Quantum phase diagram of fermion mixtures with population imbalance in one-dimensional optical lattices

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With a recently developed time evolving block decimation (TEBD) algorithm, we numerically study the ground state quantum phase diagram of fermi mixtures with attractive inter-species interactions loaded in one-dimensional optical lattices. For our study, we adopt a general asymmetric Hubbard model (AHM) with species-dependent tunneling rates to incorporate the possibility of mass imbalance in the mixtures. We find clear signatures for the existence of a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase in this model in the presence of population imbalance. Our simulation also reveals that in the presence of mass imbalance, the parameter space for FFLO states shrinks or even completely vanishes depending on the strength of the attractive interaction and the degree of mass imbalance.

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The pairing of fermions in multi-component fermi mixtures is of fundamental interest not only in condensed matter, but also in atomic, nuclear, and astrophysics. When the fermi surfaces of the component species are mismatched due to unequal densities, possibilities open up for exotic pairing mechanisms such as the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) [1, 2] and the breached pair (BP) states [3, 4]. While these interesting states of matter remain experimentally elusive, controversies about their stability have been long-standing. Recently, this subject has received renewed intense attention due to atomic physics experimental studies on population-imbalanced ultra-cold fermions [5]. The advent of techniques for precisely controlling and detecting ultra-cold atoms is making it possible to systematically study the FFLO and/or the BP states with exotic fermionic pairing, which has turned out to be impossible to do in conventional solid state superconductors.

Inspired by the experimental achievements, over the past few years a large body of theoretical studies have been reported for the exotic pairing states in ultra-cold atomic fermion systems with population imbalance [6, 7]. It has been found that both FFLO [6] and BP states [7] could exist in 3D systems. Particularly, a consensus has developed that the stability region of the 3D FFLO states is very narrow, making it very difficult to observe experimentally. In contrast, due to the Fermi surface nesting it could be much easier to observe the FFLO-type states in 1D or quasi-1D systems [6, 8]. In this work we present numerically calculated exact quantum phase diagrams for the population imbalanced 1D fermi mixtures with unequal masses for the component species.

Fermi mixture systems with mass imbalance could be characterized by the asymmetric Hubbard model (AHM) with species dependent tunneling rates. With equal spin populations, a phase diagram for the 1D AHM has been obtained with the renormalization group technique [10] and possible spin segregation in this model with repulsive interactions has been investigated with bosonization and density matrix renormalization group (DMRG) techniques [11]. Nonetheless, it is not surprising that more attention has been given to the systems with both mass and population imbalances, in which stabilities of FFLO and breached pair (BP) states in 3D systems have been extensively studied [12]. Very recently, a quantum Monte Carlo (QMC) study on finite-size fermi mixtures in 1D optical lattices with imbalanced populations and masses has been reported [13], in which evidence of 1D analog of FFLO-type states has been found. The QMC simulation also reveals that when the mass difference is large enough, instead of an FFLO-type state, the ground state of the system will become an inhomogeneous “collapsed” state.

In this paper, we report a time evolving block decimation (TEBD) numerical study on fermi mixtures with unequal masses and attractive on-site interaction in 1D optical lattices. Our study is complementary to the QMC simulation in Ref. [13], in that we obtain the phase diagrams for such fermi mixture systems. Consistent with the QMC results, we find that FFLO states are the only possible class of polarized pairing states in such systems. As the mass imbalance increases, the parameter space for FFLO states shrinks and eventually vanishes completely. Since we study the homogeneous system at the thermodynamic limit, our phase diagram does not have any inhomogeneous collapsed state, in contrast to Ref. [13].

For our simulation, we adopt the asymmetric Hubbard Hamiltonian to model the Fermi mixtures in 1D optical lattices with unequal masses:

\[ H = - \sum_{\langle i,j \rangle, \sigma} t_{\sigma} c_{\sigma i}^\dagger c_{\sigma j} + \sum_{i} U n_{\uparrow i} n_{\downarrow i} - \sum_{i} \mu (n_{\uparrow i} + n_{\downarrow i}) + \sum_{i} \delta \mu (n_{\uparrow i} - n_{\downarrow i}), \]

where \( c_{\sigma i} (\sigma = \uparrow \text{ or } \downarrow) \) stands for the annihilation operator.
We note that the asymmetric Hubbard model defined by Eq. (1) could also be realized in mixtures of same-species fermions prepared in two different internal states by engineering internal-state-dependent optical lattices [14].

To investigate the ground state properties of this Hamiltonian, we use an infinite lattice version of the TEBD algorithm [15], which allows us to study the model in the thermodynamic limit. A source of intrinsic numerical error for TEBD is due to the Trotter-Suzuki expansion (TSE) used in the decomposition of time evolution operator. (In our simulation we choose the 4th order symmetric TSE.) Furthermore, the convergence of the physical results with TEBD is mainly controlled by a cut-off parameter \( \chi \), which characterizes how well one preserves the bipartite entanglement of the system when truncating the Hilbert space. In this work, we choose \( \chi = 60 \). The convergence has been checked to be good enough (within \( \sim \mathcal{O}(10^{-4}) \) for real space correlation functions) for our purpose, as compared with \( \chi = 80 \) and 100 results.

To identify relevant (quasi-)phases for our model, we calculate the real space spin-spin (\( S^m_r \)), density-density (\( D_r \)), and pairing (\( P_r \)) correlations and their Fourier transforms \( X_k = 1/\sqrt{M} \sum_{i=0}^{M-1} X_r \cos(kr) \), where \( M + 1 \) is the number of sites involved in the transformation (for this work, we choose \( M = 100 \)) and \( X \) stands for \( S, D \) and \( P \) correlations. The real space correlation functions are defined as

\[
S^m_r \equiv \langle s^m_i s^m_{i+r} \rangle - \langle s^m_i \rangle \langle s^m_{i+r} \rangle,
\]

\[
D_r \equiv \langle n_i n_{i+r} \rangle - \langle n_i \rangle \langle n_{i+r} \rangle,
\]

\[
P_r \equiv \langle c^\dagger_{i\uparrow} c_{i+r\uparrow} c^\dagger_{i\downarrow} c_{i+r\downarrow} \rangle
\]

where the spin operators associated with site \( i \) is given by \( s^m_i \equiv c^\dagger_{i\alpha} \sigma^m_{\alpha\beta} c_{i\beta} / 2 \) with \( \alpha = \downarrow \) and \( \sigma^m = (m = x,y,z) \) standing for the Pauli matrices. In addition, we also calculate \( \langle c^\dagger_{i\sigma} c_{i+r\sigma} \rangle \) and its fourier transform, which gives the momentum distribution for the \( \sigma \)-fermion.

In Fig. 1, we present the ground state phase diagram (effective magnetic field vs. chemical potential) for Fermi mixtures based on the asymmetric Hubbard model at \( U = -4 \). In the shaded parameter regions around the centers of the diagrams, all the lattice sites are partially filled by both species of fermions and the effective magnetic field \( \delta \mu \) is not strong enough to induce any population imbalance. In these regions, the ground states of the system have either charge density wave (CDW) or singlet superfluid (SS) as the dominant quasi-long range order, depending on the filling factor. As the effective magnetic field increases, population imbalance is introduced and the system could be brought into the regions filled with solid dots as shown in the diagram. These regions are of central interest for us, since within them the ground state of the system is found to be of the FFLO type. (The pairing correlation and momentum distribution characterizing the FFLO-type states will be presented later in Fig. 3 for the sample data points marked in the phase diagrams.) In the remaining regions of the diagrams, at least one type of fermions has zero or unity occupation number at all sites (\( \langle n_{\sigma} \rangle = 0 \) or 1) and the system behaves as normal Fermi gas. The green lines in Fig. 1 show the phase boundaries of the normal states (N). (We note that our so-called normal states could be further divided into several different categories according to the particle occupation numbers and degree of polarization, e.g. vacuum state, fully occupied state, fully polarized state, etc. But as they are of limited interest, we do not distinguish them in this work.)

By comparing the diagrams corresponding to different \( t_1 \), we can make the following observations. First, the pa-
paramater space supporting the FFLO states shrinks with the increase of the imbalance in $t_\sigma$ or, equivalently, in the fermion masses. This can be understood by considering the bandwidth. A larger mass imbalance effectively leads to a narrower bandwidth ($\sim 4t_\sigma^2/U$), hence when we tune $\mu$ or $\delta\mu$ it is easier for the system to fall into the $n_1 = 0$ or 1 bands and become normal. A second observation is that the symmetry of the $t_1 \neq 1$ diagrams is different from that of the $t_1 = 1$ diagram. When $t_1 \neq 1$, the diagrams are only symmetric about the center point ($\mu = U/2, \delta\mu = 0$), reflecting the fact that the Hamiltonian is invariant under the particle-hole transformation combined with the inversion about ($\mu = U/2, \delta\mu = 0$).

In the $t_1 = 1$ case, the diagram is symmetric about the two axes $\mu = U/2$ and $\delta\mu = 0$, since the Hamiltonian now possesses an extra symmetry, namely the invariance under spin flip combined with the inversion about ($\mu = U/2, \delta\mu = 0$).

We present in Fig. 2 the ground state phase diagram for $U = -10$. One can see that the key features are the same as the $U = -4$ case. Namely, FFLO is the only partially polarized superfluid states in the phase diagram and its parameter space shrinks with the increase of mass imbalance. Furthermore, the shape and symmetry of the diagrams also resemble those of the $U = -4$ diagrams in Fig. 1. Nonetheless, there are noticeable differences.

With a stronger on-site attraction, it is harder to break the pairs. Hence we have higher critical fields $\delta\mu_c$ in the $U = -10$ case. Besides, the effects of unequal masses become more dramatic when the on-site interaction is stronger. For example, in contrast to the $U = -4$ case, when $U = -10$ and $t_1 = 0.3$ one can barely find the FFLO phase and at $t_1 = 0.15$ the parameter space for FFLO completely disappears for $U = -10$.

In Fig. 3, we show the pairing correlation functions and particle number distributions in the momentum space for six sample data points with various $\{t_1, \mu, \delta\mu\}$ in the FFLO regime of Fig. 1. FFLO pairs are known to have non-zero center-of-mass momentum and as its signature, the pairing correlation function $P_k$ for FFLO states has peaks at non-zero momentum $|k_{1F} - k_{1F}|$ with $k_{\sigma F} = (n_\sigma)\pi$ standing for the fermi momentum for non-interacting free fermions. From the solid curves in Fig. 3, we can clearly see the peaks of $P_k$ at non-zero momenta $k_p = |k_{1F} - k_{1F}|$, indicating the presence of FFLO pairing. One can also see that the particle number distribution functions $N_{1k}$ and $N_{1k}$ drop sharply at $k_{1F}$ and $k_{1F}$, respectively. Another noteworthy point is that the momentum distribution function for the “heavier” species ($\downarrow$-fermion) in an FFLO state clearly exhibits a dip at momentum $2k_{1F} - k_{1F}$.

Considering the potential interests in studying the
mixtures of $^6$Li and $^{40}$K, we also present the momentum space pairing ($P_k$) and density ($D_k$) correlations for the asymmetric Hubbard model at $U = -4$ and $t_1/t_1 = 0.15$ in Fig. 4. The two upper panels of Fig. 4 show the pairing and density correlations in the case with population imbalance, while the lower panels show the case with equal populations. From the visibility and height of the peaks in the correlation functions, one can tell which kind order is more dominant. First, we look into the case with equal populations. When the filling factor slightly deviates from half-filling, charge density wave is the dominant quasi-long range order. As an example, for $\delta\mu = 1.1$ and $\mu = -1.9$, we have $\langle n_i \rangle = 2k_F t_F = 2k_F \sim 1.09$. One can observe a sharp peak for $D_k$ located at $k \sim 0.9\pi(= 2\pi - 2k_F)$ while $P_k$ shows a much broader and lower peak at $k = 0$ indicating that CDW is more dominant than SS. When the filling factor is further away from half-filling, the single superfluid order gradually becomes more dominant. (The peak of $D_k$ moves toward $k = 0$ with its visibility and height decreasing, while the peak of $P_k$ remains at $k = 0$ and becomes sharper.) Next, we examine the case with population imbalance. From the upper left panel of Fig. 4, we can see that $P_k$ shows maxima at non-zero momenta, which are verified to be directly given by the difference in particle number density, signalling the presence of FFLO pairing. The results presented in Fig. 4 indicate that in order to observe the FFLO state in mixtures of spinless $^6$Li and $^{40}$K, one should keep the density of $^{40}$K well away from half-filling and consider avoid large inter-species interaction.

In summary, we have presented effective magnetic field ($\delta\mu$) vs. chemical potential ($\mu$) phase diagrams for 1D fermi mixtures with unequal masses and attractive on-site inter-species interactions loaded in optical lattices. We find that with mass and population imbalance the ground state of the system could be either an FFLO state or a normal state. With the increase of mass imbalance, the parameter space for the FFLO states shrinks. When the mass imbalance gets too large, the FFLO states are no longer stable.

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