma}\) such that the system is in a single homogeneous phase with the required densities \(n_{\sigma} = n\). This gives evidence for phase separation, in agreement with the general arguments above. This scenario, in which a mixture of phases has lower ground state energy \(E\) than a single homogeneous phase at \(T = 0\), is signalled in the grandcanonical framework by the existence of multiple solutions with the same grand potential per lattice site \(\Omega = E - \sum_{\sigma} \mu_{\sigma} n_{\sigma}\) for given \(\mu_{\sigma}\).

We considered several possible scenarios to build the equilibrium mixture, combining phases with pairing in different channels [38] and also explicitly suppressing superfluidity. We found that the equilibrium mixture at \(T = 0\) consists of a fraction \(\alpha\) of a two-species SF involving the species with the strongest interaction, 1–2, at densities \(n^N_{1} = n^S_{1} = n_p, n^N_{2} = 0\), and a fraction \(1 - \alpha\) of a normal phase which accommodates the remaining unpaired species, i.e. \(n^N_{\lambda} = n^S_{\lambda} = 0, n^N_{\lambda} \equiv n_u\). The energy of the mixture per lattice site is given by \(E_{mix} = \alpha E^{SF}(n_p) + (1 - \alpha) E^{N}(n_u)\) and \(\alpha = n/n_p = 1 - n/n_u\). Note that a similar scenario (though with a different \(\alpha\)) also applies for much smaller \(\lambda\), where the simple analytical picture above does not apply. Moreover, we find that the densities in the two phases in equilibrium are very different, being \(n_p \approx 0.75\) and \(n_u \approx 0.2\) for \(\lambda = 1\) and \(n = 0.16\), since a (strongly-interacting) two-species SF is in equilibrium with a spin-polarized (and therefore non-interacting) Fermi gas.

This scenario is confirmed via VMC in 2D, where we use an explicit Maxwell construction. We find that the energy \(E_{mix}\) of the SF plus normal mixture described above is lower than the energy \(E_{hom}\) of the homogeneous ACS solution for the same overall fixed densities \(n_{\sigma} = n\). We plot \(\Delta E = E_{hom} - E_{mix} > 0\) in Fig. 2a, where it is evident that the energy difference between the homogeneous solution and the equilibrium mixture is a very small fraction of \(E_{mix}\) shown in Fig. 2a. The relative energy gain from phase separation is therefore very small, probably because the kinetic energy of the unpaired fermions and the boson-fermion repulsion are of the same order \(\sim J\) (see Eq. 2). Once rescaled with the bandwidth \(W = 4D\), the DMFT and VMC values for the energy \(E^{mix}\) are in good agreement. The approximately linear scaling of \(E_{mix}\) with the density \(E_{mix} \approx n U_{1,2}\) occurs because the interaction energy in the superfluid is much larger than the kinetic energy in the superfluid or normal fluid, and \(d_{1,2} \approx n_p\) in the superfluid phase at strong-coupling.

To further characterize the equilibrium mixture, we also evaluated the SF order parameter \(P = \lim_{\mathbf{R} \to 0} P(\mathbf{R}) = \frac{1}{N_{SF}} \sum_{i} (c_{i} \ddagger c_{i+1} \ddagger c_{i+1} \ddagger c_{i+2})\), where \(N_{SF}\) is the number of lattice sites in the SF domain. As shown in Fig. 2b, \(P\) increases monotonically with the density in both 2D and 3D. Conversely, \(P\) is maximum whenever \(n_p = 0.5\), similarly to a two-component SF.
FIG. 3: (Color online) (a,b) z-integrated momentum distribution $\tilde{n}_\sigma(k_x, k_y)$ from DMFT for (a) $\sigma = 3$ in the normal phase and (b) $\sigma = 1$ (identical to $\sigma = 2$) in the SF phase. (c) Raman response $R(\omega)$ for the normal (dotted blue line) and SF component (solid red line) of the mixture. All results are for $\lambda = 1$, $n = 0.16$ and $T = 0$.

In Fig. 3 we show that the phase-separated scenario persists in the intermediate-coupling regime where the effective Hamiltonian description fails, rescaling the interactions with a factor $\lambda$ down to $\lambda = 0.3$.

Numerical results at finite temperature — To connect with experiments, we investigated the effect of finite temperature $T$ within DMFT. For finite $T$ the grand-canonical potential is given by $\Omega = E - TS - \sum_\sigma \ln(Z_\sigma)$, where the entropy $S$ is computed via the Maxwell relation $\partial n_\sigma / \partial T = \partial S / \partial \mu_\sigma$. For increasing $T$ the order parameter $P$ for the superfluid component decreases and eventually vanishes at $T = T_c$, as shown in Fig. 2.

However, phase separation persists for $T > T_c$, where both components are normal, as clearly seen from the mixing fraction $\alpha$. As explained above, this effect is due to the loss-induced constraint and scale separation. This is in contrast to (i) strong coupling in the absence of a constraint, where the trionic phase is favored and (ii) the case of symmetric interactions $U_{\sigma,\sigma'} = U$, where phase separation is favored due to a condensation energy gain in the ACS phase and disappears above the $T_c$ [15].

Experimental signatures — Clear experimental signatures of this scenario appear in the quasi-momentum distribution of the mixture, accessible in state-selective time-of-flight (TOF) measurements. Within DMFT we estimated the $z$-integrated momentum distribution $\tilde{n}_\sigma(k_x, k_y) = \int \frac{dk_z}{2\pi} n_\sigma(k)$ of the two phases in 3D at $T = 0$. For the normal phase of the unpaired species (Fig. 3b), this coincides with the Fermi distribution at $T = 0$ ($Z = 1$, where $Z$ is the quasiparticle weight). Despite smoothing due to the integration along the $z$ axis, $\tilde{n}$ vanishes identically at large $k$. If the system were in a balanced ACS phase, the jump at the Fermi surface of the unpaired species would be strongly renormalized at strong coupling ($Z < 1$) and some particles would be promoted to momenta outside the Fermi surface. The SF component (Fig. 3b) shows the weak dependence of $n_k$ on $k$ as expected for a two-color SF in the BEC regime.

Complementary signatures can be obtained using Raman spectroscopy [10], which allows us to distinguish different scenarios via the spectral gap. Within DMFT, the Raman response at zero transferred momentum $R_\sigma(\omega)$, where $\omega = \omega + \mu - \epsilon^o_{\text{out}}$ and $\epsilon^o_{\text{out}}$ is the energy of the final state, is given at $T = 0$ by $R_\sigma(\omega) = C \sum_k \delta(\omega - \mu - \epsilon^o_{\text{out}})$. As shown in Fig. 3c, $R(\omega)$ for the SF component of the mixture shows a gap $\Delta \approx 3.2W = O(U_{12})$, while for the normal (non-interacting) component $R(\omega) \propto \delta(\omega - \mu_3)$. For a balanced ACS, the Raman peak at $\omega = \mu_3$ would be broadened due to the interactions and in a trionic phase every component would be gapped with $\Delta_\sigma = O(U_{\sigma,\sigma+1} + U_{\sigma,\sigma+2})$.

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