Phases of attractive spin-imbalanced fermions in square lattices

Simone Chiesa\textsuperscript{1} and Shiwei Zhang\textsuperscript{1}

\textsuperscript{1}Department of Physics, College of William & Mary, Williamsburg, VA 23188, USA

We determine the relative stability of different ground-state phases of spin-imbalanced populations of attractive fermions in square lattices. The ground state is determined within Hartree-Fock-Bogoliubov theory, with care taken to remove finite size effects. The phases are systematically characterized by the symmetry of the order parameter and their real- and momentum-space structures. For quarter- to half-filled lattices, where the Fermi surfaces are most distorted from their spherical counterpart in the continuum, we predominantly find unidirectional Larkin-Ovchinikov-type phases. We discuss the effect of commensuration between the ordering wave vector and the density imbalance, and describe the mechanism of Fermi surface reconstruction and pairing for various orders. A robust supersolid phase exists when the ordering wave vector is diagonally directed. Charge and pairing order coexist, rather than competing, and are responsible for the opening of the gap on different portions of the Fermi surface. A variational determination of the correct pair momentum of the Larkin-Ovchinikov phases shows that phase separation does not occur in the considered regime of density and magnetization.

PACS numbers:

INTRODUCTION

There has been a surge of interest in the possibility of realizing unconventional fermionic superfluids using cold atomic gases. Amongst the many possibilities offered by the highly tunable Hamiltonians available in cold-atoms experiments, the simplest remains that of unequal populations of two hyperfine states in the presence of attractive interaction. The theoretical study of such systems dates back to Fulde and Ferrel (FF) \cite{FF} and Larkin and Ovchinikov (LO) \cite{LO} who independently suggested that the mismatch between the Fermi surfaces of the two species could result in the formation of a condensate of finite-momentum pairs. Atomic gases offer a direct route to the realization of FFLO phases, circumventing most of the difficulties of solid state systems, thanks to the possibility of controlling independently the density of the two species, the absence of disorder and, most importantly, the ability to engineer strong interactions. In spite of this, the existence of an FFLO phase in three dimensions has been argued to be confined to a small range of interaction strengths and polarizations\cite{3d}, and detection has remained elusive.

The possibility of using optical lattices has been suggested by several authors\cite{4, 5} as a key ingredient to observe FFLO-type states. The best empirical indication that this may be the case is provided by experiments on strongly-correlated-electrons materials and the fact that, when doped, these systems show a tendency toward formation of inhomogeneities in the form of spin, charge and, possibly, pairing density waves. The relevance of these experiments to the properties of attractive fermions in optical lattices stems from the belief that, in both cases, the essential physics can be captured by a one-band Hubbard model: with an on-site repulsive interaction for many of the electronic systems and an on-site attraction in an optical lattice. The attractive and repulsive cases are mapped into each other by a particle-hole transformation\cite{4} and the presence of spin-texture in the doped repulsive case translates into the occurrence of a modulated superfluid in an imbalanced population of attractive fermions, i.e. an FFLO phase. This is reinforced by recent quantum Monte Carlo results \cite{6} on the two-dimensional repulsive model showing spin-density waves with long wavelength modulation.

Despite this mapping and several works addressing the existence of a possible FFLO phase \cite{7, 8}, the nature of the ground state phases in a spin-imbalanced two-dimensional optical lattice remains largely undetermined. On the one hand, information on the repulsive model is entirely confined to the case of unpolarized systems, which maps into the attractive case at half-filling: $n_\uparrow + n_\downarrow = 1$; for the case of imbalanced fermionic population, one is interested in the more general case of a polarized system and arbitrary density. On the other hand, works addressing the physics in the lattice have either focused on the single plane-wave form of the order parameter \cite{7, 8} or on selected states \cite{9, 10} (e.g. in fixed size supercells) because of the challenge of removing large finite-size effects. Such restrictions can bias the result and lead to, for example, an incorrect pair momentum. The accurate determination of the spatial structure of the order parameter is also indispensable to addressing the issue of phase separation.

In this work we establish the correct form that FFLO phases have in the thermodynamic limit on a square lattice, and show that a proper determination of the leading pairing wave vectors in the ordered state leads to a characterization of different physical regimes based on the properties of the nodal (excess) particles. Small to moderate interaction strengths are considered, where mean-field theory is expected to capture the correct physics. In
regime of density and polarization where the presence of a lattice alters most dramatically the shape of the Fermi surfaces, we find unidirectional order and the existence of three distinct phases: 1) a nodal metallic state characterized by the presence of Fermi arcs, 2) a nodal band insulator where the densities of excess particles and nodal lines are equal and 3) a charge density wave that results in a robust supersolid phase obtained when the ordering wave vector is directed along the diagonal direction. Once the variational search for the optimal pairing wave vector includes the proper symmetry of the order parameter, the Hartree-Fock-Bogoliubov ground state does not phase separate in the parameter regime of interest.

**HARTREE-FOCK-BOGOLIUBOV THEORY**

Results presented in this work are obtained using Hartree-Fock-Bogoliubov theory so that modulations in charge, spin and pairing are all handled on the same footing. The starting Hamiltonian reads

\[ H = -t \sum_{\langle ij \rangle, \sigma} c_{i \sigma}^\dagger c_{j \sigma} - U \sum_i \left( n_{i \uparrow} n_{i \downarrow} - \mu n_i - \frac{\hbar}{2} m_i \right), \]

where \( c_{i \sigma} \) are fermionic annihilation operators of spin \( \sigma \) on site \( i \), \( n_{i \sigma} = c_{i \sigma}^\dagger c_{i \sigma} \), \( n_i = n_{i \uparrow} + n_{i \downarrow} \) and \( m_i = n_{i \uparrow} - n_{i \downarrow} \).

In order to accommodate the inhomogeneities, the calculations are performed on supercells whose shape is dictated by the symmetry of the targeted phase. The supercell is characterized by two basis vectors, \( L_1 \) and \( L_2 \), whose components are integers. Once the supercell shape is chosen, we define Bloch states as \( c_j(k) \propto \sum_L c_{j + L} \exp(ik \cdot L) \) where \( L = n_1 L_1 + n_2 L_2 \), and \( k \) is a vector that varies freely within the super-lattice first Brillouin zone. Then, using these states and the mean-field approximation, the Hamiltonian decouples into a sum of \( k \)-dependent pieces, \( H = \sum_k H(k) \), of the form

\[ H(k) = [c^\dagger \cdot c] \begin{bmatrix} H^\uparrow(k) \\ \Delta \end{bmatrix} \begin{bmatrix} \Delta^\dagger \\ -H^\downarrow T (G - k) \end{bmatrix} \begin{bmatrix} c^\dagger \cdot c \end{bmatrix}^T, \]

where \( c^\dagger \) and \( c \) represent an array (row) of operators, \( \{c_j(k)\} \) and \( \{c_{i \sigma}(G - k)\} \) respectively, with index \( i \) running over the \( N \) sites of the supercell, and \( G \) is defined below. \( H \) and \( \Delta \) are \( N \times N \) matrices with elements

\[ [H_{ij}(k)]_{ij} = -t_{ij}(k) + \delta_{ij} (D_{i \sigma} - \mu - s_\sigma \hbar/2), \]

\[ [\Delta_{ij}] = \delta_{ij} \Delta. \]

In the above, \( t_{ij}(k) = \sum_L \exp(ik \cdot L)t_{i,j + L} \), \( s_{1/4} = \pm 1 \) and \( D_{i \sigma}, \Delta_i, \mu \) and \( \hbar \) are determined by the requirement that the Free energy \( F = \langle H \rangle - TS \) is a minimum for the target average densities \( n_\sigma \). This amounts to imposing the following self-consistency conditions

\[ D_{i \sigma} = -U \int dk \langle c^\dagger_{i \sigma}(k) c_{i \sigma}(k) \rangle, \]

\[ \Delta_i = -U \int dk \langle c_{i \downarrow}(k) c_{i \uparrow}(k) \rangle, \]

\[ n_\sigma = N^{-1} \sum_i \int dk \langle c^\dagger_{i \sigma}(k) c_{i \sigma}(k) \rangle, \]

with expectation values evaluated in the supercell. Note that, although we target specific densities, the mean-field approach works in the grand-canonical ensemble.

The variable \( G \) in Eq. (2) is a vector such that \( \theta = G \cdot L \) gives the twist angle of the pairing order parameter under translation by \( L \). For collinear phases, \( \theta \) is either 0 or \( \pi \), giving periodic or anti-periodic boundary conditions on \( \langle c^\dagger_{i \sigma}(k) \rangle \). Note that uniform phases with a spiral order parameter (FF type) amount to the choice of a one-site cell and \( G \) equal to the wave-vector of the spiral modulation. Thus \( H(k) \) is specified by a \( 2 \times 2 \) matrix, and the eigenvalues and eigenvectors can be computed analytically in the spiral phase.[1]

**SYMMEtRY OF THE ORDER PARAMETER**

**Determination**

Given a set of symmetry-equivalent \( q \) vectors and assuming a continuous phase transition, linear response theory can be used to show that the onset of instabilities of the form

\[ \Delta_q = \sum_q \Delta_q e^{iq \cdot r_i}, \]

FIG. 1: Left Panel: local order parameter, max. \{\langle c^\dagger_{i \sigma} c_{i \sigma} \rangle\}, and leading wavevector (inset) versus \( U \) for \( \langle c^\dagger_{i \sigma} c_{i \sigma} \rangle \propto e^{\delta_{i \sigma} r_i} \) (Spiral), \( \langle c^\dagger_{i \sigma} c_{i \sigma} \rangle \propto \cos(q_\sigma \cdot r_i) \) (Linear), \( \langle c^\dagger_{i \sigma} c_{i \sigma} \rangle \propto \cos(q_\sigma \cdot r_i) \) (Chkbld) with \( q_\sigma = |q| (0, 1) \) and \( q_\sigma = |q| (0.1) \). Right Panel: relative energies of the three phases. Data are for \( n = 0.95 \) and \( m/n = 0.1 \). Kinetic energies are in units of \( t \).
must happen at exactly the same value of $U$, regardless of the choice of $\Delta q$. Below such value, mean field theory is guaranteed to return a normal, spin-polarized Fermi liquid. In order to determine the correct form of order parameter, we proceed as follows. We first determine $U_c$ and the associated non-zero wave-vector $q_c$ using the single plane-wave form as this allows for a quick exploration of phase space. We find that $q_c$ is directed along any of the four, symmetry-equivalent directions $(\pm 1, 0)$, $(0, \pm 1)$ and, therefore, any linear combination of the four associated plane waves is a candidate ground state order parameter just above $U_c$. To resolve which one leads to the largest lowering of energy, we proceed by solving the mean-field equations for the three cases corresponding to spiral ($\Delta_i \propto \exp(iq_\alpha \cdot r_i)$), unidirectional ($\Delta_i \propto \cos(q_\alpha \cdot r_i)$) and checkerboard ($\Delta_i \propto \cos(q_x r_i) + \cos(q_y r_i)$) pairing density wave and track the evolution of $|q|$ as a function of $U$. Explicit calculations in large simulations cells on the repulsive model (with simulated annealing starting with random initial fields[11]) have shown that instabilities involving $q$-vectors in different, non-equivalent directions, which the above approach would miss, are unlikely to occur in the range of $U$ considered here.

**Dependence on density and polarization**

Mean-field results[11] on the repulsive model and the particle-hole transformation relating the attractive and repulsive models imply the existence of the following properties at half-filling, i.e., when the average particle density is precisely one fermion per site: 1) a critical $U$ exists such that, above it, the system develops a phase with an inhomogeneous order parameter 2) the pairing order parameter is characterized by a wave vector $|q| = m\pi$ where $m = n_\uparrow - n_\downarrow$ is the average magnetization 3) both fermionic species have a gap in their single particle spectrum 4) as $U$ grows larger there is a transition from a pair-density-wave in the $(1,0)$ state to one in the $(1,1)$ direction 5) order can be arbitrarily broken into a charge or a pairing instability or a combination of the two. This last point is a consequence of the possibility of breaking spin symmetry in any of the three equivalent directions in the repulsive case. It implies that charge and pairing orders compete, in the sense that the larger one is, the smaller the other must be.

Although there have been studies on several aspects of the physics away from half-filling[10], the correct leading pairing wave vector (which requires a scan through super-
surate regime is characterized by a density of one relation holding at half-filling, precisely determined by the magnetization via the same $n > 0.95$ and for $n = 0.75$ the wavevector is directed along (1,0). The two entries in the last line in each table cell describe, respectively, the type of order just above $U_c$ and at $U = 4$ (see Fig.1’s caption for detail).

cell sizes) has not been determined. This has prevented a characterization of the nature of such phases. As a result the order of possible transitions and the related possibility of phase separation have not been resolved. We address these questions here using the strategy outlined in the previous subsection. A representative example is given in Figure 1 for the case with $m/n$ given in Figure 1 for the case with $m/n = 0.95$ and $n = 0.95$.

To understand the effects due to the significantly different shape of the Fermi surfaces in a lattice when compared to their circular counterparts in the continuum, we repeat a similar analysis in different regimes of density and polarization, $n = 0.95$, 0.75 and 0.5 and $m/n = 0.1$ and 0.4, so as to have a rather complete picture close and away from half-filling, at small and large polarization and in an interaction range that extends from $U_c$ up to $U = 4$.

The results are summarized in Table I. They are consistent with earlier results addressing the physics of FFLO phases in the continuum, which found checkerboard order close to $U_c$, thanks to an expansion in powers of the order parameter\[12\], and show that for $n \geq 0.75$ lattice effects are strong enough to return unidirectional order independently of polarization or proximity to $U_c$, as known to happen at and around $n = 1.0$. Given the difficulty in observing unconventional pairing in the continuum, the latter is the density regime where an experimental realization of the FFLO state could be more feasible. We will therefore focus on it in the following.

| $m/n$ | $n = 0.95$ | $n = 0.75$ | $n = 0.5$ |
|-------|------------|------------|------------|
| $U_c$ | 1.8        | 1.8        | 2.0        |
| $q_c$ | 0.071$\pi$ | 0.078$\pi$ | 0.066$\pi$ |
| Linear | Linear | Linear | Chkbd; Linear |
| $U_c$ | 3.6        | 3.2        | 2.8        |
| $q_c$ | 0.34$\pi$  | 0.30$\pi$  | 0.27$\pi$  |
| Linear | Linear | Linear | Chkbd; Chkbd |

Character of the Nodal Phases

Metal and band insulator at weak coupling

Figure 2 characterizes the FFLO phase at $U = 3t$ and for $m = 0.05$ in two qualitatively different density regimes. In particular, for $n > 0.95$, the wave vector is precisely determined by the magnetization via the same relation holding at half-filling, $q = mn\pi$. This commensurate regime is characterized by a density of one excess particle per node (of the order parameter) and consequent band-insulating behavior along the node. This is most clearly seen in the local density of states at the node, with both species showing a gap at the Fermi energy. Correspondingly the gradient of the momentum distribution shows no sharp lines indicative of the existence of a Fermi surface. The commensurate regime here has, however, some important distinctions from half-filling.

First, the interchangeability between pairing and charge orders is broken as soon as the average density deviates from $n = 1$, and pairing emerges as the dominant order. Second, the density is not perfectly uniform, as it is for the purely superfluid phase at half-filling. The density is instead characterized by a weak modulation that reflects the different degrees of localization of the Andreev states for the two spin species. The density profile shows weak peaks at the nodes indicating that the majority-species nodal states have stronger localization. A similar phase was found in the context of a two-dimensional array of tubes\[13\].

In the second density regime, $n < 0.95$, the majority spin species develop a finite density of states at the nodes of the order parameter. Fermi arcs appear in $|\nabla \psi_{k\downarrow}|$ in the form of sharp lines. The arc in Fig. 2B is of perfectly one-dimensional nature, indicating a complete decoupling between the metallic states living at different nodes. At larger polarization, the arcs will more strongly resemble the underlying Fermi surface of the non-interacting species. Finally, the density profile shows minima at the nodes, rather than the maxima observed in case A, as a direct consequence of the gradual emptying of the majority-spin Andreev bands visible in the local density of states. This is a potentially important experimental signature as it allows the characterization of the nature of the nodal phase, metallic or insulating, via a static local property instead of a collective property such as the distance between nodes or the presence of Fermi arcs.

Supersolid phase at intermediate coupling

Next we consider the phases at larger interaction strengths $U$. Results on the repulsive model\[11\] indicate that the ordering wave vector switches to the (1,1) direction at sufficiently small $m$ and $U > 3t$. We focus on $U = 4t$ for an extensive and systematic examination of the properties of these phases. Indeed unidirectional LO states along the diagonal direction are found; in addition, we find that the system can accommodate both pairing and charge orders as non-competing instabilities away from half-filling. The real- and momentum-space properties of the phases are shown in Fig. 3. In contrast to the (1,0)-direction states, pairing here is achieved by a more radical reconstruction of the Fermi surface. The non-interacting surface of the majority spin is stretched,
FIG. 3: Left panels: Evolution of charge $\langle n_\uparrow + n_\downarrow \rangle$ and pairing order as density is reduced, for $m = 0.05$ along the $(1,0)$ direction. Right panels: corresponding evolution of the gradient of the momentum distributions, and illustration of Fermi surface reconstruction and pairing. The pairing wave-vector, $q$, is in the $(-1,1)$-direction. The solid (green) lines give the non-interacting Fermi surface.

while that of the minority spin is compressed, along the $(-1,1)$ direction so that the reconstructed surfaces become “nested” via $k \rightarrow -k + q$ as illustrated in the middle row of Fig.3. The charge-density wave that develops at larger density is a consequence of the $(\pi, \pi)$ nesting along the $(1,1)$-direction which results from the reconstruction; its amplitude increases with the amount of nested states. The charge order is complementary to pairing, and further lowers the energy.

The new phase discussed above has an important distinction from the supersolid phase that can occur at half-filling. There both charge and pairing orders are associated with wave-vectors coupling the same regions around the Fermi surface: if pairing order happens at $q$, charge order must happen at $(\pi, \pi) - q$ and one can dial the form of the order parameter interpolating between a purely superfluid and a purely charge-density wave state. Away from half-filling, however, pairing is characterized by a polarization dependent wave-vector $q$ while charge order appears at $(\pi, \pi)$ and cannot be dialed away.

PHASE DIAGRAM

Our results are summarized in the phase diagram of Fig.4 for $U = 3t$ and $U = 4t$. We found no evidence of diagonal supersolid order at $U = 3t$ with a region of stability for the commensurate phase limited to small polarization and density close to one. At $U = 4t$, the diagonal wave vector is almost always commensurate with $m$, and pairing and charge order coexist in all but a small fraction of the phase diagram where the diagonal phase is the correct ground state. This suggests that the charge-density wave play a small but important role in stabilizing diagonal order.

Because we have accurately determined the pair momenta and the correct symmetry of the order parameter as a function of magnetization and density, we can now tackle the issue of phase separation in spin-imbalanced systems on a square lattice within Hartree-Fock-Bogoliubov theory. To do this we check the convexity of the energy by diagonalizing

$$
\mathcal{P} = \begin{bmatrix}
\frac{\partial \mu}{\partial n} & \frac{\partial \mu}{\partial h} \\
\frac{\partial h}{\partial n} & \frac{\partial h}{\partial h}
\end{bmatrix}
$$

for the same set of densities and magnetizations reported in Fig.4. The values of $\mu$, $h$ and their derivatives are
determined numerically from the Helmholtz free energy using the grid in Fig. 4. As a result, data in Fig. 4 have numerical uncertainty that we estimated to be comparable to the symbol size. These data, summarizing the case of $U = 3t$, do not suggest any tendency toward phase separation. Although the smallest eigenvalue of $P$ approaches 0 at small magnetization we do not interpret this as a signal of incipient phase separation. Because the distance between nodal lines is inversely proportional to the magnetization, the ground state at small magnetization is characterized by the presence of essentially non-interacting domain walls where the excess spin particles reside. The ground state energy is then simply determined by the energy to create one such wall multiplied by the walls density. Because the latter is proportional to the distance between nodal lines is inversely proportional to the magnetization, the energy displays linear behavior in $m$ and causes $\partial h/\partial m$ to become vanishingly small. This, in turn, is responsible for the vanishing behavior of one of the eigenvalues. These results show that, contrary to previous conclusion based on restricted searches [14] on two-dimensional lattices and contrary to the widely accepted scenario in the dilute continuum, there is no phase separation in the true Hartree-Fock-Bogoliubov ground state on a lattice in these parameter regimes.

Similar results hold for the phases at $U = 4t$ when the different order parameter patterns are separately considered. Obviously, in the global phase diagram, the different symmetry between diagonal and vertical phases implies that the transition is discontinuous and accompanied by phase separation. We have not attempted an in-depth study of how this affects the situation at $U = 4t$. However, a simpler analysis based on considering phase separation in two phases having the same density and different magnetization leads to a narrow coexistence region ($\Delta m = 0.02$ at $n = 1$) and makes it sensible to assume that the broad feature of the phase diagram are, in fact, robust.

**SUMMARY**

We have determined the type of phases that an imbalanced population of two fermionic species with attractive interactions support in the two-dimensional square lattice. Their real- and momentum-space properties are quantitatively characterized. We find that unidirectional LO states are the most stable mean field solutions in a large range of parameter regimes, and checkerboard order is only clearly favored at small density and large polarization. At lower $U$, the finite-momentum pairing wave-vector is along $(1,0)$. We have shown the insulating versus conducting nature of the nodal region of the superconducting order parameter, and its interplay with commensuration effects. Related to these effects, a new phase with supersolid order is seen when the ordering wave vector is directed along the $(1,1)$ direction. Our results suggest that, besides time of flight or Bragg spectroscopy, the different local phases we discussed are also identifiable by their local density profiles. This, in turn, should help their real-space characterization in the presence of a confining potential. Our results conclusively show that, within Hartree-Fock-Bogoliubov, there is no phase separation in the presence of a lattice for the considered density and magnetization regimes.

**Acknowledgments**

We acknowledge support from NSF (Grant no. DMR-1006217), DOE (de-sc0008627), and ARO (Grant no. 56693-PH) and computational support from the Center for Piezoelectrics by Design and by DOE leadership computing through an INCITE grant.

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