Competing superfluid and density-wave ground-states of fermionic mixtures with mass imbalance in optical lattices

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(Dated: November 24, 2018)

We study the effect of mass imbalance on the phase diagram of a two-component fermionic mixture with attractive interactions in optical lattices. Using static and dynamical mean-field theories, we show that the pure superfluid phase is stable for all couplings when the mass imbalance is smaller than a limiting value. For larger imbalance, phase separation between a superfluid and a charge-density wave takes place when the coupling exceeds a critical strength. The harmonic trap induces a spatial segregation of the two phases, with a rapid variation of the density at the boundary.

PACS numbers: 71.10.Fd, 03.75.Lm, 32.80.Pj, 71.30.+h

The remarkable advances in handling ultra-cold atomic gases have given birth to the new field of “condensed matter physics with light and atoms”\(^1\). Cold atoms in optical lattices, with tunable and controllable parameters, have been studied in many different contexts (for reviews, see [1]). Mixtures of two-component atoms with different masses (e.g. \(^{6}\)Li, \(^{40}\)K) introduce an additional parameter, namely the difference between the hopping amplitudes associated with each species in the optical lattice. This may affect the stability of the possible quantum phases or even induce new ones. Recently, a phase diagram has been worked out in the one-dimensional (1D) case [2].

In this article, we consider such fermionic mixtures in higher dimensions, with an attractive on-site coupling. Using analytical and numerical techniques, we establish a ground-state phase diagram as a function of coupling strength and mass imbalance, in all regimes of couplings. We also consider the experimentally relevant effect of the trap potential, which is shown to induce a spatial segregation between superfluid and density-wave phases.

Under conditions discussed, e.g., in Refs. [1, 3, 4], fermionic mixtures are described by a Hubbard model:

\[
H = - \sum_{\langle i,j \rangle, \sigma} t_{\sigma} (c_{i\sigma}^+ c_{j\sigma} + \text{h.c.}) - |U| \sum_i n_{i\uparrow} n_{i\downarrow} \tag{1}
\]

The (pseudo-) spin index \(\sigma\) refers to the two different species. Feshbach resonances between \(^{6}\)Li and \(^{40}\)K are currently under investigation [5], and would allow for an attractive interaction with a tunable strength, as assumed in (1). For an example of hetero-atomic resonances in the boson-fermion case, see e.g [6]. In the following, a bipartite optical lattice made of two inter-penetrating (\(A, B\)) sublattices (such as a cubic lattice) is considered. For simplicity, we consider an equal number of atoms for each species, leaving for future work the study of imbalanced populations.

In order to study the ground-state phase diagram of model (1), we use dynamical mean field theory at zero temperature (DMFT) [7], together with analytical mean-field calculations for both weak and strong coupling. Let us anticipate the DMFT phase diagram of the uniform system, displayed in Fig. 1. When the fermions have the same mass, the ground-state is a superfluid (SF) for all \(|U|\). A competing ordering exists, namely a charge density wave (CDW), considered here in the simplest (commensurate) case in which the charge is modulated with an alternating pattern on the A and B sublattices. At half-filling (\(\langle n_{\uparrow} + n_{\downarrow} \rangle = 1\)), it is well known that the SF and CDW states are degenerate. This no longer applies in the ‘doped’ system away from half-filling: for equal masses, the SF phase is stabilized by doping for all \(|U|\), but a large mass imbalance favors the CDW phase over a SF state in which the Cooper pairs must be formed by fermions with different mobilities. Hence the SF/CDW competition becomes more interesting in the presence of mass imbalance. As displayed on Fig. 1, we find that the uniform system has a SF ground-state for all values of \(|U|\) as long as the mass imbalance \(z \equiv (t_{\uparrow} - t_{\downarrow})/(t_{\uparrow} + t_{\downarrow})\) is smaller than a limiting value \(z_c\) (which depends on the average density). For \(z > z_c\), a (first-order) phase boundary is crossed as \(|U|\) is increased, beyond which the uniform system undergoes a phase separation (PS) between a SF and a CDW phase. As discussed later in this paper, this implies that, in the presence of a harmonic trap, the CDW and SF phases may both exist in different regions of the trap.

DMFT is a quantum generalization of classical mean-field theories, which takes the full local quantum dynamics into account, while spatial fluctuations are neglected. It maps a lattice model onto an effective ‘quantum impurity model’ (a single interacting site which hybridizes with an uncorrelated bath), subject to a self-consistency condition [7]. DMFT and its extensions have been used to study the attractive Hubbard model with equal masses [8]. It is convenient to work with Nambu’s spinors \(\psi^\dagger = (c_{\uparrow}^+, c_{\downarrow})\). The key quantity considered in DMFT is the local (on-site) Green’s function:
\( \hat{G}(\tau) = \langle T_\tau \psi_i(\tau)\psi_i^\dagger(0) \rangle \) and its Fourier transform for imaginary frequencies:

\[
\hat{G}(i\omega) = \begin{bmatrix}
G_A(i\omega) \\
G_B(i\omega)
\end{bmatrix} = \begin{bmatrix}
F_A(i\omega) \\
F_B(i\omega)
\end{bmatrix} - G_A(-i\omega)
\]  

The superfluid order parameter is then given by \( \Delta_{SF} = \langle c_\uparrow c_\downarrow \rangle / F(\tau = 0) = \sum_\omega F(i\omega). \) In the CDW state, the local Green's function takes different values (\( \hat{G}_A \) and \( \hat{G}_B \)) on each sublattice. The self-consistency conditions of DMFT relate the (frequency-dependent) 'Weiss fields' \( \hat{G}_{A,B}(i\omega) \) entering the effective 'impurity model' on one sublattice, to the Green’s functions, through [7]:

\[
\hat{G}^{-1}_{A,B}(i\omega) = i\omega 1 + \hat{T} \hat{G}_{A,B}(i\omega) \hat{T},
\]

where \( \hat{T} = \text{diag}[t_\uparrow, -t_\downarrow] \) and \( \hat{\mu} = \text{diag}[\mu_\uparrow, -\mu_\downarrow] \) are diagonal matrices associated with the hopping and chemical potential of each species. As written, (3) assumes for simplicity a semi-circular density of states, but is easily generalized to an arbitrary lattice. Eq.(3) allows for the study of both SF and CDW orders, and for their possible coexistence. The ground-state energy of the different phases is evaluated as \( (H) = \langle K \rangle + U \sum_\sigma \langle n_{\uparrow \sigma} n_{\downarrow \sigma} \rangle \), with the kinetic energy \( (K) \) in the SF and the CDW phases reading, respectively:

\[
(K)_{SF} = \beta^{-1} \sum_\omega \sum_\sigma t_{\sigma}^2 [G_{\sigma}^2(i\omega) - F^2(i\omega)] \\
(K)_{CDW} = \beta^{-1} \sum_\omega \sum_\sigma t_{\sigma}^2 G_{\sigma}(i\omega) G_{\overline{\sigma}}(i\omega)
\]

We performed DMFT calculations [12] spanning the whole range of coupling \(|U|\) and imbalance \(z\). We focused on the vicinity of half-filling, and found the phase diagram of the uniform system (Fig. 1) to be qualitatively independent of the 'doping level' \( \delta = (n_\uparrow + n_\downarrow - 1) \). For small enough values \( z < z_c(\delta) \) of the mass imbalance, a pure SF solution is stable for all \(|U|\). In contrast, for \( z > z_c \), the pure SF phase is stable only for small interactions (below the line drawn in Fig. 1). Above this line which depends on \( \delta \), the pure SF solution becomes unstable towards phase separation between a SF and a CDW phase. (Note that we did not find a homogeneous CDW solution out of half-filling, except at \( z = 1 \). This means that it is more convenient to separate the system into a fraction \( 1 - x \) with CDW order and \( x = 0 \), and a fraction \( x \) with SF order accommodating the rest of the particles. This conclusion is reached by minimizing over \( x \) the expression \( E_{PS}(x) = (1 - x)E_{CDW} + xE_{SF} \). We note that the SF phase is more stable than in the 1D case [2] (in which nesting favors a CDW with \( Q = 2k_F \)).

In the following, we describe analytical mean-field calculations for both weak and strong coupling which help in understanding the DMFT phase diagram established numerically. We first present a strong-coupling analysis, which holds for \( |U| \gg t_\uparrow, t_\downarrow \). In order to analyze this limit, we find it useful to resort to a particle-hole transformation (Table I) and work in the repulsive-\( U \) framework. We emphasize that we are not switching to truly repulsive interactions, but we simply exploit a mapping. Under this mapping, our model is transformed, at large

\[
\begin{array}{ll}
-|U| < 0 & |U| > 0 \\
\begin{array}{c}
\begin{array}{c}
c_{\pi \uparrow}, c_{\pi \downarrow} \\
n_{\pi \uparrow}, n_{\pi \downarrow}
\end{array}
\end{array}
\begin{array}{c}
\begin{array}{c}
d_{\pi \uparrow}, (-1)^{\gamma}d_{\pi \downarrow} \\
n_{d \uparrow}, 1 - n_{d \downarrow}
\end{array}
\end{array}
\end{array}
\]

\[
\begin{array}{c}
\begin{array}{c}
\delta \equiv n_c - 1 \equiv (n_\uparrow + n_\downarrow) - 1 \\
\text{chemical potential} : \mu_c \\
h_c
\end{array}
\begin{array}{c}
\begin{array}{c}
\delta \equiv n_d - 1 \equiv (n_\uparrow + n_\downarrow) - 1 \\
\text{field} : h_d = \mu_c - |U|/2 \\
\mu_d = h_c + |U|/2
\end{array}
\end{array}
\end{array}
\]

\[
\begin{array}{c}
\begin{array}{c}
\text{SF} : (c_{\pi \uparrow}, c_{\pi \downarrow}^+) \\
\text{CDW} : (-1)^{\gamma}(n_{\pi \downarrow})
\end{array}
\begin{array}{c}
\begin{array}{c}
\text{SDW} \downarrow : (-1)^{\gamma}(d_{\pi \uparrow}^+, d_{\pi \downarrow}) \\
\text{SDW} \uparrow : (-1)^{\gamma}(S_{\pi \downarrow}^+)
\end{array}
\end{array}
\end{array}
\]

\[
\begin{array}{c}
\begin{array}{c}
\text{TABLE I: Particle-hole transformation mapping the } \langle U \rangle < 0 \\
\text{model with } \langle n_\pi \rangle = \langle n_d \rangle \text{ onto a half-filled } U > 0 \text{ model with a magnetic field.}
\end{array}
\end{array}
\]

\[
|U| \gg t_\uparrow, t_\downarrow, \text{ into an XXZ quantum spin-1/2 model [2, 4]:}
\]

\[
H = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + \gamma J \sum_{\langle i,j \rangle} S_i^x S_j^x - h \sum_i (2 S_i^z - m)
\]

in which \( \vec{S} = \frac{1}{2}d_\alpha^\dagger \vec{\sigma}_\alpha d_\beta \), \( J = 4t_\uparrow t_\downarrow / |U| \) and \( \gamma = (t_\uparrow - t_\downarrow)^2 / 2 t_\uparrow t_\downarrow = 2z^2 / (1 - z^2) \). Hence, the mass imbalance turns into a spin exchange anisotropy. The uniform magnetic field \( h \) corresponds to the original chemical potential \( \mu = |U|/2 \) and the magnetization to the doping \( \delta \) (cf. Table I). The mean-field approach [9] amounts to treat the spin variables as classical, and minimize the energy over the angles \( \theta_A, \theta_B \) describing the orientation of the spins in the two sublattices. The energy per site reads (with \( \zeta \) the lattice connectivity and

\[
\begin{array}{c}
\begin{array}{c}
\text{FIG. 1: Phase diagram of the uniform system in the } (z,|U|) \\
\text{plane, obtained from DMFT. Below the curves (displayed here}
\end{array}
\end{array}
\]

\[
\begin{array}{c}
\begin{array}{c}
\text{for two 'doping' levels } \delta \equiv n - 1 = 0.05,0.1, \text{ the superfluid is}
\end{array}
\end{array}
\]

\[
\begin{array}{c}
\begin{array}{c}
\text{stable. Above the curves, the system is phase-separated into a}
\end{array}
\end{array}
\]

\[
\begin{array}{c}
\begin{array}{c}
\text{half-filled CDW and a SF. The arrows indicate the strong-coupling}
\end{array}
\end{array}
\]

\[
\begin{array}{c}
\begin{array}{c}
\text{values obtained analytically. The dotted lines are}
\end{array}
\end{array}
\]

\[
\begin{array}{c}
\begin{array}{c}
\text{the weak-coupling mean-field approximation (see text). } |U| \text{ is}
\end{array}
\end{array}
\]

\[
\begin{array}{c}
\begin{array}{c}
\text{normalized to the bandwidth } W \text{ of } (e_{k\uparrow} + e_{k\downarrow})/2.
\end{array}
\end{array}
\]
The phase diagram is characterized by the competition between the $xy$ spin-density wave (SDW$_{xy}$) with order parameter $\Delta_{xy} = \langle (-1)^i S^x_i \rangle$ (corresponding to SF ordering for $U < 0$), and Néel order (SDW$_z$), $\Delta_z = \langle (-1)^i S^z_i \rangle$ (corresponding to CDW). The solution changes according to the magnetization $m$ of the system (i.e. the doping of our physical model). The $m$ vs. $h$ curve has a discontinuity of amplitude $m_c = \sqrt{7/(\gamma + 2)} = z$. For $m = 0$ (half-filling $\delta = 0$), a SDW$_z$ (CDW) phase separation takes place between the two types of ordering. Thus, when working at fixed magnetization (corresponding to fixed doping $\delta$), one finds a SF for $z < z_c = m = \delta$ and phase separation for $z > z_c = \delta$. This strong coupling value (indicated by arrows on Fig. 1) agrees very well with our DMFT results.

We now turn to the opposite weak-coupling limit. We decouple the interaction term in the SF and the CDW channels, and determine the regions of stability of each. We first consider the BCS decoupling of the interaction, introducing the order parameter $\Delta$. We first compare the ground-state energies of two mean-field solutions: the homogeneous SF, and the SF/half-filled CDW phase-separated solution obtained from a Maxwell construction. The resulting phase boundary (Fig. 1) is seen to be qualitatively reasonable, and even quantitatively accurate (in comparison to the numerical DMFT result) for some intermediate range of $z$. Indeed, the weak-coupling mean-field is justified when $|U| \lesssim t_1$, i.e. $|U|/W \lesssim (1 - z)$. In Fig. 2, we perform a more detailed comparison of the ground-state energies of three mean-field solutions: the homogeneous SF, the phase separated SF/CDW, and the homogeneous CDW with $\delta \neq 0$ (when it exists). This comparison yields a small region of parameters, for large $z$, in which a homogeneous CDW with a density different from one atom per site is stable. This pure CDW pocket might be unstable to SF ordering, yielding a candidate for a supersolid region, but we did not check this explicitly. Anyhow, this solution is stabilized in a region where the reliability of weak-coupling mean-field is questionable. The lack of such a solution in DMFT may lead to the conclusion that the CDW (or supersolid) is an artefact of weak-coupling mean-field, but it must also be noted that the DMFT solution has a finite numerical resolution, and that the energetic balance involved is very delicate. Hence, we cannot reach a definitive conclusion on this issue. Exactly for $z = 1$ the “down spin” atoms are no longer mobile and we have a Falicov-Kimball model, which has a pure CDW ground state [10].

We finally discuss the effect of the trap potential. For simplicity, we perform an explicit calculation only in the strong coupling limit, using again the particle-hole trans-
formation (Table I) and considering the effective spin model (4). A harmonic trap potential yields a position-dependent chemical potential which corresponds, under the particle-hole transformation to a spatially varying magnetic field $h(r) = h_0 r^2 / R_0^2$. Here $R_0$ is the radius of the circular trap, $h_0 = m c^2 R_0^2 / 2$ and $h = \mu - |U|/2$ is related to the chemical potential at the center of the trap, which must be adjusted so that the local density $n(r)$ integrates to the total number of atoms. We start from a local density approximation (LDA), and also compare with a Monte Carlo solution of the strong-coupling model in the presence of $h(r)$. As described above, the strong coupling analysis of the uniform system yields a critical magnetic field (chemical potential) at which $m(h)$ is discontinuous. For $|h| < h_c = J \zeta \sqrt{\gamma(\gamma + 2)} = \frac{\sqrt{2} \zeta}{1 - 2 |\zeta|}$, we have a SDW$_z$ (CDW) phase, otherwise we have a SDW$_{xy}$ (SF) phase. Within the LDA approximation, this implies that in a region where $|h(r)|$ is smaller (resp. larger) than $h_c$ we locally observe SDW$_z$/CDW ordering (resp. SDW$_{xy}$/SF). According to the values of the parameters $h$ and $h_0$, and noting that $h - h_0 < h(r) < h$, one finds several different regimes:

(i) $h - h_0 > h_c$ or $h < -h_c$. The trap potential is always larger than $h_c$, or smaller than $-h_c$, so that the system is in a SDW$_{xy}$ (SF) phase everywhere inside the trap, and the density profile varies smoothly. (ii) $h > h_c$ and $|h - h_0| < h_c$: in this case, $h(r) > h_c$ inside a circle of radius $R_1 = R_0 \sqrt{(h - h_c) / h_0}$ centered at $r = 0$. Hence, one has phase separation into two distinct regions: SDW$_{xy}$ (SF) ordering within this circle, and SDW$_z$ (CDW) in the outer ring (Fig. 3, left panel). (iii) $h - h_0 < -h_c$ and $|h| < h_c$: we find again phase separation, with the opposite spatial arrangement. The SDW$_{xy}$ (SF) part is stable out or a circle of radius $R_2 = R_0 \sqrt{(h + h_c) / h_0}$ inside which there is a SDW$_z$ (CDW) phase (Fig. 3, middle panel). (iv) $h > h_c$ and $h - h_0 < -h_c$. Then, the magnetic field profile crosses both $h_c$ and $-h_c$, so that there are three spatial regions: $R < R_1$ where we find SDW$_{xy}$ (SF), then the ring $R_1 < r < R_2$, where SDW$_z$ (CDW) establishes, and finally an outer ring $r > R_2$ with SDW$_{xy}$ (SF) ordering (Fig. 3, right panel).

In the three last cases (ii-iv), in which phase separation occurs, the LDA approximation predicts a jump of the magnetization at the phase boundaries $R_1$ and $R_2$, corresponding to a jump of the density in the original $U < 0$ model (see also [11]). In order to test this prediction and assess the validity of LDA, we performed a classical Monte Carlo simulation of model (4) in the presence of a spatially dependent field $h(r)$. For simplicity, this test was performed in a one-dimensional geometry. We find a remarkable agreement between the LDA density profiles and the Monte Carlo solution, which confirms that very sharp variations of the local density indeed takes place at the boundary between domains in cases (ii-iv).

In conclusion, for attractive interactions, the dominant effect of the mass imbalance is to induce a competition between superfluid and density-wave ordering. In the presence of an inhomogeneous trap potential, both phases can be stabilized in different regions of the trap, with rapid variations of the local density at the phase boundaries. We note finally that, in the case of the $^6$Li/$^{40}$K mixture, a simple estimate shows that the mass imbalance $z$ can be varied over a large range by changing the lattice depth $V_0/E_R$ ($z < 1$ at small $V_0/E_R$ and $z \sim 0.9$ for $V_0/E_R \sim 15$), so that the effects discussed in this work may indeed be observable in this system.

We are grateful to I. Carusotto, F. Chevy, P. S. Cornglia, T. Giamarchi, D. Rohe, C. Salomon and F. Schreck for useful discussions. Support was provided by the ANR under contract "GASCOR", by CNRS, Ecole Polytechnique and MIUR-PRIN Prot.200522492.

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