Populations imbalanced lattice fermions near the BCS-BEC crossover: I. The breached pair and metastable FFLO phases

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We study s-wave superconductivity in the two dimensional attractive Hubbard model in an applied magnetic field, assume the extreme Pauli limit, and examine the role of spatial fluctuations in the coupling regime corresponding to BCS-BEC crossover. We use a decomposition of the interaction in terms of an auxiliary pairing field, retain the static mode, and sample the pairing field via Monte Carlo. The method requires iterative solution of the Bogoliubov-de-Gennes (BdG) equations for amplitude and phase fluctuating configurations of the pairing field. We establish the full thermal phase diagram of this strong coupling problem, revealing $T_c$ scales an order of magnitude below the mean field estimate, highlight the spontaneous inhomogeneity in the field induced magnetization, and discover a strong non monotonicity in the temperature dependence of the low energy density of states. We compare our results to the experimental phase diagram of the imbalanced Fermi gas at unitarity. This paper focuses on the magnetized but homogeneous (breached pair) superconducting state, a companion paper deals with the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) regime.

I. INTRODUCTION

For an electron system in a superconducting state the Meissner effect characterizes the response to a magnetic field. In type II superconductors there is flux penetration beyond a threshold $h_{c1}$ in the form of an Abrikosov lattice before superconductivity (SC) is finally lost at the 'orbital critical field' $h^{orb}_{c2}$. The magnetic field also couples to the spin of the electrons, and tends to break an $\uparrow \downarrow$ pair. This effect is detrimental to SC, and, if orbital effects were irrelevant, SC would order to some 'Pauli limiting' field $h^{P}_{c2}$, say\cite{1}. The ratio of these critical fields, $\alpha = h^{orb}_{c2}/h^{P}_{c2}$, defines the Maki parameter and is roughly $\Delta_0/\epsilon_F$, where $\Delta_0$ is the zero temperature gap in the SC state and $\epsilon_F$ is the Fermi energy.

In most superconductors $\alpha \ll 1$, so the Pauli suppression effects never show up. There are however three scenarios where it becomes relevant. (a) If $\epsilon_F$ is suppressed strongly by correlation effects, as in heavy fermions where the suppression factor can be $\sim 10^3$ due to Fermi liquid correction\cite{2}, (b) for two dimensional systems, the layered organics, say, orbital effects are irrelevant for an 'in plane' field, and (c) for neutral Fermi gases, as in cold atomic systems, the magnetic effects would be related only to spin. Recent discoveries on the heavy fermions\cite{3,4,5} CeCoIn$_5$, the $\kappa$-BEDT based layered superconductors\cite{6,7}, iron pnictides\cite{8,9}, and population imbalanced cold Fermi gases\cite{10,11}, make the Pauli limit relevant.

Early extensions\cite{12,13} of the BCS scheme to finite Zeeman field (neglecting orbital effects) predicted that, in the continuum, the superconducting $T_c$ decreases with applied field up to a critical value, $h_1$, say, and the thermal transition remains second order. Beyond $h_1$, one would have expected a SC state with a first order thermal transition, but the ground state actually becomes modulated, in the spirit predicted by Fulde and Ferrell (FFLO)\cite{14} and Larkin and Ovchinnikov (LO)\cite{15}, and stays so till all order is lost at some $h_{c2}$. The FFLO state is characterized by periodic spatial modulation of the superconducting order parameter and magnetization. The modulations in these quantities are complementary and the nodes of the superconducting order parameter correspond to the maximum of the magnetization, and vice versa. The zero temperature and $h < h_1$ system is an 'unpolarised superfluid' (USF), its finite temperature counterpart is a 'breached pair' (BP) state and the $h_1 < h < h_{c2}$ window is FFLO. The BP phase is the finite temperature extension of the USF, with homogeneous superconducting order spatially coexisting with finite uniform polarization. The original scenario does not support any first order transition between the BP phase and the normal state.

Experiments bear out some features of this scenario with solid state studies focused on probing the FFLO state while cold atom experiments probe the general effect of imbalance on pairing. The FFLO signatures in CeCoIn$_5$ include specific heat\cite{16}, magnetic torque\cite{17}, muon spin relaxation\cite{18}, NMR\cite{19} and magnetic neutron scattering\cite{20}, while in the $\kappa$-BEDT based organics there is indirect evidence\cite{21,22} for a modulated state

![FIG. 1. Color online: (a) Comparison of $T_c$ scales obtained from the mean field calculation (upper curve) and our static auxiliary field (SAF) Monte Carlo technique (lower curve). In the SAF data BP-II represents a breached pair state that undergoes a second order transition to the partially polarized Fermi liquid (PPFL), while BP-I undergoes a first order thermal transition to the PPFL. Beyond BP-I the system exhibits FFLO order up to some critical field. (b) Polarization vs- temperature phase diagram inferred from the SAF calculation, plotted in the spirit of the experimentally obtained unitary Fermi gas result\cite{23}. The ‘unstable’ region is phase separated.]

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at large in-plane fields. In KFe$_2$As$_2$ also thermal expansion and magnetostriction suggests the occurrence of Pauli limited superconductivity\cite{29}. For cold atoms, fermionic superfluidity with population imbalance has been probed in detail with the Fermi gas tuned to unitarity\cite{32} revealing an ‘universal’ phase diagram.

The microscopic models for superconductivity (or superfluidity) in these systems are widely different but they share the features of (i) a ‘homogeneous’ magnetized superfluid state near $T_c$ at intermediate fields, (ii) a possible FFLO state at higher fields, and (iii) being in a coupling regime well beyond the reach of mean field theory (at least for the atomic gases). Taking (iii) as our point of departure we address these issues by studying the Zeeman field dependence in the attractive two dimensional Hubbard model at intermediate coupling, $U/t = 4$ (see later). This corresponds roughly to the maximum $T_c$ in the BCS-BEC crossover window, and crucially involves amplitude and phase fluctuations in describing the thermal physics\cite{30,31}. Our main results, using a recently developed Monte Carlo (MC) approach, are the following:

1. We observe that in the imbalanced problem, as in the case of balanced Fermi gases\cite{30,33}, the fluctuation effects suppress $T_c$ scales by a factor of more than 4 compared to widely used mean field theory.

2. Intermediate fields allow for a temperature window over which the superfluid supports significant magnetization which, although homogeneous on the average, shows noticeable configurational fluctuation.

3. At high fields the superfluid shows a first order transition to the normal state on heating, but cooling in this field window inevitably traps the system into a metastable FFLO state.

4. The spin resolved density of states shows a pseudogap (PG) feature that is strongly non monotonic in temperature: the pseudogap weakens initially with increasing temperature and then deepens again beyond a scale $T_{\text{max}}$. The applied field dramatically suppresses $T_{\text{max}}$.

We characterize the thermal state via real space maps, the structure factors associated with the superfluid and magnetic order, the spin resolved momentum distribution of the fermions, and the density of states.

The rest of the paper is organized as follows. In Section-II we discuss the model and the methods used to study it. Section-III contains the results. Section-IV discusses possible limitations of our numerical scheme, suggests the connection to Ginzburg-Landau phenomenology, and relates our predictions to some cold atom experiments. Section-V concludes with our key observations. An appendix describes the Hubbard-Stratonovich transformation and the related approximations in detail.

II. MODEL AND METHOD

A. Model

We study the attractive two dimensional Hubbard model (A2DHM) on a square lattice in the presence of a Zeeman field:

$$H = H_0 - h \sum_i \sigma_{iz} - |U| \sum_i n_{i\uparrow} n_{i\downarrow}$$

with, $H_0 = \sum_{ij,\sigma} (t_{ij} - \mu \delta_{ij}) c_{i\sigma}^\dagger c_{j\sigma}$, where $t_{ij} = -t$ only for nearest neighbor hopping and is zero otherwise. $\sigma_{iz}$ is the chemical potential and $h$ is the applied magnetic field in the $z$ direction. $U > 0$ is the strength of on-site attraction. We will use $U/t = 4$.

We wish to explore the physics beyond weak coupling, i.e., short coherence length. This requires retaining fluctuations well beyond mean field theory (MFT). We accomplish that as follows. We use a ‘single channel’ Hubbard-Stratonovich (HS) decomposition of the interaction term in terms of an auxiliary complex scalar field $\Delta_i(\tau) = |\Delta_i(\tau)| e^{i\theta_i(\tau)}$. A complete treatment of the resulting problem handles the full spatial and imaginary time, $(i, \tau)$, dependence of the $\Delta$ - this is possible only within quantum Monte Carlo - while mean field theory imposes a spatially periodic pattern and ignores the $\tau$ dependence. We ignore the ‘time’ dependence of the $\Delta$, but completely retain the spatial dependence. This, as we shall see, makes our method ‘mean field’ at zero temperature, $T = 0$, but retains the crucial thermal fluctuations of the amplitude and phase of $\Delta_i$ that control $T_c$ scales, etc. We discuss the formal structure of this approximation in detail in the Appendix, and its limitations in the Discussion section.

The static $\Delta_i$ problem is described by the coupled effective Hamiltonian:

$$H_{\text{eff}} = H_0 - h \sum_i \sigma_{iz} + \sum_i (\Delta_i c_{i\uparrow}^\dagger c_{i\downarrow} + h.c) + H_{cl}$$

where $H_{cl} = \sum_i \frac{|\Delta_i|^2}{2}$ is the stiffness cost associated with the now ‘classical’ auxiliary field. The equation above indicates how the fermions see the pairing field. The pairing field configurations in turn are controlled by the Boltzmann weight:

$$P\{\Delta_i\} \propto \text{Tr} e^{-\beta H_{\text{eff}}}$$

This is related to the free energy of the fermions in the configuration $\{\Delta_i\}$. For large and random $\Delta_i$ the trace needs to be computed numerically. We generate the equilibrium $\{\Delta_i\}$ configurations by a Monte Carlo technique (see later) diagonalising the fermion Hamiltonian $H_{\text{eff}}$ for every attempted update of the auxiliary fields.

B. Numerical method: Monte Carlo and variational calculation

Mean field theory has been the standard tool for exploring the effect of a Zeeman field on the superconductor. However,
even though MFT may be reasonable in capturing the ground state, inclusion of amplitude and phase fluctuations is essential as one moves beyond the $U/t \ll 1$ window. This issue has been widely discussed in the context of the zero field BCS to BEC crossover.

Fluctuation effects have been found to suppress the $T_c$, compared to MFT estimates, both at intermediate and strong coupling. Measurements on the 3D unitary gas indicates a peak $T_c/E_F \sim 0.167$, while various theoretical estimates at unitarity include (a) a mean field based result suggesting $T_c/E_F \sim 0.6$ (b) a $T$-matrix based result suggesting $T_c/E_F \sim 0.16$, (c) fluctuation corrected mean field theory yielding $T_c/E_F \sim 0.245$, and (d) Monte Carlo estimates yielding $T_c/E_F \sim 0.15 - 0.25$. A very recent experiment on a 2D cold Fermi gas indicates a peak $T_c/E_F \sim 0.16$, while an interpolative theory estimate suggests $T_c/E_F \sim 0.1$. Results on the 2D Hubbard model indicate $T_c/E_F \sim 0.16$. Corrections beyond mean field theory, it is obvious, are essential for an accurate description beyond weak coupling.

We include thermal fluctuations via our static auxiliary field (SAF) scheme, which, implemented using Monte Carlo, can access system sizes larger than typical quantum Monte Carlo (QMC) calculations. This has several advantages: (i) it provides an accurate estimate of the $T_c$, (ii) at high fields it helps in accessing spatially modulated (FFLO) paired states which may have a large wavelength, and (iii) it allows calculation of dynamical properties without the need for any analytic continuation.

In order to make the study numerically less expensive the Monte Carlo is implemented using a cluster approximation, in which instead of diagonalising the entire $L \times L$ lattice for each local update of the $\Delta_i$ a smaller cluster, of size $L_c \times L_c$, surrounding the update site is diagonalised. We mostly used $L = 24$ and $L_c = 6$ for the results in this paper. The cluster approximation has been extensively benchmarked, and used successfully in the zero field case. We will discuss the limitations of the SAF approach and cluster based update at the end of the paper.

At zero temperature within the SAF scheme the energy is minimized over static configurations of the field $\Delta_i$. We have carried out variational calculations at several fixed values of $\mu$, at different $h$, exploring the following kinds of periodic configuration: (i) ‘axial stripes’ $\Delta_i \sim \Delta_0 \cos(q x_i)$, and diagonal stripes $\Delta_i \sim \Delta_0 \cos(q(x_i + y_i))$, and (ii) two dimensional modulations, $\Delta_i \sim \Delta_0 (\cos(q x_i) + \cos(q y_i))$, and of course (iii) the unpolarised superfluid (USF) state $\Delta_i = \Delta_0$. We minimize the energy with respect to the $q$, and $\Delta_0$ (assumed real). This paper focuses on the uniform state, the FFLO regime is discussed in detail in a companion paper.

C. Parameter regime and indicators

Any real space numerical calculation requires a system with linear dimension $L \gg \xi_0$, where $\xi_0$ is the $T = 0$ coherence length, to accurately capture the SC state. Since $\xi_0$ increases with reducing $U/t$, this puts a limit on the $U/t$ window that we can explore. The results in this paper are at $U = 4t$, both within Monte Carlo and the variational scheme. We have also explored $U = 2t$ variationally but it requires $L \sim 48$ to access modulated phases so we have not been able to do MC in that regime. At $U/t = 4$ we have explored the $h - T$ dependence at multiple values of $\mu$ below half-filling (the physics above half-filling can be inferred from this) but the qualitative features are independent of the choice of $\mu$ so this paper focuses on $\mu = -0.2t$, where the density is $n \approx 0.94$ (independent, roughly, of $h$ or $T$). We have studied the temperature dependence at a large number of fields in the window $h/t \sim [0.5]$. Beyond the global features of the $h - T$ phase diagram, we will discuss three field values, typical of three response regimes.

We use the following indicators to characterize the system: (i) Monte Carlo snapshots of $|\Delta_i|$, the phase correlation $\cos(\theta_0 - \theta_i)$ where $\theta_0$ is the angle at a fixed reference site on the lattice, the magnetization variable $m_i = \langle n_{i\uparrow} - n_{i\downarrow} \rangle$, and particle number $n_i = \langle n_{i\uparrow} + n_{i\downarrow} \rangle$. These explicitly highlight the spatial fluctuation with increasing temperature, and the modulated nature in the FFLO window. (ii) We keep track of the structure factors, $S_\Delta(q)$ and $S_m(q)$, defined as:

$$S_\Delta(q) = \frac{1}{N^2} \sum_{i,j} \langle \Delta_i \Delta_j^\ast \rangle e^{i q(r_i - r_j)}$$

$$S_m(q) = \frac{1}{N^2} \sum_{i,j} \langle m_i m_j \rangle e^{i q(r_i - r_j)}$$

where, $N = L^2$. (iii) We monitor the bulk magnetization and the SC order parameter, $S_\Delta(q = 0; T, h)$. (iv) We compute the momentum occupation number $\langle |\langle n_{\mathbf{k}\sigma} \rangle | \rangle$ that carries the signature of imbalance and FFLO modulation. Finally, (v) we compute the spin resolved and total fermionic density of states (DOS).

III. RESULTS

In what follows we first highlight the huge difference between the mean field results and that of our Monte Carlo approach.
proach due to that of thermal fluctuations in this coupling regime. We then take a step back to illustrate the working of the variational approach to the ground state and the \( \mu - h \) phase diagram that emerges. Following this we move on to a detailed discussion of thermal properties, in particular the difference between ‘cooling’ and ‘heating’ the system, suggestive of the presence of metastable states. We show detailed results for what we feel are three broad field regimes: (i) Weak field, where the \( T_c \) is only modestly modified with respect to \( h = 0 \), the thermal transition is second order, and there is hardly any magnetization for \( T < T_c \). (ii) Intermediate field, where \( T_c \) is noticeably lower, the thermal transition is still second order, but there is a window \( \delta T = T_c - T > 0 \) where the system simultaneously shows superfluid order and magnetization, characteristic of the ‘breached pair’ state. (iii) Strong field, where the SC shows a first order thermal transition, and there is a metastable FFLO state over a wide temperature window.

Fig.1 presents the primary contrast between MFT and the MC result. Fig.1.(a) presents the \( h - T \) phase diagram indicating regions of first and second order thermal transition and the regions of BP and FFLO character. A much more detailed phase diagram will be shown in Fig.4.

Fig.1.(b) shows the MC phase diagram in terms of the inferred magnetization and temperature to create a parallel with cold fermionic systems, where the physics is probed for a fixed population imbalance (“magnetization”) rather than a fixed applied field. At \( T = 0 \) the entire USF window, \( 0 < h < 0.85t \), collapses to the origin, and the first order jump to the LO state involves a magnetization discontinuity \( m \sim 0.28 \). Magnetization in the LO ground state is up to \( m \sim 0.37 \) beyond which we have the ‘normal’ partially polarized Fermi liquid. The BP state is the finite \( T \) extension of the USF and occupies a widening window as \( T \) increases and then shrinks again as \( T \to T_c \). The ‘unstable’ region is the magnetization discontinuity between the high temperature PPFL state and the low \( T \) nearly unpolarised state in the 1st order transition window. The LO \( T_c \)'s are small and the LO phase occupies a small low temperature sliver in the large \( m \) region. This picture helps understand the cold atom experiments where the population imbalance, rather than the applied field, is the primary variable. We will take up this comparison at the end of the paper. Fluctuations suppresses the \( T_c \) to well below the MF value, as observed earlier in balanced Fermi gases.\(^{31,35}\) The presence of imbalance (or an applied field) suppresses the \( T_c \) more rapidly.

We have used the variational approach described earlier to determine the ground state, in the same spirit as Chiesa et al.\(^{24}\), wherein diagonal, uniaxial and checkerboard patterns of \( \Delta \) were compared to determine the ground state.

Fig.2.(a) and Fig.2.(b) shows the dependence of the energy on the ‘magnitude’ \( \Delta_0 \), of the pairing field, for several values of \( q \). Panel (a) is for intermediate field, \( h = 0.5t \), where the ground state is still homogeneous, \( i.e. \) at \( q = (0, 0) \). Panel (b), at \( h = 0.95t \) shows an absolute minimum at \( q = (\pi/3, 0) \), an axial Larkin-Ovchinnikov state.

The variationally determined \( \mu - h \) phase diagram is shown in Fig.3. At low \( h \) the system is a homogeneous unmagnetised superfluid (USF). One may have expected this to undergo a transition to a partially polarized Fermi liquid (PPFL) at a field \( h_c = \Delta_0/\sqrt{2} \), the naive Pauli limit. However, as predicted by Fulde and Ferrell\(^{40}\) and Larkin and Ovchinnikov\(^{42,43}\) and confirmed by several later studies, we find that a \( \Delta \) modulated state with finite magnetization intervenes between the USF and the PPFL. We designate the USF to LO transition as \( h_{c1} \) and the LO to PPFL transition as \( h_{c2} \). Both these fields increase with \( \mu \). We will discuss the detailed behavior within the LO window elsewhere.

\[ \text{FIG. 3. Color online: Ground state } \mu - h \text{ phase diagram obtained from the variational scheme, showing the unpolarised superfluid (USF), modulated (LO) and partially polarized Fermi liquid (PPFL) regions. There is no homogeneous superfluid state with finite magnetization, } i.e. \text{ BP, at } T = 0. \]

**A. Overview of thermal phase diagram**

Mean field theory for \( s \)-wave superconductors in a magnetic field indicate that (in the continuum case) the normal to SC thermal transition continues to be second order from \( h = 0 \) to a finite field, beyond which the system shows a first order transition, but now to a modulated superfluid phase.\(^{42,44,45}\)

The simultaneity of the second to first order change and transition from the \( q = (0, 0) \) to a finite \( q \) state is probably specific to continuum mean field theory. Additionally, the MF prediction of \( T_c \) scales, etc, is valid only in the weak coupling limit.

In the presence of an underlying lattice, even MFT suggests a field window over which one can have a first order SC to normal transition, see Fig.1, although the transition temperature is badly overestimated. Beyond another higher field the lattice based MFT predicts a modulated state.

Fig.4 shows the phases revealed by heating from the mean field ground state (left) and cooling (right) from a disordered high temperature state. The thermal transition from the SC to normal state is second order up to a field \( h_1 \sim 0.7t \) beyond which it becomes first order (with the ordered state still being at \( q = (0, 0) \)). For \( h < 0.7t \) the results are path independent but for \( 0.7t < h < 0.85t \) the system gets trapped in a LO state on cooling although the ground state is still USF. Beyond
FIG. 4. Color online: The field-temperature, $h - T$, behavior suggested by (a) heating from the variational ground state, and (b) cooling from a random high temperature state. We show the phases that emerge, the $T_c$ scales, as well as the dominant fluctuation in the disordered regime (following a convention described in the text). In both panels the change from a second order to first order BP to PPFL thermal transition occurs consistently at $h \approx 0.7t$. In the heating process the first order BP-PPFL transition encounters a region with strong LO fluctuations. This regime shows LO fluctuations on cooling as well and the system remains trapped in a fragmented LO state, rather than transit to the BP phase, as $T$ is lowered. The USF to LO transition in the ground state occurs at $h \sim 0.85t$. The ‘LO’ window in (a) refers to the genuine ground state, while in (b) it also includes the metastable LO region.

\[
h \sim 0.85t,
\]
where the ground state is LO the results are again path independent.

In the first order transition window, $h_1 < h < h_{c1}$, the USF ground state thermally evolves into BP at finite $T$ and then shows a transition to a PPFL state where the fluctuations, surprisingly, have LO character. On cooling down from a disordered state the system fails to attain a $q = (0,0)$ state and instead shows strong LO signatures. This MC inferred LO state is energetically higher than the variational USF state so this is a sign of metastability. We would characterize this state in terms of the various indicators in a later section.

1. Fluctuation regime

While long range order is only observed for $T \lesssim 0.2t$, we wanted to probe if there is a significant window above $T_c$, where fluctuation effects of $q = (0,0)$ or finite $q$ pairing can be seen. We define the cut off to the fluctuation regime as the temperature at which the ratio between the highest magnitude of the structure factor peak to that at the neighboring $k$-point is $\approx 1.5$. The regimes of strong BP fluctuation and strong LO fluctuation are marked in Fig. 4 in this spirit.

2. Thermodynamic properties

Fig. 5 shows the thermal evolution of $q = (0,0)$ structure factor peak, $S(0,0)$, and magnetization $m(T)$ for the magnetic fields characteristic of the low, intermediate and high field regimes. The two panels on top show the MC based results while the lower panels are based on MFT. The MC and MFT results have a gross similarity but (i) the MF $T_c$ scales are four times larger, (ii) even on a normalized, $T/T_c$ scale, the MC order parameter shows a quicker drop with temperature associated with the $O(2)$ nature of the superconducting problem, while the MF plot is much flatter due to absence of phase fluctuations, (iii) the MF magnetization has

FIG. 5. Color online: (a)-(b) Monte Carlo results for the temperature dependence of (a) $S(0,0)$ and (b) the magnetization, for heating (solid line) and cooling (open circle). (c)-(d). Mean field results on the order parameter (c), and the magnetization (d). Note that the $T$ range in (c)-(d) is about 5 times larger than in (a)-(b). Also, the MC based order parameter shows an almost linear drop with $T$ at low temperature while the MF order parameter is expectedly flat. The magnetization results, (b)-(d), despite their overall similarity differ in the low $h$, $T > T_c$ window.
effects show up. The thermal transition is reversible and no thermal history dependence of the following indicators: (a) the pairing amplitude $|\Delta(x, y)|$, (b) phase correlation $\cos(\theta_0 - \theta_{x,y})$ where $\theta_0$ is the phase at a reference site, (c) pairing structure factor $S_\Delta(q)$, (d) magnetization $n(x, y)$, (e) magnetic structure factor $S_m(q)$, and (f) number density $n(x, y)$. (a), (b), (d) and (f) are for a single MC snapshot, while (c) and (e) are thermally averaged. The $T_c$ in this case is $\sim 0.13t$.

We characterize this phase in Fig.7 through the $T$ dependence of the following indicators: (a) the pairing amplitude $|\Delta(x, y)|$, (b) phase correlation $\cos(\theta_0 - \theta_{x,y})$ where $\theta_0$ is the phase at a reference site, (c) pairing structure factor $S_\Delta(q)$, (d) magnetization $n(x, y)$, (e) magnetic structure factor $S_m(q)$, and (f) number density $n(x, y)$. (a), (b), (d) and (f) are for a single MC snapshot, while (c) and (e) are thermally averaged. The $T_c$ in this case is $\sim 0.13t$.

We have calculated the momentum occupation number $n_\sigma(k) = \langle \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle\rangle$. In Fig.8 we show $n_1(k)$ and $n_1(k)$ at $h = 0.5t$ for different temperatures. At low temperature where the system is unpolarised the Fermi surfaces are of equal sizes. As one increase the temperature the system develops an imbalance in the population of the up and down fermionic species, the signature of which is observed in the increasing size mismatch between the two Fermi surfaces. There is already a weak signature at $T \sim 0.11t$, a clear signature at $T \sim 0.13t \sim T_c$ (not shown here), and a prominent difference at $T = 0.2t$ and $T = 0.3t$.

FIG. 6. Color online: Thermal evolution of the superfluid ($S_\Delta(q)$) and magnetic ($S_m(q)$) structure factor at $h = 0.2t$. By the time the magnetization picks up a reasonable value (extreme right) the superfluid order has been lost.
FIG. 7. Color online: Thermal evolution of the various indicators at $h = 0.5t$. Starting from the top we show maps of $|\Delta|$, phase correlation, pairing structure factor, magnetization $m_i$, magnetic structure factor, and number density. The temperature, along the row, is marked at the bottom of the figure. Between $T = 0.10t$ and $0.13t$, see Fig.5, there is both significant superfluid order as well as magnetization.

D. High field: appearance of metastable FFLO states

In the high field regime, $0.7t < h < 0.85t$, the region of first order USF to normal transition, the system seems to encounter competing minima in the energy landscape. The state we obtain depends on the thermal history of the system. We highlight the effects at a typical field $h = 0.8t$.

Fig.9 shows the standard spatial and Fourier space indicators on a cooling run. The results on heating from the USF are qualitatively similar to what we have seen at $h = 0.5t$. On cooling from high $T$ the system encounters $q \neq 0$ fluctuations and instead of transiting to a $q = (0, 0)$ low $T$ state it actually enters a modulated state! This state has higher energy than the variational USF state which suggests its metastable character. We show the real space patterns at the lowest $T$ further on. While real space features are not very illuminating down to $T = 0.05t$, the pairing structure factor shows a clear finite $q$ feature. The spatial character becomes clearer at even lower $T$.

FIG. 8. Color online: Thermal evolution of the momentum occupation number $n^s_{\sigma}(k)$ at $h = 0.50$. The up and down spin distributions are same at $T = 0$, slightly different for $T \lesssim T_c$ (2nd row), and noticeably different at high temperature.
FIG. 9. Color online: Thermal evolution of the various indicators on cooling the system at $h = 0.8t$. From top to bottom we have plotted the spatial map of $|\Delta|$, phase correlation, the pairing structure factor, magnetization, magnetic structure factor and number density. This illustrates the emergence of a strong LO signature in the pairing structure factor, when the ground state is actually USF. The pattern at the lowest temperature: $T = 0.001t$ is shown later.

$T$ as we show below.

We compute the momentum occupation numbers for the up and down fermionic species through the heating and cooling cycles. Apart from the evolution of the mismatch between the up and down distributions with temperature one can also see the modification in the Fermi surface shape with respect to what one would expect in the simple tight binding case. The straight Fermi surface segments at low $T$ in Fig.10 result from line-like LO correlations as we show in the Fig.11. The rise in temperature wipes out this feature.

What does this metastable LO state look like in real space? We computed the amplitude, phase, magnetization and number density maps for MC snapshots and show a typical set at low temperature in Fig.11. As can be seen, real space periodic
FIG. 10. Color online: Momentum occupation numbers $n_{\sigma}(k)$ at different temperatures through the heating and the cooling cycle computed at $h = 0.8t$. Notice the ‘size difference’ persisting to low temperature in the cooling run - suggesting a finite m ‘ground state’ (actually metastable in this case). For $T > T_c$ the heating and cooling results are essentially similar.

FIG. 11. Color online: Spatial maps characterizing the metastable LO state through (a) $|\Delta|$, (b) phase correlation, (c) magnetization and (d) number density distribution at $T = 0.001t$. Modulations are observed in both the superfluid order parameter and local magnetization. The order parameter exhibits a nodal, domain wall like structure, in the nodes of which reside the unpaired fermions giving rise to a finite magnetization. A ‘node’ in the $|\Delta|$ corresponds roughly to a peak in the local magnetization.

Before we end this section we show the ideal momentum occupation number $n_{\sigma}(k)$ corresponding to the metastable state at $h = 0.80t$ in Fig.12. A weaker variant of the same has been observed and presented in Fig.10. Fig.12 prominently shows the anisotropic deformation of the Fermi surfaces in presence of an underlying modulated pairing order.

E. Density of states

Pseudogap features in the density of states, and momentum resolved spectral functions, have been explored experimentally in the balanced ‘continuum’ Fermi gas at unitarity. There is also a body of associated theory\cite{56,75}. Unfortunately there are no such detailed spectral experiments in the imbal-

FIG. 12. Color online: Momentum occupation function for an ideal diagonal stripe phase to mimic the pattern that we observe in Fig.11. Fig.11 modulations have a 2D character (rather than simple diagonal stripe) so the actual $n(k)$ in Fig.10 has an approximate fourfold look.
FIG. 13. Color online: Temperature dependence of the DOS at \( h = 0.2t, 0.5t, 0.8t \) (left to right). The top row shows \( N_\uparrow(\omega) \) and the bottom row shows the total DOS \( N(\omega) \). \( N_\downarrow(\omega) \) is just a shifted version of \( N_\uparrow(\omega) \). While the main feature in (a) is slow filling up of the gap (with increasing \( T \) the gap converts to a pseudogap already below \( T_c \)), (b) and (c) reveal that at higher fields this ‘filling up’ process is non monotonic. We quantify the relevant temperature scales later in Fig.16.

anced case. Our coupling corresponds roughly to what would be considered ‘unitary’ (see the Discussion section), but we are working on a lattice, at densities far from the continuum end. To check the usefulness of our approach in capturing the qualitative features of this well studied end we compared our ‘balanced’ results to those in the literature. We found that the dispersion and damping share several features (we will put this up separately) providing confidence that our lattice results would have value in analysing imbalanced continuum gases as well.

Fig.13 shows the spin resolved and total density of states at low, intermediate, and high fields, \( h = 0.2t, 0.5t, 0.8t \), respectively. We focus on the ‘up spin’ DOS, since the ‘down spin’ DOS is symmetrically shifted (and the total is simply a sum of these two) and define ‘low energy’ as \( \omega \sim -h \).

Fig.14 shows the \( T \) dependence of the spin up DOS at the shifted Fermi level for up spin fermions. Right: a color map of the DOS at \( \omega = -h \) for varying \( h \) and \( T \). The non monotonic \( T \) dependence is clearly visible in the large \( h \) regime.

FIG. 14. Color online: (Left) Temperature dependence of the DOS at the shifted Fermi level for up spin fermions. Right: a color map of the DOS at \( \omega = -h \) for varying \( h \) and \( T \). The non monotonic \( T \) dependence is clearly visible in the large \( h \) regime.
FIG. 15. Color online: Field dependence of the $N\uparrow(\omega + h)$, the total DOS $N(\omega)$ and $P(|\Delta|)$. Top row: $T = 0.05\,t$, bottom row $T = 0.15\,t$. The shift in $N\uparrow$ is to gauge out the field dependent shift of origin and the resulting clutter in the plot.

which the spin resolved DOS at $\omega = \pm h$ has its maximum.

Fig.15 shows $h$ dependence at fixed temperatures, highlighting the effect on the DOS as the system evolves from the

‘balanced’ situation to the highly magnetized (hence weakly paired) state. At $T = 0.05\,t$, top row, which is $\sim 0.37T_c$, the pseudogap in the DOS vanishes at $h \sim t$ while at $T = 0.15\,t$, bottom row, the PG seems to persist even at $h = 1.5\,t$ where the ground state is an unpaired Fermi liquid!

In panels (c) and (f) we show $P(|\Delta|)$ for the same field values as in the DOS panels. At $T = 0.05\,t$ the $P(|\Delta|)$ remains almost unchanged for $h$ between $\sim 0 - 0.6t$. The resulting DOS also remains essentially unchanged over this field window. At $h = 0.8t$ the center of $P(|\Delta|)$ is at a noticeably smaller value, and as $h$ increases the peak and the mean value of $|\Delta|$ shift to progressively lower value. At $h = 1.5t$ the peak value is $\sim 0.25\Delta_0$ and the $P(|\Delta|)$ cannot generate a pseudogap in the spectrum.

At $T = 0.15\,t$ the peak location of $P(|\Delta|)$ and the mean shift to lower value with increasing $h$. All the data, except at $h = 0, 0.2t$, are at $T > T_c$. However, at this temperature the mean value at high fields is significantly larger than what we see at $T = 0.05\,t$. At $h = 1.5t$ the peak of $P(|\Delta|)$ is at $\sim 0.5\Delta_0$, almost twice the $T = 0.05\,t$ value.

As a result, even though the high field system starts at low $T$ as essentially an ‘uncorrelated’ partially polarized Fermi liquid (within our scheme) the thermally generated correlation effects are strong enough to generate a pseudogap with increasing temperature. The spin resolved DOS at large $h$ starts gapless (at $T = 0$) but transits to an interaction induced weak pseudogap phase at high $T$. This pseudogap has nothing to do with long range order in the ground state.

FIG. 16. Color online: Temperature scales associated with the behavior of the spin resolved DOS. The low $T$ hard gap in the superconductor converts to a pseudogap at a temperature $T_{pg1} < T_c$, while the ‘ungapped’ partially polarized Fermi liquid at large $h$ develops a pseudogap at $T = T_{pg2}$. The entire window above $T_{pg1}$ and $T_{pg2}$ is pseudogapped. The DOS at the center of the pseudogap ($\omega = \pm h$) shows a maximum at $T_{max}$.
Tracking the field dependence of the pseudogap formation scale, starting from the low temperature end, allows us to construct the PG feature based ‘phase diagram’ in Fig.16. It reveals several intriguing features: (i) Although the $T = 0$ gap in the spectrum remains the same for $h = 0 - 0.85t$ the temperature $T_{pg1}$, at which this gap converts to a pseudogap, collapses as $h \to h_{c1}$ the USF-FFLO boundary. (ii) Although the mean field ground state has no pairing for $h \gtrsim 1.3t$, and is therefore gapless, fairly modest temperature $\sim 0.07t$ generates an weak pseudogap due to thermal generation of pairing fluctuations. (iii) The PG in the spin resolved DOS survives to a high temperature, certainly greater than $T \sim 0.5t$ that we have probed, although at large $h$ it is a weak feature. This survival to high $T$ is a consequence of the large interaction $U = 4t$ that we have chosen, and has a parallel in the PG observations made on the imbalanced cold Fermi gas at unitarity[22].

IV. DISCUSSION

Till now we have mainly focused on our specific results. In what follows we touch briefly on a few broader issues. These include: (a) the reliability and limitations of our method, (b) a conceptual framework for understanding the numerical data, (c) the connection between our intermediate coupling lattice results and the unitary continuum gas, (d) qualitative comparison with cold atom and solid state experiments, and (e) the wider possibilities of our method in exploring imbalanced superfluids in other situations.

A. Issues of method

Our results are based on (i) a Hubbard-Stratonovich decomposition of the interaction in the pairing channel, (ii) approximating this auxiliary pairing field $\Delta$, as classical, (iii) a cluster algorithm based Monte Carlo sampling of the $\Delta$, field, (iv) use of finite size, as is inevitable in any calculation of this kind. (ii), (iii) and (iv) introduce errors and we comment on these in the paragraphs below.

1. Hubbard-Stratonovich decomposition

The analytic basis of the HS based method is discussed in the Appendix.

2. The static approximation

The static auxiliary field approximation is exact as $T \to \infty$ and in principle becomes less and less accurate as $T \to 0$ (as the energy difference between the bosonic Matsubara frequencies reduce). However, when the ground state has some kind of long range order, as in both the balanced and unbalanced fermion cases, the static mode succeeds in capturing much of the interaction effects. This keeps our $T = 0$ results qualitatively valid. A comparison in the balanced case revealed that by the time $T \sim T_c$, the static mode captures most of the thermal effects, and anyway for $T \gg T_c$ it should describe the problem exactly. Overall, in the current problem, the static approximation by itself is not a serious limitation.

3. Single channel decomposition

A single field decomposition that is static cannot in general capture instabilities in all channels. In the FFLO regime the pairing, density, and magnetic channels are in principle all relevant. However, we find that for our chosen mean density, the density modulations in the FFLO phase are very weak so ‘density channel’ effects are not important (they would be very important if $n = 1$). The presence of an additional magnetic channel may make a quantitative difference to our results. While these additional channels are readily incorporated within MFT a non Gaussian fluctuation theory, like ours, involving all these modes is difficult to construct. We have opted to stay with a simple decomposition so that the fluctuation theory can be better handled.

For the homogeneous BP phase we have found that there is no density wave ordering tendency at $n = 0.94$ and the field regime that we have considered. Fluctuations in density are present, as evidenced in Figs.7 and 9, but are small since the field induced magnetization suppresses the density wave susceptibility. In a more elaborate calculation the fluctuations could be numerically larger, without changing the qualitative features of our result.

4. Monte Carlo: cluster algorithm and size dependence

The MC implementation using the Bogolubov-de Gennes scheme requires repeated diagonalisation of the fermion problem. Done exactly this computation scales as $N^4$ where $N$ is the system size, limiting one to $N \sim 10 \times 10$, hardly adequate to access complex phases. This is a primary limitation in FFLO studies and limits most finite temperature studies to mean field theory. We can access much larger size (up to $40 \times 40$, say) since we use a cluster based update scheme, discussed in the text. Unfortunately the cluster size introduces another length scale, that affects access to FFLO phases, but does not seem to have much impact on the uniform SC state. So, as far as the present study is concerned, size limitations have not been significant. We have checked the quality of the MC in the $h = 0$ problem earlier by comparing to full QMC[49].

B. Landau-Ginzburg framework

It is useful to put up a Ginzburg-Landau (GL) framework for qualitatively understanding our results, focusing on a $\Delta_i$ only theory rather than the ‘fermion + $\Delta_i$’ problem. At weak coupling GL theory could have been systematically derived[56][58], here it serves as a phenomenological construct.
The free energy density suggested by Casalbuoni et al.\cite{casalbuoni1} for the superfluid in the presence of a magnetic field, is:

\[
\mathcal{F} = \frac{1}{2} \alpha |\Delta|^2 + \frac{1}{4} \beta |\Delta|^4 + \frac{1}{6} \gamma |\Delta|^6 + \epsilon |\nabla \Delta|^2 + \frac{\eta}{2} |\nabla^2 \Delta|^2
\]

The complicated form, involving a 6th order amplitude term and \(\nabla^2 \Delta\), is retained since \(\beta\) and \(\epsilon\) which are positive in the \(h = 0\) case can change sign when \(h \neq 0\).

In the \(h = 0\) functional involving only \(\alpha\), \(\beta\) and \(\epsilon\), we have \(\beta > 0\). The sign change of \(\alpha\) drives a second order transition to a \(q = (0, 0)\) state since the gradient term penalizes spatial modulation.

\(\beta\) changing sign from positive to negative leads to a first order transition, again to an uniform state if \(\epsilon > 0\), and one retains a positive \(\gamma\). On the other hand if \(\epsilon\) changes sign the system would head towards a modulated state, whose wave number has to be decided by the presence of a positive \(\eta\). This would be the thermal transition to some FFLO state.

In the continuum weak coupling limit it turns out that \(\beta\) and \(\epsilon\) change sign from positive to negative at the same point.\cite{casalbuoni1,forbes2}

In that situation one has a second order normal to SC transition at weak field, crossing over to a first order normal to FFLO transition beyond a critical field.

Our lattice mean field results at \(U = 4t\) indicate that a first order thermal transition need not be necessarily to an FFLO state. We do have a window of a first order normal to uniform SC transition. This distinction is probably a lattice versus continuum difference. It shows up in the MC results as well, with \(T_c\) scales suppressed due to amplitude and phase fluctuations.

The MC results suggest the rough behavior of the various GL coefficients in terms of \(h\) and \(T\) but the observed metastability is harder to pin down. For that a more elaborate functional, derived by tracing out the fermions from the coupled problem, and expanded about \(Q\) and \(\mathcal{F}\) (the FFLO wave vector) would be needed. For \(h < h_1\) that free energy has the deepest minimum at \(q = 0\), and also uniquely reaches this state on thermal cycling. For \(h_1 < h < h_{c1}\) the absolute minimum is still at \(q = 0\) but it seems that the minimum at \(Q\), although metastable, dominates the energy landscape. When one cools from the high \(T\) state the system seems to first encounter this \(q \neq 0\) minimum and tracks this state down to \(T = 0\).

\[\text{C. Connection to continuum unitary gas}\]

While we have motivated our lattice model in terms of experiments on the continuum unitary Fermi gas there are issues which need highlighting. These are (i) the notion of ‘unitarity’ in the 2D lattice model (and its relation to BCS-BEC crossover), and (ii) the access to continuum ‘universal’ effects via lattice simulations.

**Unitarity:** The primary scale quantifying the strength of interaction in cold Fermi gases is the two body \(s\)-wave scattering length: \(a_D\), where \(D\) denotes the spatial dimensionality. The dimensionless coupling constant can then be written in terms of \(k_F a_D\), where \(k_F\) is the Fermi wavevector. We quickly comment on unitarity and the BCS-BEC crossover issue in the continuum and lattice contexts and then see what information lattice simulations can yield.

In the 3D continuum Fermi gas the scattering length \(a_{3D} \to \infty\) as the interaction \(g \to g_c\). \(g_c\) is a finite in 3D, and defines the interaction for which a two body bound state first forms in vacuum. The (inverse) dimensionless coupling \(1/k_F a_{3D} = 0\) at \(g_c\). This is also the point near which the transition temperature of the 3D Fermi gas has its maximum, with \(T_{c\text{max}}/E_F \sim 0.15\). On the 3D Hubbard lattice an equivalent critical interaction for bound state formation can be worked out and yields \(U_c/t \sim 7.9\). Again, the \(T_c\) is found to be maximum for \(U/t \sim 8\) (from QMC), remarkably close\cite{casalbuoni1} to \(U_c\).

In the 2D continuum a two body bound state forms in the presence of an arbitrary attractive interaction so \(a_{2D}(g) \to \infty\) for \(g \to 0\). This is however in the deep BCS regime where a weak coupling description in terms of fermionic quasiparticles is sufficient. As \(g\) increases the pair size shrinks and in the Bose limit \(a_{2D} \to 0\). The crossover coupling in the 2D case is defined via \(ln(k_F a_{2D}) \to 0\), i.e., the scattering length being comparable to inter particle separation. We are not aware of a 2D continuum QMC calculation for the \(T_c\), but interpolation between the BCS and BEC end suggests that the maximum \(T_c\) occurs for \(ln(k_F a_{2D}) \to 0\), with \(T_{c\text{max}}/E_F \sim 0.1\).

On the 2D Hubbard lattice a two body bound state would form at arbitrary weak attraction, i.e, \(U_c/t \to 0\). The notion of \(k_F\) is not very meaningful on the lattice, particularly away from low density, but following the cases above one may identify the crossover as the region of maximum \(T_c\). The \(T_c\) is well established via QMC and the maximum occurs for \(U/t \sim 5\). For \(U/t = 4\) that we use the \(T_c\) is \(\sim 0.9\) of the maximum value\cite{casalbuoni1}.

Overall, the two body bound state based unitary point in 3D also corresponds to a regime where (i) neither the fermionic nor the bosonic quasiparticle description suffices, and (ii) the \(T_c/E_F\) is maximum. In 2D the simple two body argument would put this regime at extreme weak coupling but (i) and (ii) above indicate that \(ln(k_F a_{2D}) \to -\infty\), rather than \(a_{2D} \to \infty\), is the relevant choice.

Our interaction strength is not far from what would be considered the ‘unitary’ value in the 2D lattice case. Can we comment on the universal physics one would have seen in the continuum case, on which, remarkably, there is now an experiment?

**Continuum universality from lattice physics:** The first difficulty is with our density choice, we have used \(n \sim 0.9\) to maximize \(T_c\) (at the same time avoiding the density wave instability at \(n = 1\)). At this density the lattice effects are very prominent and the Fermi surface is distinctly non circular. Even if we had used lower density, \(n \sim 0.1\), say, where the Fermi surface is indeed circular and \(\epsilon_F \sim k^2\) is a good approximation access to continuum effects is difficult. If the interaction were weak, i.e, \(U \ll 4t\), the physics would have been insensitive to the high energy band cutoff. However, ‘unitarity’ requires \(U \sim 5t\) and even if the Fermi level is at the lower edge of the band, scattering effects couple in states at the upper edge. The high energy states are lattice specific, and as the paper by Privitera et al.\cite{casalbuoni1} demonstrates...
The suppression of $T_\text{c}$ of the zero field (balanced) behavior$^{51,53–55}$ near the tricritical point occurs at 53. Using the measured zero imbalance $T$, the magnetic field is significantly lowered with respect to mean field theory. Superfluid (SF) state cannot occur at $m = 0$ for normal Fermi liquid. At $m = 0$, the SF to unstable transition occurs at $T = 0$, and the unstable to LO transition at $m = 0$. It must be noted that the unstable region essentially is a phase separated region, marked by discontinuity in density, and characterized by the absence of homogeneous superfluid phase. The LO state has not been observed experimentally in the 2D geometry, possibly due to additional fluctuations in the absence of a lattice. Our tricritical point is at $m \sim 0.15$ and $T_{\text{tricrit}} \sim 0.07T_0 \sim 0.4T_0$. Given that we are in a regime where the Fermi surface is significantly non circular the overall correspondence of phase boundaries and temperature scales is reasonable. We have predictions about spectral properties on the $m - T$ plane that we will present separately.

2. Superconductors

The solid state systems in which Pauli limited behavior is observed, for example CeCoIn$_5$ and the organic superconductors, are non s-wave materials and have low energy fermionic degrees of freedom even in the ordered state. In our model, however, the fermions are gapped, or have a strong pseudogap, due to the large on site attraction - unless the population imbalance is large. As a result, despite the overall similarity in the look of our theory phase diagram and those observed in experiments$^{9,10,19}$, the comparison of indicators like specific heat, $C_V(T,h)$, and magnetization, $m(T,h)$, reveals differences in detailed behavior. We have made these comparisons but do not present the data here.

D. Comparison with experiments

1. Atomic superfluids

Our model finds it most appropriate experimental counterpart in imbalanced cold Fermi gases, studied at strong attractive interaction promoting s-wave pairing. There are still differences, e.g., (i) our results are on a lattice theory, the experiments are in the ‘continuum’, (ii) there is a trap present in the experiments, and (iii) dimensionality (the experiments are in three dimensions). Nevertheless, the similarities are striking. Fig.17 presents the experimental phase diagram$^{32}$ of the unitary Fermi gas in terms of magnetization $m = (n_{\uparrow} - n_{\downarrow})/(n_{\uparrow} + n_{\downarrow})$ and temperature, constructed by the experimental group by ‘gauging out’ the effect of the trap. Next to it we show our $m - T$ phase diagram, constructed at $n \sim 0.9$ by varying $h$ (hence $m$).

The experiments infer (i) a homogeneous magnetized superfluid (SF), (ii) an unstable region, and (iii) a magnetized normal Fermi liquid. At $T = 0$ the SF to unstable transition occurs at $m = 0$, suggesting that a finite $m$ homogeneous SF state cannot occur at $T = 0$, while the ‘unstable’ to normal transition occurs at $m \sim 0.35$. The $T_c$ of the unitary Fermi gas is significantly lowered with respect to mean field theory$^{32}$ and using the measured zero imbalance $T_c$ as the reference scale, the tricritical point occurs at $m \sim 0.2$ and $T_{\text{tricrit}} \sim 0.4T_0$. The suppression of $T_c$ in presence of imbalance is an extension of the zero field (balanced) behavior$^{51,53–55}$. The presence of imbalance makes the suppression rapid.

The $m - T$ picture that emerges from our data already has the fluctuation effects built in on $T_0$. In the ground state the SF to ‘unstable’ transition occurs at $m = 0$+ and the unstable to LO transition at $m \sim 0.28$ and the LO to normal transition at $m \sim 0.37$. It must be noted that the unstable region essentially is a phase separated region, marked by discontinuity in density, and characterized by the absence of homogeneous superfluid phase. The LO state has not been observed experimentally in the 2D geometry, possibly due to additional fluctuations in the absence of a lattice. Our tricritical point is at $m \sim 0.15$ and $T_{\text{tricrit}} \sim 0.07T_0 \sim 0.4T_0$. Given that we are in a regime where the Fermi surface is significantly non circular the overall correspondence of phase boundaries and temperature scales is reasonable. We have predictions about spectral properties on the $m - T$ plane that we will present separately.

E. Extensions of the present method

The present work was focused on understanding a part of a larger phase diagram. As a natural extension of this we have studied the thermal properties of the large $h$ FFLO states in detail. We have also computed the momentum resolved spectral functions of the BP, PPFL, and FFLO phases over the entire $h - T$ window. We will present these results separately.

A natural extension of the present method, involving a ‘two field’ decomposition, can handle the effect of disorder$^{54,55}$ on the FFLO state, including the thermal effects which are in general difficult to access. Finally, cold Fermi gases involve a trapping potential and a non trivial spatial dependence of the region where the fluid is magnetized. While experimental optical lattice sizes $\sim 100 \times 100$ are hard to access using our MC technique, we hope to access the physics at least in the BP regime using a local density scheme grafted on to our Monte Carlo solver.

V. CONCLUSION

We have used a real space Monte Carlo technique based on static pairing field approximation to study the behavior of a Pauli limited superconductor in the BCS to BEC crossover regime. We find that the $T_c$ scales are strongly suppressed...
with respect to mean field predictions, there is a wide window of metastable FFLO states in which the system gets trapped when the true ground state is a homogeneous superfluid, and the spin resolved density of states shows a non monotonic low energy character. We do not know of Pauli limited solid state systems with s-wave pairing, but ultracold unitary gases suggest an universal phase diagram quite similar to what we observe. This paper probes the lower field ‘breached pair’ state in detail, companion papers discuss the FFLO regime and the spectral features expected with changing imbalance.

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VI. APPENDIX: HUBBARD-STRATONOVICH TRANSFORMATION AND MONTE CARLO SAMPLING

The primary numerical technique we use is a Monte Carlo implementation of a ‘single channel’ static auxiliary field decomposition of the A2DHM. Below we discuss about the various aspects of our numerical technique.

The Hubbard model at strong interaction requires a non perturbative solution. The exponential growth in the dimension of the Hilbert space rules out the use of exact diagonalization except for very small sizes. The ‘exact’ tool of choice is quantum Monte Carlo (QMC) against which all approximations are bench marked. While QMC can be implemented via various approaches, the method below easiest reveals the connection to our approach.

The Hubbard partition function is written as a functional integral over Grassmann fields $\psi_{i\sigma}(\tau), \bar{\psi}_{i\sigma}(\tau)$.

\[
Z = \int D\psi D\bar{\psi} e^{-S[\psi, \bar{\psi}]}
\]

\[
S = \int_0^\beta d\tau \sum_{ij,\sigma} \left( \psi_{i\sigma}(0) \delta_{\tau, \delta_{ij}} + t_{ij} \psi_{j\sigma} \right) - |U| \sum_i \bar{\psi}_{i\uparrow} \psi_{i\uparrow} \bar{\psi}_{i\downarrow} \psi_{i\downarrow}
\]

Only quadratic path integrals can be exactly evaluated. Since the interaction generates a quartic term in the $\psi$’s the partition function cannot be immediately evaluated.

The quartic term is ‘decoupled’ exactly through a Hubbard-Stratonovich transformation in terms of pairing fields $\Delta_i(\tau), \bar{\Delta}_i(\tau)$. This introduces a term $\Delta_i(\bar{\psi}_{i\uparrow}(\tau) \bar{\psi}_{i\downarrow}(\tau))$ in the action.

\[
Z = \int D\Delta D\bar{\Delta} e^{-S[\Delta, \bar{\Delta}, \Delta^*]} \]

\[
S_1 = \int_0^\beta d\tau \sum_{ij,\sigma} \left( \bar{\psi}_{i\sigma}(\partial_{\tau} \delta_{ij} + t_{ij}) \psi_{j\sigma} \right) + \sum_i \left( \Delta_i(\tau) \bar{\psi}_{i\uparrow}(\tau) \bar{\psi}_{i\downarrow}(\tau) + h.c + \frac{|\Delta_i|^2}{|U|} \right)
\]

The $\psi$ integral is now quadratic but an additional integration over the field $\Delta_i(\tau)$ has been introduced. The ‘weight factor’ for the $\Delta$ configurations can be determined by integrating out the $\psi, \bar{\psi}$, and using these weighted configurations one goes back and computes fermionic properties. Formally

\[
Z = \int D\Delta D\bar{\Delta} e^{-S_2[\Delta, \bar{\Delta}^*]} \]

\[
S_2 = \log[Det[G^{-1} - \Delta]] + \frac{|\Delta|^2}{|U|}
\]

where $G$ is the Greens function associated with the non interacting $H$. The weight factor for an arbitrary space-time configuration $\Delta_i(\tau)$ involves computation of the fermionic determinant in that background. If we write the auxiliary field $\Delta_i(\tau)$ in terms of its Matsubara modes, as $\Delta_i(\Omega_n)$, then the various approximations can be readily recognized and compared.

- Quantum Monte Carlo retains the full $\{i, \Omega_n\}$ dependence of $\Delta$ computing $log[Det[G^{-1} - \Delta]]$ iteratively for importance sampling. The approach is valid at all $T$, but does not readily yield real frequency spectra.
- Mean field theory restricts $\Delta_i(\Omega_n)$ to a spatially uniform (or periodic) and time independent ($\Omega_n = 0$) mode, i.e, $\Delta_i(i\Omega_n) \rightarrow \Delta$. The free energy is minimized with respect $\Delta$. When the MF order parameter vanishes at high temperature the theory trivializes.
- Our static auxiliary field (SAF) approach retains the full spatial dependence in $\Delta$ but keeps only the $\Omega_n = 0$ mode, i.e, $\Delta_i(\Omega_n) \rightarrow \Delta$. It thus includes classical fluctuations of arbitrary magnitude but no quantum ($\Omega_n \neq 0$) fluctuations. One may consider different temperature regimes: (1) $T = 0$: since classical fluctuations die off at $T = 0$, SAF reduces to standard Bogoliubov-de Gennes (BdG) MFT. (2) At $T \neq 0$ we consider not just the saddle point configuration but all configurations following the weight $e^{-S_2}$ above. These involve the classical amplitude and phase fluctuations of the order parameter, and the BdG equations are solved in all these configurations to compute the thermally averaged properties. This approach suppresses the order much quicker than in MFT. (3) High $T$: since the $\Omega_n = 0$ mode dominates the exact partition function the SAF approach becomes exact as $T \rightarrow \infty$.
- DMFT: for completeness we mention that DMFT retains the full dynamics but keeps $\Delta$ at effectively one site, i.e, $\Delta_i(\Omega_n) \rightarrow \Delta(\Omega_n)$.

Overall, our method reduces to BdG mean field theory only at $T = 0$ but retains all the classical thermal fluctuations at $T \neq 0$. As a result it is only as good as MFT at $T = 0$ but is far superior in estimating $T_c$, and essentially exact as $T \rightarrow \infty$. It does use BdG iteratively as a tool but on all fluctuating configurations not just the mean field state.
In contrast to Chiesa and Zhang, who do a mean field theory in pairing, density, and spin channel, we decouple the Hubbard term only in the pairing channel. This would lead to different results in parts of the FFLO regime but has no effect on the USF ground state.

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