Fulde-Ferrell-Larkin-Ovchinnikov pairing as leading instability on the square lattice

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We study attractively interacting spin-$\frac{1}{2}$ fermions on the square lattice subject to a spin population imbalance. Using unbiased diagrammatic Monte Carlo simulations we find an extended region in the parameter space where the Fermi liquid is unstable towards formation of Cooper pairs with non-zero center-of-mass momentum, known as the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state. In contrast to earlier mean-field and quasi-classical studies we provide quantitative and well-controlled predictions on the existence and location of the relevant Fermi-liquid instabilities. The highest temperature where the FFLO instability can be observed is about half of the superfluid transition temperature in the unpolarized system.

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Fifty years after the initial prediction by Fulde, Ferrell, Larkin, and Ovchinnikov (FFLO) [1,2], superconducting phases with spontaneously broken translational invariance are still at the center of interest in such diverse fields as solid state physics, cold atomic gases, nuclear physics, and dense quark matter in neutron stars [3–7]. While the underlying mechanism is generic enough to apply to any partially polarized Fermi system, it has proven surprisingly difficult to unambiguously observe such phases in nature. Recently, however, experimental evidence has been mounting for their existence in heavy fermion compounds [8–10] and layered organic materials [11–15]. On the other hand, experiments with ultracold atoms, which are among the cleanest imbalanced Fermi systems without the need for a magnetic field, so far failed to demonstrate inhomogeneous superfluidity [16, 17] — although there is some evidence for such a phase in one dimension (1D) [18] — possibly due to small extent of the parameter region where an FFLO phase may exist in three dimensions (3D) and difficulties in reaching sufficiently low temperatures [19].

On the theoretical side, results on the existence and nature of FFLO phases based on well-controlled microscopic theories are scarce, with the exception of 1D systems, where exact analytical and numerical studies are possible [19,20], and where finite-momentum pairing is a generic feature of the spin-imbalanced phase diagram. In higher dimensions, most studies are based on effective field theories in the neighborhood of critical points or resort to quasi-classical or mean-field approximations. For 3D Fermi gases, many features of the mean-field phase diagram [20] have been corroborated by fixed-node diffusion quantum Monte Carlo calculations [21]; whether the FFLO phase does exist in a small sliver of the phase diagram, as predicted by the mean-field theory, is however still subject to debate.

The FFLO state is expected [22,23] to occupy a larger parameter region in two dimensions (2D), and lattice effects may further increase its stability [28,29]. Correspondingly, mean-field calculations [30,31] and real-space dynamical mean-field theory (DMFT) for fermions in anisotropic optical lattices find a stable and extended spatially modulated superfluid [32,33]. However, such approximations are particularly questionable in 2D. The only numerically exact study to date is a determinantal quantum Monte Carlo simulation of the attractive Hubbard model [35], showing a finite-momentum peak in the pair-momentum distribution in large parts of the polarization–temperature phase diagram. Unfortunately, this study is severely limited by the negative sign problem and could not reach low enough temperatures to establish phase coherence of the pairs. Therefore, the question of whether or not an FFLO phase with (quasi-)long-range order can emerge in a given microscopic model remains open.

In this Letter we employ the unbiased diagrammatic Monte Carlo (DiagMC) method [36–38] to identify superfluid instabilities of spin-imbalanced fermions on a 2D lattice in a controlled way at lower temperatures than hitherto accessible. Our main result is that, for attractive interactions of the order of half the bandwidth, there is an extended region in two dimensions (2D), and lattice effects may further increase its stability [28,29]. Correspondingly, mean-field calculations [30,31] and real-space dynamical mean-field theory (DMFT) for fermions in anisotropic optical lattices find a stable and extended spatially modulated superfluid [32,33]. However, such approximations are particularly questionable in 2D.

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FIG. 1. (all figures: color online). Phase diagram for $U/t = -4$ at quarter filling: The white region is a Fermi liquid. In the blue shaded region, the Fermi liquid is unstable towards conventional ($Q = 0$) pairing. In the red shaded region there is an exclusive FFLO instability with finite pair momentum $Q_\star$. Open symbols indicate whether zero- (blue circles) or finite-momentum pairing (red diamonds) is dominant (black squares: no significant difference). The black dotted line separates the two regimes. All lines are guides to the eye.

such that $P = 1$ corresponds to a fully polarized system. In the following, we present results for $U = -4$ at quarter filling $n = (n_{i\uparrow} + n_{i\downarrow}) = 0.5$.

Our DiagMC algorithm \cite{37, 38} stochastically samples many-body Feynman diagrams (built on the bare Green’s function) for the self-energy and the two-particle-irreducible pairing vertex directly in the thermodynamic limit. Due to the diagrammatic sign problem, in practice a cutoff $N_\star$ on the maximum addressed diagram order is introduced and independence of the results on $N_\star$ is checked by varying the cutoff. We identify continuous phase transitions to ordered phases by monitoring the divergence of the corresponding susceptibilities on approach to the phase boundary from the normal phase. According to the Bethe-Salpeter equation, the susceptibility $\chi_c = \chi_c^{(0)} + \chi_c^{(0)} \Gamma_c \chi_c = \chi_c^{(0)} / \left[ 1 - \chi_c^{(0)} \Gamma_c \right]$ in a given channel $c$ (with, e.g., zero or non-zero center-of-mass momentum) diverges when the largest eigenvalue of the kernel $\chi_c^{(0)} \Gamma_c$ reaches unity. Here, $\chi_c^{(0)}$ denotes the product of two one-particle propagators and $\Gamma_c$ the two-particle-irreducible pairing vertex, see Refs. \cite{39, 40} for details. In the present case, we are primarily interested in pairing of $\uparrow$- with $\downarrow$-particles, which gives rise to both the conventional BCS and the FFLO phases, and hence concentrate on the superconducting channels with total spin projection $S_z = 0$ first. We refer to these as “singlet” channels \cite{41} and compute their pairing eigenvalues $\lambda_Q$ for different pair momenta $Q$.

FIG. 2. (top) Temperature dependence of the leading pairing eigenvalues for zero momentum (open symbols/dashed lines) and finite momentum $Q_\star$ (filled symbols/solid lines) for different polarizations $P$. (center) Estimates of the critical polarization for the two channels from varying diagram order cutoff $N_\star$ for temperatures $T = 0.5$ (black), $T = 0.1$ (green), and $T = 0.025$ (cyan). The left-most data points show our extrapolations $N_\star \to \infty$. (bottom) Difference between FFLO and conventional pairing eigenvalues for varying polarization. The corresponding temperatures are indicated to the right of the curves. Circles and diamonds on the curves indicate the critical polarization where zero- and finite-momentum eigenvalues respectively cross unity. Also shown is the pair momentum magnitude $Q_\star$ (red dots).

It is possible that the transition to an FFLO state is actually first-order due to appearance of solid-type order. In this case, the transition temperature extracted from the Bethe-Salpeter equation would correspond to a lower bound. However, the FFLO transition on the 2D lattice is generally believed to be continuous, at least in the neighborhood of the temperature where the FFLO instability first emerges \cite{30, 31, 42, 44}.

In the following we compare the pairing eigenvalues at
$Q = 0$ and at a non-zero candidate momentum $Q_*$ (to be defined below). Studying their temperature dependence, shown in the top panel of Fig. 2 we find that a non-zero polarization strongly suppresses the singlet superfluid instabilities as soon as the temperature is low enough to resolve the mismatch between the Fermi surfaces (FSs) of the minority and majority species: While the transition temperature in the unpolarized system is roughly $T_c = 0.15$, a moderate polarization of $P = 0.2$ may only lead to a transition (in the FFLO channel) at the lower end of the considered temperature range, $T_c \lesssim 0.025$. At larger polarizations $P \gtrsim 0.3$ all the singlet eigenvalues seem to saturate below unity, indicating the absence of a transition in the considered channels at any temperature.

Comparing eigenvalues for zero and non-zero pair momentum, one may differentiate three regimes: At high temperatures the FSs are so blurred that the two channels are essentially degenerate. In the region where the effects of the FS mismatch first become noticeable, there is a small advantage of zero-momentum pairing. Here a configuration where all parts of one FS are close to the other FS, even if the two never intersect, is apparently more favorable than the alternative with some matching parts and others that are very far apart. At an even lower temperature, finally, the zero-momentum eigenvalue starts decreasing whereas the finite momentum one continues growing, although with a decreasing rate. Depending on polarization, the following scenarios are generically realised when the system is cooled down: (a) For small polarization, the $Q = 0$ eigenvalue grows to unity before it is overtaken by the $Q_*$ eigenvalue. (b) For larger polarization, the FFLO eigenvalue will reach unity first. (c) For even larger polarization, all singlet eigenvalues saturate below unity, i.e. the Fermi liquid phase remains stable until triplet pairing emerges at exponentially low temperatures (see below).

By tracking the growth of the pairing eigenvalues with decreasing polarization at fixed temperature $T$, we find the critical polarization $P_c(T)$ for superfluidity. Its extrapolation in the diagram-order cutoff, the uncertainty of which is indicated by horizontal error bars on the phase boundaries of Fig. [1] is shown in the central panel of Fig. [2]. The bottom panel of Fig. [2] shows the difference between non-zero- and zero-momentum pairing eigenvalues. A positive (negative) difference corresponds to dominant FFLO (conventional) pairing fluctuations in the Fermi liquid phase, indicated by red diamonds (blue circles) in the phase diagram. Non-zero-momentum pairing fluctuations are dominant at large polarization and low temperature, which is in accord with the large region found in Ref. [35] where the pair momentum distribution function is peaked at finite momenta. For temperatures $T \lesssim 0.05$, the difference is positive at the critical polarization $P_c(T)$ implying that the FFLO instability is reached before the conventional superfluid one in this region of the phase diagram [45]. We cannot reliably compute the extent of the FFLO phase because our diagrammatic approach is not valid inside an ordered phase, but we can estimate the region of onset of conventional order in the absence of an FFLO phase by extrapolating the growth of the corresponding pairing eigenvalue from the Fermi liquid phase. As means of extrapolation we use the finite-order eigenvalue estimates inside the superfluid phase, drawn in lighter shades in Fig. 2.

In our study, the optimal pair momentum of the FFLO state $Q_*$ could only be determined approximately because an optimization of the pairing eigenvalue $\lambda_Q$ over $Q$ would be too costly within DiagMC. To this end we replace the irreducible vertex in the Bethe-Salpeter equation by the bare interaction $U$, such that the approximate pairing eigenvalue $\tilde{\lambda}_Q = -U\chi(Q)$ only depends on $Q$ via

![Fig. 3. Influence of density shown for $n = 0.8$ (top row) and $n = 0.1$ (center row) with polarization $P = 0.3$ and temperature $T = 0.025$. Left panels show majority spin momentum distribution (colors, from blue=unoccupied to red=occupied) and minority FS (dashed contour), as well as the latter shifted by the optimal pair momentum $Q_*$ (solid contour). The other panels illustrate the dependence of the one-particle propagator product $\chi(Q)$ on the pair momentum $Q$. (bottom) Dependence of the optimal pair momentum $Q_*$, extracted from the one-particle propagator product $\chi(Q)$, on density $n$ and polarization $P$. Dotted lines indicate the weak-coupling form for an isotropic dispersion, dashed lines for a square-shaped Fermi surface.](image-url)
the product of single-particle propagators

\[ \chi(Q) = T \sum_n \int \frac{d^2 k}{4\pi^2} G_n(k, i\omega_n)G_T(Q - k, -i\omega_n), \]

which can easily be evaluated numerically. The optimal pair momentum is always found to lie on the coordinate axes of the Brillouin zone. This is most easily understood close to half filling (top row of Fig. 3), where the FSs are almost squares. Then, a pair momentum of the form \( Q_\pm = (Q_\pm, 0) \) (and those related by point-group symmetry) can connect two sides of the minority FS to the corresponding majority FS patches, whereas, say, a diagonal pair momentum could only connect one side of each FS. For dilute systems (center row of Fig. 3), the FSs are almost isotropic such that the majority and minority FS can at best touch in one tangential point. The difference between pair momenta with the same magnitude is rather small, but for finite filling we always find a slight preference for pair momenta along the lattice axes. The bottom panel of Fig. 3 plots this pair momentum \( Q_* \) found by numerical optimization for different site fillings and polarizations. In general, there is no closed expression for \( Q_* \), but one can consider two limiting cases: (a) For circular FSs the respective Fermi momenta are \( k_F = \sqrt{4\pi n}\sigma \), so the \( \uparrow \) and \( \downarrow \) FSs are connected by \( Q_\sigma = k_F^\uparrow - k_F^\downarrow = 2\pi n(\sqrt{1 + P} - \sqrt{1 - P}) \). (b) For square-shaped FSs, whose corners lie on the coordinate axes at \( k_F^\sigma = \sqrt{\pi^2 n}\sigma \), the optimal pair momentum is \( Q_* = \sqrt{\pi^2 n}(\sqrt{1 + P} - \sqrt{1 - P}) \). These estimates are indicated by dotted and dashed lines, respectively, in the bottom panel of Fig. 3. The data obtained by numerical optimization lie quite consistently between the two extreme estimates. While the approximation \( \lambda_Q \) will in general strongly overestimate the pairing eigenvalue due to the neglect of correlation effects in the vertex, the extracted pair momentum \( Q_* \) is expected to be accurate because the momentum dependence of the vertex is typically much weaker than that of the propagators. Strictly speaking, we cannot exclude the (unlikely) existence of a stronger instability at a different momentum. This means that our phase diagram is conservative in the sense that the region of the FFLO phase might become only larger if additional pair momenta are relevant.

At strong polarization and at weaker interaction, all singlet-pairing eigenvalues saturate below unity. Here, triplet pairing, which is not susceptible to the FS mismatch, will emerge at (exponentially) low temperatures \[ 10 \] due to an effective interaction between identical particles mediated by the other species, just as in the case of a spin-dependent hopping anisotropy \[ 39 \]. In principle, either the majority or the minority species may have the dominant instability. In second-order perturbation theory at quarter filling, the majority species always reach the superfluid transition first, independent of the polarization. We have confirmed this with DiagMC calculations for \( P = 0.2 \) (Fig. 4) and \( P = 0.4 \) (not shown). In Fig. 4 we compare the eigenvalues in five different channels: Among the singlet-pairing eigenvalues, the pair momentum \( Q_* \) dominates at low temperatures, whereas the conventional \( Q = 0 \) channel saturates below \( T \lesssim 0.2 \). A further candidate, \( Q_\times \), which is the optimal pair momentum on the BZ diagonal within the approximation \[ 2 \], is always subdominant to \( Q_* \). The triplet eigenvalues, on the other hand, are by an order of magnitude smaller at the temperatures considered here, but exhibit the logarithmically-diverging growth with decreasing temperature that is standard for a weak-coupling Cooper instability. As in the weak-coupling calculation, pairing between majority particles clearly dominates over minority pairing.

Phase diagrams at densities \( n = 0.8 \) and 0.9 look very similar to the quarter filled case, indicating that the FFLO instability is not very sensitive to particle density. For nearly half-filled bands, density-wave instabilities may however become relevant due to nesting in the particle-hole channel; the full phase diagram in the vicinity of half filling is therefore left for further studies. We have not systematically studied other interactions, but expect \( U/t = -4 \) to be close to the optimal case for observation of FFLO order: At smaller \( |U| \), transition temperatures and the width of the FFLO instability will decrease quickly \[ 17 \], whereas in the strong-coupling regime a (coherent or incoherent) mixture of tightly bound pairs and unpaired excess particles may be more stable than an FFLO phase. Note that a well-known particle-hole transformation relates the attractive and repulsive Hubbard models to each other \[ 38 \]. Under this transfor-
The Many Electron Problem.

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Some questions concerning the extent and character of the FFLO state cannot be answered definitively by our study since we cannot enter the broken-symmetry phase. This concerns in particular the type of order (single-Q vs. multi-Q) and possible transitions between different ordered phases. We have not detected any hints of phase separation in the polarization vs. magnetic field curves, but we cannot conclusively rule this scenario out — even though previous studies on 2D lattices generally find direct and continuous transitions to the FFLO phase.

In summary, we have presented the first well-controlled numerical evidence for the presence of a Fermi liquid instability towards FFLO order in the spin-imbalanced phase diagram of attractively interacting fermions on a 2D lattice. For moderate on-site interaction $U/t = -4$, the instability is present in an extended region of the temperature–polarization plane. The largest temperatures where this instability is observable are roughly by a factor of two smaller than the Kosterlitz-Thouless transition temperature in the corresponding spin-balanced system, similar to DMFT results for anisotropic optical lattices [34]. At large polarization there does not seem to be any singlet superfluid order and triplet pairing is found at exponentially low temperatures. Our quantiative predictions may be checked by experiments with cold atoms in optical lattices, where the breaking of translational symmetry can be observed by in-situ imaging [50–52] and the pair-momentum distribution by time-of-flight measurements [53–56] or in noise correlations [57, 58]. We acknowledge numerous enlightening discussions with N. Prokof’ev and B. Svistunov and thank them for

We acknowledge numerous enlightening discussions with N. Prokof’ev and B. Svistunov and thank them for helpful comments on the manuscript. We used the ALPS libraries for simulations and data evaluation [59–60]. Simulations were performed on the Mönch and Brutus clusters of ETH Zurich. This work was supported by FP7/ERC Starting Grant No. 306897, ERC Advanced Grant SIMCOFE and by the Simons Collaboration on the Many Electron Problem.

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