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. The highest temperature where the FFLO instability can be observed is roughly one half of the superfluid transition temperature in the unpolarized system.

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Fifty years after their 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 [3–6]. While the basic mechanism is generic enough to apply to any 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 [7–9] and, in particular, layered organic materials [10–14]. 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 [15, 16] — although there is some evidence for such a phase in 1D [17] — possibly due to smallness of the parameter region where an FFLO phase may exist in 3D and/or difficulty in reaching sufficiently low temperatures [4].

On the theory side, in spite of decades of intense work, results on the existence and nature of FFLO phases from well-controlled microscopic theories are scarce, with the exception of 1D systems, where exact analytical and numerical studies are possible [18–20], 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, the ground state phase diagram obtained from the mean-field theory [21] has been corroborated by fixed-node diffusion quantum Monte Carlo calculations [22]; whether the FFLO phase exists in a small sliver of the phase diagram is not resolved yet.

The FFLO state is expected [3] to occupy a larger parameter region in 2D, and lattice effects may further increase its stability [23, 24]. Correspondingly, mean-field calculations [25] and real-space dynamical mean-field theory (DMFT) for fermions in anisotropic optical lattices find a stable and extended spatially modulated superfluid [26–28]. 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 [29], 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 diagrammatic Monte Carlo (DiagMC) method [30–32] 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 the temperature–polarization plane, indicated by red shading in Fig. 1, where the Fermi liquid is unstable exclusively towards FFLO superfluidity. Specifically, we simulate the Hubbard model on a square lattice

$$H = -t \sum_{\langle i,j\rangle,\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + h.c. \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \qquad (1)$$

with nearest-neighbor hopping amplitude $t = 1$ setting the scale of energy, on-site attraction $U < 0$, fermionic creation and annihilation operators $c^\dagger_{i\sigma}$ and $c_{i\sigma}$, respectively, with spin $\sigma = \uparrow, \downarrow$, and occupation numbers $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$. Spin imbalance is quantified by the polarization

$$P = \frac{\langle n_{i\downarrow} - n_{i\uparrow}\rangle}{\langle n_{i\downarrow} + n_{i\uparrow}\rangle}, \qquad (2)$$

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

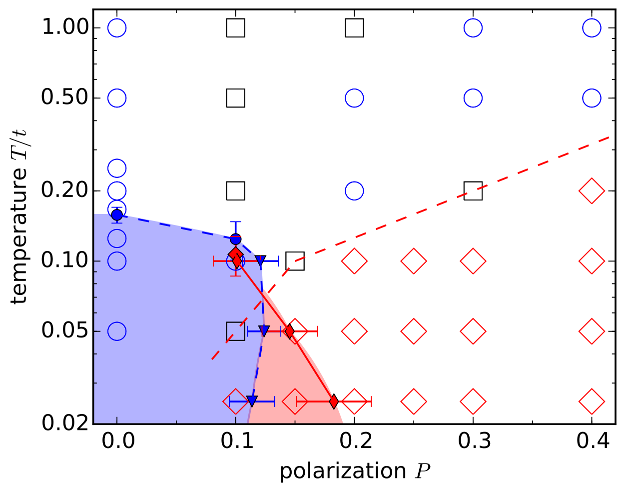

FIG. 1. (all figures: color online). Phase diagram for $U/t = -4$ at quarter filling: The white region is a Fermi liquid. In the blue shaded region, the Fermi liquid is unstable towards conventional ($\boldsymbol{Q} = 0$) pairing. In the red shaded region there is an exclusive FFLO instability with finite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

With DiagMC we sample bare many-body Feynman diagrams for the proper self-energy and the two-particle-irreducible pairing vertex directly in the thermodynamic limit. Due to the factorial complexity of the diagrammatic space at high order, the series needs to be restricted to diagrams below a cutoff order $N \leq N_*$ and convergence of the results is checked by varying the cutoff. As explained in Refs. [33, 34], we identify continuous phase transitions by monitoring the leading eigenvalues of the Bethe-Salpeter kernel on approach to the phase boundary. The transition to an FFLO state may be first-order due to the appearance of solid-type order. The transition temperature extracted from the Bethe-Salpeter equation would then correspond to a lower bound. However, the FFLO transition in 2D is generally believed to be continuous, at least in the neighborhood of the temperature where the FFLO instability first emerges [35–37]. In the present case, we are primarily interested in the "singlet" [38] superconducting channels and compute hence the pairing eigenvalues $\lambda_{\boldsymbol{Q}}$ for different pair momenta $\boldsymbol{Q}$. When the first eigenvalue reaches unity, the corresponding pairing susceptibility diverges and the Fermi liquid becomes unstable towards a superfluid transition with this center-of-mass momentum.

Studying the temperature dependence of the leading pairing eigenvalues, as shown in the top panel of Fig. 2, we find that a finite polarization strongly suppresses the singlet superfluid instabilities as soon as the temperature is low enough to resolve the mismatch between

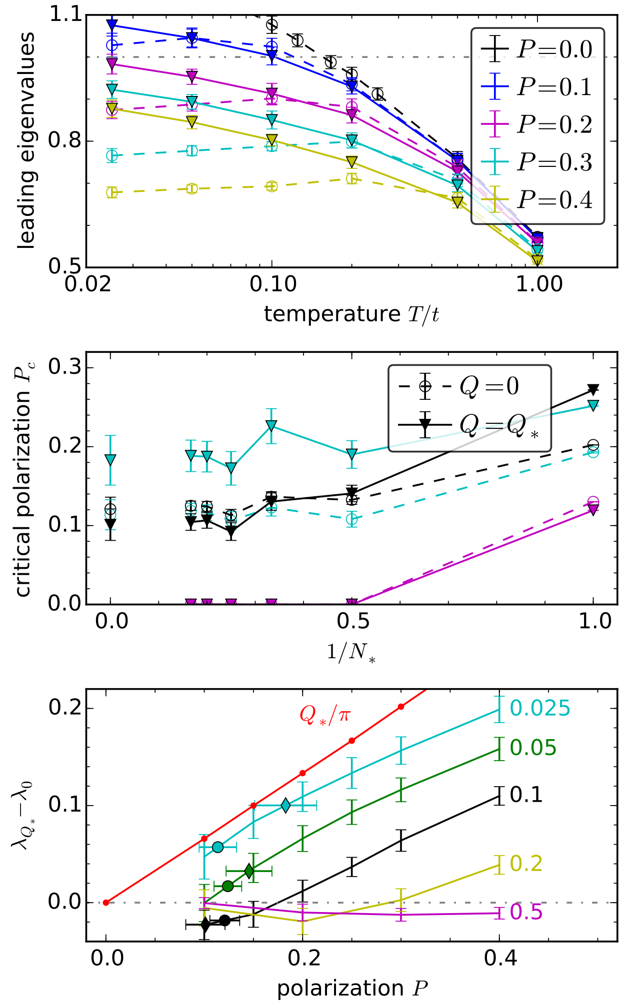

FIG. 2. *(top)* Temperature dependence of the leading pairing eigenvalues for zero momentum (open symbols/dashed lines) and finite momentum $\boldsymbol{Q}_*$ (filled symbols/solid lines) for different polarizations $P = 0, \ldots 0.4$. *(center)* Estimates of the critical polarization for the two channels from varying diagram order cutoff $N_* = 1, \ldots 6$ for temperatures $T = 0.5$ (magenta), $T = 0.1$ (black), and $T = 0.025$ (cyan). The left-most data points show our extrapolations determining the phase boundaries in Fig. 1. *(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_* (red dots).

the Fermi surfaces (FSs) of the minority and majority species: While the transition temperature in the unpolarized system is roughly $T_c/t = 0.15$, 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 eigenvalues seem to saturate below unity, indicating the absence of a transition in the considered channels at any temperature. Comparing eigenvalues for zero and finite pair momentum, one may differentiate three regimes: At very large temperatures the FSs are so blurred that the two channels are basically degenerate. Then, in the region where the effects of the FS mismatch are first noticeable, there is a small advantage of the zero-momentum eigenvalue over the other. 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 decreasing rate. Depending on polarization (and interaction), one of three cases may thus happen when the system is cooled down: (a) For small polarization, the $\boldsymbol{Q} = 0$ eigenvalue may grow to unity before it is overtaken by the $\boldsymbol{Q}_*$ eigenvalue. (b) For larger polarization, the FFLO eigenvalue will reach unity first. (c) For even larger polarization, all singlet eigenvalues may saturate below unity. In other words, either of the instabilities may develop first, or the Fermi liquid phase may remain stable until triplet pairing emerges at exponentially low temperatures (see below).

By tracking the pairing eigenvalues' growth with decreasing polarization at fixed temperature T, we find the critical polarization $P_c(T)$ for superfluidity. Its extrapolation, which is indicated by horizontal error bars on the phase boundaries of Fig. 1, in the diagram-order cutoff is shown in the central panel of Fig. 2. The bottom panel of the latter figure shows the difference between finite- 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. Finite-momentum pairing fluctuations are dominant at large polarization and low temperature, which is in accord with the large region found in Ref. [29] 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 [39].

The optimal pair momentum $\boldsymbol{Q}_*$ could only be determined approximately because an optimization of the pairing eigenvalue $\lambda_{\boldsymbol{Q}}$ over arbitrary pair momenta 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 $\tilde{\lambda}_{\boldsymbol{Q}} = -U\chi(\boldsymbol{Q})$ only depends on $\boldsymbol{Q}$ via the product of single-particle propagators

$$\chi(\boldsymbol{Q}) = T\sum_n \int \mathrm{d}^2k\, G_\downarrow(\boldsymbol{k}, i\omega_n) G_\uparrow(\boldsymbol{Q}-\boldsymbol{k}, -i\omega_n), \quad (3)$$

which can easily be evaluated numerically. The optimal

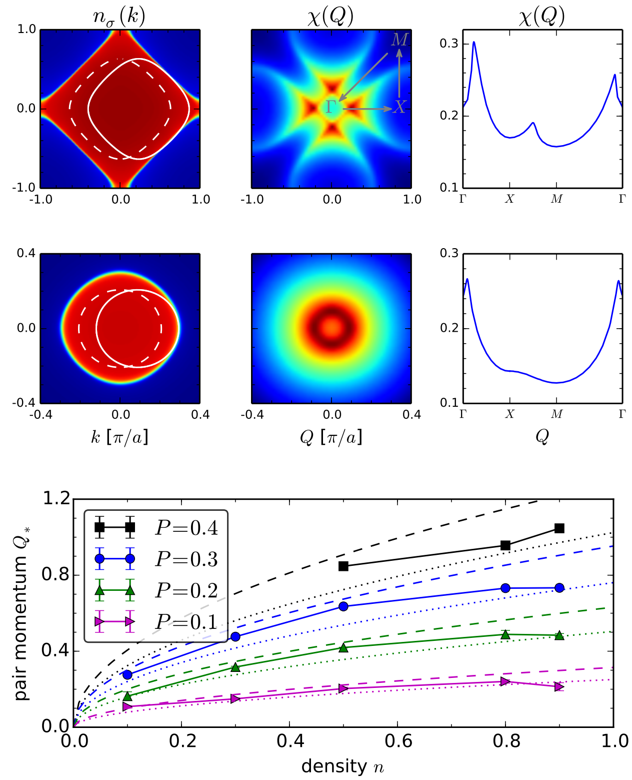

FIG. 3. Finite pair momenta for densities $n = 0.8$ (top row) and $n = 0.1$ (center row) with polarization $P = 0.3$ and temperature $T = 0.025$. Left panels show majority spin momentum distribution (colors, from blue=unoccupied to red=occupied) and minority FS (dashed contour), as well as the latter shifted by the optimal pair momentum $\boldsymbol{Q}_*$ (solid contour). The other panels illustrate the dependence of the one-particle propagator product $\chi(\boldsymbol{Q})$ on the pair momentum $\boldsymbol{Q}$. Brillouin zone plots for $n = 0.1$ are zoomed to the central region $k_{x,y} \in [-0.4\pi, 0.4\pi]$. *(bottom)* Dependence of the optimal pair momentum Q_*, extracted from the one-particle propagator product $\chi(\boldsymbol{Q})$, 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.

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 $\boldsymbol{Q}_* = (Q_*, 0)$ (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 mo-

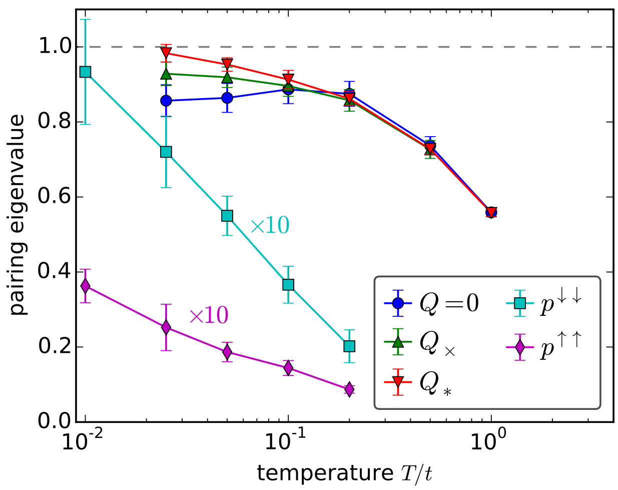

FIG. 4. Pairing eigenvalues for different channels at quarter filling and polarization $P = 0.2$. Shown are the singlet pairing eigenvalues with pair momenta $\boldsymbol{Q} = 0$, $\boldsymbol{Q}_*$ (i.e. on the coordinate axis) and $\boldsymbol{Q}_\times$ (on the BZ diagonal) as well as the p-wave triplet eigenvalues for zero-momentum pairing of the majority ($p^{\downarrow\downarrow}$) and minority ($p^{\uparrow\uparrow}$) species, respectively.

mentum 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 $k_F^\sigma = \sqrt{4\pi n_\sigma}$, so the ↑ and ↓ FSs are connected by $Q_* = k_F^\downarrow - k_F^\uparrow = \sqrt{2\pi n}(\sqrt{1+P} - \sqrt{1-P})$. (b) For square-shaped FSs, whose corners lie on the coordinate axes at $k_F^\sigma = \sqrt{2\pi^2 n_\sigma}$, 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 lies quite consistently between the two extreme estimates. While the approximation $\tilde{\lambda}_{\boldsymbol{Q}}$ 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 usually much weaker than that of the propagators. Still, we cannot strictly speaking exclude the (unlikely) existence of stronger instabilities at different momenta. This means that our phase diagram is conservative in the sense that the regions containing an FFLO instability might become larger when additional pair momenta are considered.

At strong polarization and at weaker interaction, all singlet-pairing eigenvalues saturate below unity before a pairing instability is reached. Here, triplet pairing, which is not susceptible to the FS mismatch, will emerge at low temperatures due to an effective interaction between identical particles mediated by the other species, just as in the case of a spin-dependent hopping anisotropy [33]. 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 reaches 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 $\boldsymbol{Q}_*$ dominates at low temperatures, whereas the conventional $Q = 0$ channel saturates below $T \lesssim 0.2t$. A further candidate, $\boldsymbol{Q}_\times$, which is the best momentum on the BZ diagonal within the approximation (3), is always subdominant to $\boldsymbol{Q}_*$. The triplet eigenvalues, on the other hand, are by an order of magnitude smaller at the temperatures considered here, but exhibit the logarithmic growth with decreasing temperature expected for a weak-coupling Fermi liquid instability. As in the weak-coupling calculation, pairing between majority particles clearly dominates over minority pairing.

We have also collected data for $n = 0.8$ and 0.9 and the corresponding phase diagrams look very similar to the quarter filled case, indicating that the FFLO instability does not depend very sensitively on the 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. Note that a well-known particle-hole transformation relates the attractive and repulsive Hubbard models to each other [40, 41]. Under this transformation, the magnetization nP assumes the role of doping $x = n - 1$ and vice versa, whereas the FFLO instability translates into an instability to a striped phase.

Some questions concerning the extent and character of the FFLO phase cannot be answered authoritatively by our study since we cannot enter the broken phase. This concerns in particular the type of order (single-Q vs. multi-Q) and its stability with respect to low-energy fluctuations [42, 43]. 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 in 2D generally find direct and continuous transitions to the FFLO phase [25, 35–37].

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 [28]. At large polarization there does not seem to be any singlet superfluid order and triplet pairing may be found at very low temperatures.

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