Pair formation and collapse in imbalanced fermion populations with unequal masses

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Abstract – We present an exact quantum Monte Carlo study of the effect of unequal masses on pair formation in fermionic systems with population imbalance loaded into optical lattices. We have considered three forms of the attractive interaction and find in all cases that the system is unstable and collapses as the mass difference increases and that the ground state becomes an inhomogeneous collapsed state. We also address the question of canonical vs. grand canonical ensemble and its role, if any, in stabilizing certain phases.

Introduction. – The properties of fermionic systems with imbalanced populations have long been of interest for a variety of reasons. Of particular importance is the pairing mechanism resulting in composite bosonic particles and leading to superconductivity/superfluidity. The original focus [1,2] was on polarized superconductors with an imbalance between the two spin populations where it was predicted that the Cooper pairs form with a center-of-mass momentum equal to the difference of the Fermi momenta of the two populations. This Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase [1,2] proved to be difficult to observe in solids and was only achieved recently in heavy-fermion systems [3].

The recent experimental realization of trapped ultracold fermionic atoms with tunable attractive interactions has intensified interest in this problem. Experiments, in which two hyperfine states of ultra-cold fermionic atoms play the role of up and down spins, have demonstrated the presence of pairing in the case of unequal populations [4,5]. This has spurred much theoretical work using a variety of approaches such as mean field [6–15], effective Lagrangian [16] bosonisation [17] and Bethe ansatz [18] applied to the uniform system with extensions to the trapped system using the local density approximation (LDA).

For the uniform case, the controversy continues on the details of the paired state: FFLO pairs forming with non-zero momentum vs. breached pairing (BP) at zero momentum [14,15,19] and on the robustness of such phases. Distinguishing features between these two possibilities include the presence, for FFLO, of spatial modulations (inhomogeneity) in the pairing order parameter, and consequently a peak at non-zero momentum in the pair momentum distribution function as opposed to the coexistence of a superfluid and normal component in a translationally invariant and isotropic state in the BP scenario. In addition, excitations are gapped for the FFLO phase but not so for BP.

No general consensus has emerged on which pairing type dominates. However, recent exact numerical work on the ground state of one-dimensional Fermi systems with imbalanced populations loaded into optical lattices has found that FFLO is the only pairing mechanism both in the uniform [20–22] and in the trapped [20,21,23,24] systems. Similar results have been found without the optical lattice [25]. On the other hand, approximate dynamical mean field (DMFT) results appear to indicate that no FFLO phase is present in the three-dimensional system [26].

In addition to the above equal-mass cases, of relevance in condensed matter and trapped ultra-cold atomic systems, there is great interest in the case of unequal masses. This arises naturally in trapped mixtures of
The difference atomic species, e.g. K-Rb, and also in cold dense quark matter where the $c$, $b$ and $t$ quarks are much heavier than the $u$, $d$ and $s$ quarks. It was argued theoretically that such mass and population imbalance leads to the BP phase [27,28] with gapless excitations which can be stabilized by longer-range interactions [29]. In this paper we examine this question with exact quantum Monte Carlo (QMC) simulations. We focus on the one-dimensional system loaded into an optical lattice governed by the extended Hubbard Hamiltonian

$$\hat{H} = -\sum_{i,\sigma} t_\sigma (c_{i+1,\sigma}^\dagger c_{i,\sigma} + c_{i,\sigma}^\dagger c_{i+1,\sigma}) + \sum_{i,j,\sigma,\sigma'} U_{ij,\sigma\sigma'} n_{i,\sigma} n_{j,\sigma'},$$

where $c_{j,\sigma}^\dagger$ ($c_{j,\sigma}$) are fermion creation (annihilation) operators on spatial site $j$ with the fermionic species labeled by $\sigma = 1, 2$ and $n_{j,\sigma} = c_{j,\sigma}^\dagger c_{j,\sigma}$ is the corresponding number operator. The unequal masses are embodied in the unequal hopping parameters. We set the energy scale by taking $t_1 = 1$ and studying the system as $t_2$ gets smaller ($m_2$ gets larger). In general, the interaction term $U_{ij,\sigma\sigma'}$ can couple all fermions on all sites; in what follows we shall consider three different forms.

For our simulations, we use a continuous imaginary-time canonical “worm” (CW) algorithm where the total number of particles is maintained strictly constant [30]. In this algorithm, two worms are propagated, one for each type of fermion, which allows the calculation of the real-space Green functions of the two fermionic species, $G_\sigma$, and the pair Green function, $G_{\text{pair}}$.

$$G_\sigma (l) = \langle c_{j+l,\sigma}^\dagger c_{j,\sigma} \rangle,$$

$$G_{\text{pair}} (l) = \langle \Delta_{j+l,1} \Delta_j \rangle,$$

where $\Delta_j = c_{j,1} c_{j,2}$. It is then immediate to obtain the momentum distributions $n_\sigma (k)$ and $n_{\text{pair}} (k)$ from their Fourier transforms. We emphasize that this algorithm is exact: there are no approximations and the only errors are statistical (which typically correspond to the size of the symbols). The polarization is given by $P = (N_2 - N_1)/(N_2 + N_1)$, where $N_1$ ($N_2$) is the minority (majority) particle numbers. The associated Fermi wave vectors are $k_{F\sigma} = \pi N_\sigma / L$. We ran our simulations at $\beta = 2L$, where $L$ (typically $L = 32$) is the number of lattice sites. We have verified that these values are large enough to yield the ground-state properties, which is our focus. Typical runs take a day or two on a desktop computer.

**Heavy majority:** $t_1 > t_2$. - We begin with the simplest form for the interaction term, $U_{ij,\sigma\sigma'} = U \delta_{ij} (1 - \delta_{\sigma,\sigma'})$, i.e. only contact attraction ($U < 0$) between the two species. Figure 1 shows what happens to the minority (left) and majority (right) momentum distributions as $t_2$ is decreased for fixed $U = -3t_1$ and $N_1 = 9$, $N_2 = 11$. For $t_2 = 0.9t_1$, $n_\sigma (k)$ drops sharply at the respective Fermi momenta, $(k_{F1}, k_{F2})$ while at the same time, the pair momentum distribution, $n_{\text{pair}} (k)$, exhibits a maximum at $k = |k_{F1} - k_{F2}|$ (fig. 2, left). This indicates pair formation at non-zero center-of-mass momentum and thus an FFLO phase [20–24]. As the mass of the majority particles increases, $t_2$ decreases, the attractive interaction effectively increases because $|U|/t_2$ increases. The increased binding is demonstrated by $\langle n_{11} n_{12} \rangle$ which takes values between $N_1 N_2 / L^2$ (no binding) and $N_1 / L$ (all minority particles have formed pairs) [20]. This quantity is shown in fig. 2 (triangles, right panel) scaled by 4 for better visibility. Clearly, as $t_2$ decreases, $\langle n_{11} n_{12} \rangle$ increases toward its upper limit. As a consequence of this increased binding, the FFLO effect first intensifies, its peak at $k = |k_{F1} - k_{F2}|$ increases in height, reaches a maximum for $t_2 = 0.4t_1$, then decreases and disappears as shown in fig. 2 (circles, right panel).

Note, for example, that for $t_2 = 0.1t_1$ the peak of $n_{\text{pair}} (k)$, fig. 2 (left), is at $k = 0$. 

![Fig. 1: (Color online) The momentum distribution for the minority (left) and majority (right) populations.](image1.png)

![Fig. 2: (Color online) Left: the pair momentum distribution function. Right: the circles show the height of $n_{\text{pair}} (k)$ vs. $t_2$, the triangles show $\langle n_{11} n_{12} \rangle$ scaled by 4 for better visibility.](image2.png)
Also noteworthy is the appearance of a dip in $n_2(k)$, at $k \approx k_{F1}$, whose depth increases with decreasing $t_2$, reaching a maximum for $t_2 = 0.4t_1$, corresponding to the maximum FFLO effect. Further decreasing $t_2$ washes this out. This feature can be understood as follows. As $t_2$ decreases, the interaction between the minority and majority effectively increases ($|U|/t_2$), thus increasing the depletion of $n_\sigma(k < k_{F\sigma})$. Most of the depletion for both $n_1(k)$ and $n_2(k)$ happens for $k < k_{F1}$ since this is where most of the minority resides. This depletion for $k < k_{F1}$ leaves $n_2(k)$ with a bump for $k_{F1} < k < k_{F2}$.

At first glance, it might seem that the disappearance of the FFLO peak, $n_{\text{pair}}(k = |k_{F1} - k_{F2}|)$, as $t_2$ decreases and the appearance of a peak $n_{\text{pair}}(k = 0)$ signal pair formation at $k = 0$ and thus a BP phase. However, a simple argument offers another option. The Fermi momentum of the majority is $k_{F2} = \pi N_2/L$; consequently, as these particles get heavier, $t_2$ smaller, their kinetic energy becomes negligible and can be ignored. To minimize its free energy, the system will then optimize the potential and kinetic energies of the light particles. The optimal potential energy is obtained when the light particles are on the same sites as the heavy ones. On the other hand, the kinetic energy is optimized when the light particles are delocalized. Both these energies can be optimized if the heavy particles coalesce, forming a contiguous region with one heavy particle per site, $n_{12} = 1$. This region, then, acts as a platform on which the light particles can delocalize over its entire extent while always being in contact with the heavy particles thus minimizing their potential energy. This is indeed what happens as the density profiles, $n_{11}$ and $n_{12}$, show in Fig. 3 for two polarizations. To summarize, as $t_2$ decreases, the system goes from an FFLO phase to a spatially collapsed one.

To quantify this collapse, we define the quantity

$$\delta n \equiv \sum_i (n_{i1}) - N_1/L$$

which is essentially zero when the system is uniform ($n_{i1} = N_1/L$) and grows as the collapse happens. In Fig. 4 we show $\delta n$ vs. $t_2/|U|$ for three polarizations and three couplings in each case. We see that, indeed, the system collapses as $t_2$ decreases and that for a given polarization, this collapse appears to happen at approximately the same value of $t_2/|U|$. Also, the larger the polarization, the easier it is to trigger the collapse (larger $t_2$). This behavior holds for all the parameters we examined, specifically $-13 < U < -1$, and polarizations $0.1 \leq P \leq 0.55$.

We, therefore, conclude that in the presence of only contact attraction, the BP phase is not realized as the majority population is made heavier; instead the system collapses. To counter the tendency of the heavy particles to clump together as in Fig. 3, we introduce longer-range interaction. It is reasonable to suppose that near-neighbor (nn) repulsion between particles of the same species would tend to oppose such collapse. To this end we redid the above study but with the interaction term $H_I = \sum_i U n_{i1} n_{i2} + V \sum_{i,\sigma} n_{i\sigma} n_{i+1\sigma}$ with $U < 0$ and $V > 0$. We studied this for $0.1 \leq P \leq 0.44$ for $-10t_1 \leq U \leq -4t_1$ and found that, indeed, the stability of the system against collapse is extended to smaller values of $t_2$ but that eventually the system always collapses. Furthermore, before the collapse, the system always exhibits FFLO pairing while after collapse, the nn repulsion term, $V$, produces density oscillations as the presence of near neighbors is opposed. Therefore, this second form of the interaction also fails to produce the BP phase.

We now turn to the third interaction form which was proposed in ref. [29] and argued to yield the BP phase. This form extends beyond the contact term and acts only between particles from different species. The idea is based on the assumption of three competing homogeneous phases: a normal state of free fermions, a fully gapped BCS superfluid and a gapless BP phase. It was argued that by giving the interaction term structure in momentum space, one may be able to stabilize the...
The contact interaction is \( V = -0.25t_1 \), \( U = -4t_1 \), \( N_1 = 5 \), \( N_2 = 7 \), \( L = 32 \). In our simulations we used a Gaussian dependence on distance. In fact, with the longer-range attraction, the system is unstable as can be easily understood by the real-space argument presented above for the contact interaction case.

**Heavy minority:** \( t_1 < t_2 \). – So far, we have considered the case where the heavy particles are the majority which leads to collapsed configurations like those in fig. 3. The question then is: will the system still collapse when the heavy particles are the minority and what form will the collapsed configurations take? We now consider this case with a heavy minority population \( N_1 = 9 \), and a lighter majority, \( N_2 = 13 \), on a 32-site lattice with \( \beta = 64 \). As before, we fix the light population hopping \( t_2 = 1 \) to define the energy scale and we study the collapse as a function of the heavy minority hopping parameter, \( t_1/t_2 \), and the attractive interaction, \( U/t_2 < 0 \). In the top panel of fig. 6 we show, like in fig. 4, \( \delta n \) as a function of \( t_1/|U| \) for five different values of the interaction, \( U \). The behavior is similar to that in fig. 4; we find that for these values of \( N_1 \) and \( N_2 \), \( \delta n \) increases sharply for \( t_1/|U| \approx 0.03 \) signalling spatial collapse in the system. One candidate for the collapsed configuration is that, as before, the heavy particles (the minority in this case) form a contiguous region thus providing a platform for the lighter particles. This would then result in a contiguous region with one heavy and one light particle per site and the excess light majority particles spread over the rest of the system. This, however, does not minimize the energy because the light particles residing on the heavy-particle platform are blocked: they are in a Mott state and have zero kinetic energy. In the bottom panel of fig. 6 we show a typical density profile of a collapsed configuration. It is easy to understand energetically why this density wave structure is favored over the previous candidate: the light particles are never blocked in a Mott region and can always hop to neighboring sites to optimize the free energy.

We note that the configuration in fig. 6 corresponds to phase separation: in one region the system is in a charge density wave phase, in the other region it has free fermions. These two phases coexist. On the other hand, the configurations in fig. 3 correspond to spatial collapse: the system has regions void of particles and regions where all the particles reside.

**Canonical vs. grand canonical.** – Finally, we consider the question of canonical vs. grand canonical ensembles. It has been suggested [15,29] that the stability of BCS, FFLO or BP phases can depend on whether one fixes the populations or the chemical potentials. All the above results have been obtained with the CW algorithm where \( N_1 \) and \( N_2 \) are kept strictly fixed. An alternative is to add the chemical potential term, \( \sum (-\mu_1 n_1 - \mu_2 n_2) \), to the Hamiltonian, eq. (1), and use a grand canonical QMC algorithm such as the determinant quantum Monte Carlo.
Carlo (DQMC) algorithm [31]. We compare in fig. 7 the momentum distributions obtained with the CW and the DQMC algorithms with $\mu_1$ and $\mu_2$ chosen to give average fillings corresponding to the fixed fillings in the canonical case. There is no disagreement between the two; in particular, the FFLO phase is seen to be stable whether one fixes the populations or the chemical potentials. Of course, if one changes $t_2$ while holding the chemical potentials fixed, the average populations, $\langle N_1 \rangle$ and $\langle N_2 \rangle$, will change. Nonetheless, whatever $\langle N_1 \rangle$ and $\langle N_2 \rangle$ one has obtained by fixing $\mu_1$ and $\mu_2$, one will obtain the same physics in the canonical ensemble by fixing the populations to the corresponding values, as seen in fig. 7. One is free to study these phases and their stability in either ensemble.

Conclusions. — In summary, we have studied, using exact QMC simulations, the effect of mass differences between two imbalanced fermion populations. For the case where the majority population is heavier, we performed our study with three possible attractive interaction terms. In all three cases, we have found the system to be unstable and to collapse when the mass disparity is large enough: the BP phase is not realized by tuning the mass ratio between the two populations. For the case where the minority is heavier, we showed that the system still collapses when the mass difference is large enough, but in this case it forms density wave structures. We have also shown that fixing the populations or the chemical potentials leads to the same physics. The stabilization of sought-after phases is not favored by one ensemble rather than another.

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