Spin and mass imbalance in a mixture of two species of fermionic atoms in a 1D optical lattice

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In this paper, we study the role of both “spin”(species) and mass imbalance in a mixture of two species of fermionic atoms with attractive interaction in an one-dimensional optical lattice. Using the bosonization approach, quantum phase transitions between a liquid phase and phase separated states are studied under various conditions of interaction, spin imbalance, and mass imbalance. We find that, in the phase-separated region, there exists two kinds of phase separation and a special quantum phase transition might exist between them in the large $U$ limit. On the other hand, the singlet superconducting correlation dominates in the liquid phase. The pairing behavior has been also demonstrated that there is oscillating behavior in real space. We find both the spin and mass imbalance are in favor of the formation of Fulde-Ferrell-Larkin-Ovchinnikov state.

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I. INTRODUCTION

Ultracold atoms trapped in optical lattices have been increasingly used to simulate the rich physics in strongly correlated condensed matter systems. In particular, the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state [1, 2] in a magnetized superconductor, in which spin imbalance of electrons leads to Cooper pair formation and condensate in states with nonzero momentum (inhomogeneous distribution in real space), was proposed four decades ago. However, the observation of the FFLO state in solids has been proven to be extremely difficult due to the Meissner effect, and was only achieved recently in a heavy fermion system [3].

Experimentally, two hyperfine states of ultracold fermionic atoms play the roles of up and down spins. Their population could be controlled by using radio-frequency field, such that the hope of observing the FFLO state in cold atomic systems has been renewed recently [4, 5, 6]. Since the dimensionality of the cold atomic systems can be easily tuned, and indeed cold atoms have already been successfully trapped in one-dimensional (1D) waveguide, it seems natural to consider these nonhomogeneous pairing behaviors in this low dimensional systems.

So far, much attention has been paid to 1D spin-polarized fermionic systems with attractive interaction by using different methods and techniques, such as Bethe-ansatz [7], density-matrix renormalization-group [8], Quantum Monte Carlo [9], and bosonization [10]. All of these studies are based on approximating the system by the 1D Hubbard model in either uniformly distributed or harmonic trap cases respectively. In uniformly distributed case, the dominant order in the ground state is singlet superconducting (SS) [9], and existence of FFLO state [8, 9, 10], which is oscillating in real space and peak in momentum space (Non-zero momentum of cooper pairs). As polarization increasing gradually, phase separation will happen gradually in the Harmonic trap, like FFLO & fully paired wings, FFLO & polarized wings and Chandrasekhar-Clogston limit [7].

Recently, Taglieber et al [11] have successfully trapped a quantum degenerate Fermi-Fermi mixture, i.e. $^6$Li and $^{40}$K, by evaporating cooled bosonic $^{87}$Rb gas. The advance raises a new and interesting question. What is the influence of mass difference to the spin polarized fermionic system or does it become easier to observe the FFLO state in such a system. In Ref. [12], the influence of mass difference has been discussed with $N_1=N_2$. They found that there is a phase transition between SS and charge density wave (CDW) in the negative $U$ case, and phase separation exists in the positive $U$ case. The bosonization study [13] showed that the phase boundary between the density-wave phase and phase separation scales like $U^2$ in the weak coupling region. The results are consistent with previous numerical studies [14] by the exact diagonalization and density-matrix renormalization group technique.

The main purpose of this paper is to study the role of both “spin”(species) and mass imbalance in a mixture of two species of fermionic atoms with attractive interaction in optical lattices. We use the 1D asymmetric Hubbard model (AHM) as an effective model to describe such a mixture in the optical lattice, and then study the phase separation, dominant order and pairing behavior in the context of different spin populations and negative $U$ region using the bosonization approach. We find that if the system is partially polarized, there can exist two different phase-separated states, and the FFLO state might be more stable in the presence of mass imbalance.

The paper is organized as follows. In section II we obtain the bosonized form of the 1D asymmetric Hubbard model, then simplify it under conditions of away from half filling $n<1$ and $U<0$. In section III we study the ground-state phase diagram, and the effects of spin imbalance, and mass imbalance. In section IV we discuss dominant order and pairing behavior in our interested system. Finally, we summarize our results in section VI.

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II. THE ASYMMETRIC HUBBARD MODEL AND ITS BOSONIZED FORM

Here we consider a mixture of two species of fermionic atoms loaded in a 1D optical lattice. In experiments, such an optical lattice potential can be written as
\[
V(x,y,z) = V_0 \sin^2(kx) + V_\perp \sin^2(ky) + \sin^2(kz)
\]  

(1)

where \(V_0(V_\perp) = v_0(v_\perp)E_R\) in unit of the recoil energy \(E_R = \hbar^2k^2/2m\). If \(v_\perp \gg v_0\), the hopping process in the \(yz\) plane is frozen; while along \(x\) direction, the hopping integrals depend on the mass of atoms. So the system is quasi one-dimensional. Without loss of generality, we use “spin” \(\sigma = \uparrow, \downarrow\) to denote the type of atoms. For sufficiently low temperatures, the atoms will be confined to the lowest Bloch band, then the system can be described by the 1D AHM, whose Hamiltonian reads \([12,13,14]\)

\[
\mathcal{H} = -\sum_{\sigma,j} t_\sigma c_{j,\sigma}^\dagger c_{j+1,\sigma} + h.c. + U \sum_j n_{j\uparrow} n_{j\downarrow}.
\]

(2)

where \(c_{j,\sigma}^\dagger, c_{j,\sigma}\) are fermion creation (annihilation) operators at site \(j(j=1, \ldots, L)\), \(n_{j\sigma} = c_{j,\sigma}^\dagger c_{j,\sigma}\), and \(U\) the on-site inter-

action between two species of atoms. In the following we set \(t_\uparrow\) as unit, \(N_\sigma = \sum_j n_{j\sigma}\), band filling \(n = (N_\uparrow + N_\downarrow)/L\), mass ratio \(\iota = t_\uparrow/t_\downarrow = m_\uparrow/m_\downarrow\), mass imbalance \(z = (t_\uparrow - t_\downarrow)/(t_\uparrow + t_\downarrow)\), and polarization \(P = |N_\uparrow - N_\downarrow|/(N_\uparrow + N_\downarrow)\).

In the standard bosonization method \([15,16]\), the AHM can be expressed in terms of canonical Bose fields and their dual counterparts as

\[
\mathcal{H}_B = \frac{v_c}{2} \int dx \left[ \frac{1}{K_c} (\partial_x \phi_c)^2 + K_c \pi_c^2 \right] + \frac{v_s}{2} \int dx \left[ \frac{1}{K_s} (\partial_x \phi_s)^2 + K_s \pi_s^2 \right] + \frac{U}{2\pi^2 a} \int dx \cos \left[ \sqrt{8\pi} \phi_c + 2(k_{F\uparrow} + k_{F\downarrow})x \right] + \frac{U}{2\pi^2 a} \int dx \cos \left[ \sqrt{8\pi} \phi_s + 2(k_{F\downarrow} - k_{F\uparrow})x \right] + \Delta v \int dx [\pi_c \pi_s + \partial_x \phi_c \partial_x \phi_s],
\]

(3)

where all parameters take the following forms

\[
v_c = a \sqrt{t_\perp \sin(k_{F\uparrow}a) + t_\uparrow \sin(k_{F\downarrow}a)} \left[ t_\uparrow \sin(k_{F\uparrow}a) + t_\downarrow \sin(k_{F\downarrow}a) + \frac{U}{2\pi} \right],
\]

(4)

\[
v_s = a \sqrt{t_\perp \sin(k_{F\downarrow}a) + t_\downarrow \sin(k_{F\uparrow}a)} \left[ t_\downarrow \sin(k_{F\downarrow}a) + t_\uparrow \sin(k_{F\uparrow}a) - \frac{U}{2\pi} \right].
\]

(5)

\[
\frac{1}{K_c} = \sqrt{1 + \frac{2\pi [t_\uparrow \sin(k_{F\uparrow}a) + t_\downarrow \sin(k_{F\downarrow}a)]}{U}},
\]

(6)

\[
\frac{1}{K_s} = \sqrt{1 - \frac{2\pi [t_\downarrow \sin(k_{F\downarrow}a) + t_\uparrow \sin(k_{F\uparrow}a)]}{U}},
\]

(7)

\[
\Delta v = a [t_\uparrow \sin(k_{F\uparrow}a) - t_\downarrow \sin(k_{F\downarrow}a)].
\]

(8)

Here the bosonic fields \(\phi_c, \phi_s\) characterize the charge and spin degree of freedom, respectively. \(k_{F\uparrow}\) and \(k_{F\downarrow}\) are the Fermi wavevectors for up- and down-spin atoms, which are determined by number density of each component, and \(a\) is the lattice constant. \(v_{c,s}\) are the propagation velocities of the charge and spin collective modes of the decoupled systems (\(\Delta v = 0\)), and \(K_{c,s}\) are the stiffness constants.

There are two oscillating terms, Umklapp and backward terms, in our low energy effective Hamiltonian. If \(k_{F\uparrow} + k_{F\downarrow} \neq \pi/a\) or \(k_{F\uparrow} \neq k_{F\downarrow}\), they will vanish after performing such integrals. Physically, quasi-momentum conservation laws do not hold in the low energy region for these two processes. Even if both of them survive, it does not mean that they will contribute significantly in the long wavelength scale. According to renormalization-group analysis \([15]\), Umklapp term \(\cos(\sqrt{8\pi} \phi_c)\) contributes effectively only for \(U > 0\) case, there will be a gap in the charge excitation spectrum. On the other hand, backward term \(\cos(\sqrt{8\pi} \phi_s)\) contributes effectively only for \(U < 0\) case there will be a gap in spin excitation spectrum. Therefore, both of them will disappear in our systems, i.e., spin imbalance and attractive on-site interaction \(U < 0\). After do one loop approximation, the effective Hamiltonian can be written as

\[
\mathcal{H}_{eff} = \frac{v_c}{2} \int dx \left[ \frac{1}{K_c} (\partial_x \phi_c)^2 + K_c \pi_c^2 \right] + \frac{v_s}{2} \int dx \left[ \frac{1}{K_s} (\partial_x \phi_s)^2 + K_s \pi_s^2 \right] + \Delta v \int dx [\pi_c \pi_s + \partial_x \phi_c \partial_x \phi_s].
\]

(9)

Here we want to emphasize that the coupling constant \(\Delta v\)
depends on both spin polarization and mass difference. Unlike the Hubbard model, here \( N_1 > N_1 \) and \( N_1 < N_1 \) will be related to different cases because up- and down-spin atoms can be distinguished from each other due to mass difference. In the following, we try to study the consequences of mass imbalance and spin imbalance for phase separation and dominant orders.

As \( \Delta \nu \to 0 \), \( \nu_+ \to \max(\nu_-, \nu_+) \), \( \nu_- \to \min(\nu_-, \nu_+) \), and here \( \nu_+ < \nu_- \). As \( \Delta \nu \) increases, \( \nu_- \) decreases until it vanishes at the points:

\[
\Delta \nu_1^2 = \nu_c \nu_p K_s K_s \tag{11}
\]

\[
\Delta \nu_2^2 = \nu_c \nu_p \frac{1}{K_s K_s}. \tag{12}
\]

At these points, the freezing of the lower bosonic (mixture of real spin and charge) mode is accompanied by a divergence in the charge and spin response functions. The static charge compressibility \( \kappa \) diverges at \( \Delta \nu = \Delta \nu_1 \) or \( \Delta \nu = \Delta \nu_2 \). It behaves as

\[
\kappa = \kappa_0 \left[ 1 - \frac{\Delta \nu}{\Delta \nu_1(2)} \right]^{-1}, \quad \kappa_0 = \frac{2K_s}{\pi \nu_c}. \tag{13}
\]

Beyond these points, the susceptibilities become negative. This behavior of the static response functions together with the vanishing of the collective mode velocity indicates that the ground state becomes unstable \cite{17} and undergoes a first-order phase transition \cite{18}. The instability is known as phase separation and has been shown to occur in the extended Hubbard Model and in the \( t - J \) model \cite{19, 20}. In our case, we obtain

\[
\Delta \nu_1 = a(t_{11} \sin(k_F a) + t_1 \sin(k_F a)), \tag{14}
\]

\[
\Delta \nu_2 = \pm \sqrt{[a(t_{11} \sin(k_F a) + t_1 \sin(k_F a))]^2 - \frac{U^2}{4\pi^2 a^2}}, \tag{15}
\]

It is obvious that if \( \Delta \nu^2 \geq \Delta \nu_2^2 \), the system is in PS region. After doing some calculations \cite{13}, we arrive at the condition of phase separation:

\[
\cos \left[ \frac{(N_e - N_e)\pi}{N} \right] - \cos \left( \frac{N_e \pi}{N} \right) \leq \frac{U^2}{8\pi t_1 t_1}. \tag{16}
\]

It seems that up- and down-spin are symmetric in above expression (Bosonization method only work in the weak coupling region). However, it is not the case in the large \( U \) limit. In the following, we will discuss these two cases in more details.

### III. PHASE SEPARATION

The quadratic effective Hamiltonian [Eq. 9] can be diagonalized in terms of two new fields \( \phi \), which are combinations of spin and charge degrees of freedom. The corresponding velocities have been obtained

\[
\nu^2_{c+, -} = \frac{\nu^2_c + \nu^2_c}{2} + \Delta \nu^2 \pm \sqrt{\left( \frac{\nu^2_c - \nu^2_c}{2} \right)^2 + \Delta \nu^2 \left[ \nu^2_c + \nu^2_c + \nu_c \nu_c \left( K_c K_s + \frac{1}{K_c K_s} \right) \right]} \tag{10}
\]

![FIG. 1: The phase boundary between the phase separation (below the line) and liquid phase (above the line) in the \( t - |U| \) plane. Here the polarization \( P = 0.5 \), band filling \( n = 0.8 \), and \( U < 0 \).](image)

In negative \( U \) case, atoms with opposite spin try to form singlet pairs and lower the ground-state energy further. Singlet pairs can be regarded as a kind of quasi-particle of mass \( m_1 + m_1 \). Generally speaking, there are three kinds of particles, up- and down-spin atoms, and bound pairs. The reason for phase separation is the large difference of their mass, i.e., heavy atoms will stay together and give more space for other atoms to hop more freely. In Fig. 1 we show the boundary of phase separation in the weak coupling limit based on the Bosonization approach for fixed polarization \( P = 0.5 \), the more large interaction \( U \) is, the more pairs are (more occupied sites); and the heavier down-atoms are, the difference of mass between these three kinds of particles will large. Both of these two situations will lead to phase separation easily. Here the phenomena we obtained is very similar to observations in experiments \cite{4, 5, 6}.

The phase boundary in the \( t - P \) plane under fixed interaction is obtained similarly. If the polarization is larger under fixed band filling, there will be less down-particles, and the system will be easily in phase separation region composed of up-particles and bound pairs. The phase transition boundary
FIG. 2: The phase boundary between the phase separation (below the line) and liquid phase (above the line) in the $t - P$ plane. Here band filling $n = 0.8$.

FIG. 3: The phase boundary (solid line) between the phase separation (top-right region above the solid line) and a liquid phase (bottom-left region below the solid line) in the $P - |U|$ plane for $t = 0.5$ (a) and $t = 0.2$ (b). The Bosonization method is only valid on the left side of the dashed lines. Here the band filling $n = 0.8$.

is shown in Fig. 2. Two phase diagrams in the $U - P$ plane for both cases of $t = 0.5$ and $t = 0.2$ are shown in Fig. 3. In both cases, if the polarization $P$ is large, the phase separation state becomes more stable. If we compare two cases, the mass imbalance will also strongly affect the phase boundary, which will dragged to the left as the mass imbalance becomes larger.

IV. PHASE SEPARATION IN STRONG COUPLING LIMIT

Bosonization approach can not provide explicit information in the phase separation region except for indicating the phase boundary. Therefore, we try to obtain some insights about configurations in phase separation region by analyzing the strong coupling limit, i.e. $U \rightarrow -\infty$. In this case, all of dilute particles are paired with their partner. It is easy to realized that there are two possible configurations (See Fig. 4).

![FIG. 4: Two possible configurations in strong coupling limit, one is pairs staying together and unpaired particles moving; another one is dilute particles moving in the background of dense particles that are congregated together.]

...that there are two possible configurations (See Fig. 4).

It is obvious that there are two cases, more light particles and more heavy particles. Now we consider the former firstly. In this case, there are two dominant configurations for the phase separation, i.e. the configuration I of all atom pairs staying together and unpaired light atoms moving in free space, and the configuration II of heavy atoms staying together and light atoms moving in the background of heavy atoms (See Fig. 4). Since the interaction is infinite (only kinetic energy–just tight bonding model), the ground-state energy of the two configurations can be calculated by

$$E_I = \frac{t^I_1}{2} \left[ 1 - \frac{\cos \left( \frac{(N_i - N_s) \pi}{N - N_s + 1} \right) - \cos \left( \frac{(N_i - N_s + 1) \pi}{N - N_s + 1} \right)}{1 - \cos \left( \frac{N_i \pi}{N_s + 1} \right)} \right]$$

$$E_{II} = \frac{t^I_1}{2} \left[ 1 - \frac{\cos \left( \frac{N_i \pi}{N_s + 1} \right) - \cos \left( \frac{(N_i + 1) \pi}{N_s + 1} \right)}{1 - \cos \left( \frac{N_i \pi}{N_s + 1} \right)} \right],$$

respectively. We show the ground-state energies for both configuration, i.e. $E(I)$ and $E(II)$, as a function of the polarization in Fig. 5(a). From the figure, we can see that $E_I$ is always smaller than $E_{II}$. Therefore, the configuration I is the
ground state. It can be understood in the following way. For light atoms, the hoping integral is large, so they can effectively lower the ground-state energy. While, in the configuration II, motion of heavy particles contribute less to the ground-state energy. So the configuration I is favorable.

On the other hand, if the heavy particles is dense, then

\[ E_I = \frac{t_1}{2} \left[ \cos \left( \frac{N_l - N_r \pi}{N_l + 1} \right) - \cos \left( \frac{N_l - N_r + 1 \pi}{N_l + 1} \right) \right] \]

\[ E_{II} = \frac{t_1}{2} \left[ 1 - \frac{\cos \left( \frac{N_r \pi}{N_r + 1} \right) - \cos \left( \frac{N_r + 1 \pi}{N_r + 1} \right)}{1 - \cos \left( \frac{\pi}{N_l + 1} \right)} \right]. \]

The two energies are shown in Fig. 5(b). In this case, if \( P < 0.65 \), the ground state is dominated by configuration II, while if \( P > 0.65 \), it is by configuration I. In configuration I, more heavy particles will contribute to the total energy, even if the value of contribution of each heavy particle is smaller. In the configuration II, value of contribution to total energy from each light particle is larger contribute to the total energy, but the number of light particles is smaller. Therefore, there is a transition point between two phase separated states. We show the phase diagram in Fig. 6. Here we would like to point out that the two phase separated states, i.e. I and II, are qualitatively different. For the configuration I, the pair-pair correlation function \( \langle n_{1\sigma} n_{1\sigma'} \rangle \) has a non-vanishing long-range behavior. So it is a true long-range order. While for the configuration II, the correlation function decays algebraically.

V. DOMINANT ORDER AND PAIRING BEHAVIOR IN THE LIQUID PHASE

As we known, the ground state is SS in standard Hubbard model with negative \( U \). In Ref. [12], there is phase transition from SS to CDW driven by different mass in negative \( U \) case but with \( N_l = N_r \). And now we want to find the modification of spin and mass imbalance to the pattern in ground state. For this purpose, we need to calculate the correlation functions related such kinds of order, like CDW, SDW, and SS. They are defined as:

\[ R_\sigma (x, x') = \langle O_\sigma (x) O_\sigma^\dagger (x') + h.c. \rangle \]

where

\[ O_{CDW}(x) = \sum_\sigma e^{-2ik_F x} \psi_{R\sigma}^\dagger (x) \psi_{L\sigma} (x), \]

\[ O_{SS}^\perp (x) = \sum_\sigma e^{-2ik_F x} \psi_{R\sigma}^\dagger (x) \psi_{L\sigma} (x), \]

and

\[ O_{SS} (x) = \sum_\sigma e^{i(k_F x - k_F' x')} \psi_{R\sigma}^\dagger (x) \psi_{R\sigma} (x'), \]

for CDW, SDW, and SS, respectively. In 1D Fermi liquid, it is well known that there is no true long-range order, and the correlation function usually has the behavior of a power-law decay.

\[ R_\sigma (x, x') \sim \frac{1}{|x - x'|^{\nu_\sigma}}. \]

In Fig. 7 we show the dependence of three correlation exponents on \( P, |U|, \) and \( z \) respectively. From the figure, we can see that the SS correlation dominates in all three cases. Unlike the case in Ref. [12], there is no phase transition from SS to CDW now. We believe that the system will come into phase separation region before this transition happens.

At the same time, we can obtain oscillating behavior of pairs very easily. In our system, pair correlation mainly comes from singlet pair correlation because of on-site attractive interaction. Therefore, SS correlation function is just expected now. It is obvious that pair correlation function will take the following form:

\[ R_{SS} (x) = 2 \cos [(k_{F1} - k_{F2}) x] \frac{1}{|x|^{\alpha_{SS}}} \]

If and only if \( N_l \neq N_r \), the pair correlation will take the oscillation form, and different mass will modify the correlation exponent \( \alpha_{SS} \) together with spin imbalance. This state has non-homogeneous distribution in real space, and it is called FFLO state. From Fig. 7 we can see that the exponent \( \alpha_{SS} \) is suppressed, hence the FFLO state becomes favorable, as the mass difference increases. Therefore, we believe that the mass imbalance is good for the FFLO state.

VI. SUMMARY

In this paper, from the bosonized form of the 1D asymmetric Hubbard model, we have studied the role of spin imbalance and mass imbalance at zero temperature under various conditions. The conditions of phase separation have been presented, and the effects of spin imbalance, different mass and interaction are also discussed in detail. We find that more-light-particle case is same as the more-heavy-particle one at the weak coupling limit. And they are different in the strong
The SS order is always dominating in the liquid phase.

coupling limit. In the liquid phase, SS is always dominant and there is no phase transition from SS to CDW. Finally, our results show that the mass imbalance might be in favor of the FFLO state.

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