Strong coupling s-wave superconductors in the extreme Pauli limit: I. The breached pair and metastable FFLO phases

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We study s-wave superconductivity in the attractive Hubbard model in an applied magnetic field and assume the extreme Pauli limit where the orbital critical field is much greater than the Zeeman critical field. We work at a coupling corresponding roughly to the peak \( T_c \) in the BCS to BEC crossover window and retain the crucial amplitude and phase fluctuations. At low field, as expected, the superconductor undergoes a second order thermal transition to the normal state, and is only weakly magnetized near \( T_c \). At intermediate fields the thermal transition is still second order, but the magnetization is significantly larger, characteristic of a ‘breached pair’ state. At strong field, the thermal transition is first order and our Monte Carlo reveals the presence of a metastable Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state. At even higher fields we observe the true FFLO ground state. We present the full ‘field-temperature’ phase diagram of this strong coupling problem, revealing \( T_c \) scales an order of magnitude below the mean field estimate, compute the superconducting and magnetic order parameters, and map out the directly measurable magnetic structure factor. We compare these trends to results on the Pauli limited heavy fermion CeCoIn$_5$, and the cold atomic Fermi gas at unitarity. This paper focuses primarily on the homogeneous superconducting state, another deals with thermal effects in the 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 \( h_c \) in the form of an Abrikosov lattice, before superconductivity (SC) is finally lost at the ‘orbital critical field’ \( h_{c2}^{orb} \). The magnetic field also couples to the spin of the electrons, and tends to break an ‘\( ↑↓ \)’ pair (assuming a singlet superconductor). This effect is detrimental for SC, and, if orbital effects were irrelevant, SC order would be lost at some ‘Pauli limiting’ field, \( h_{c2}^{P} \) say. The ratio of these critical fields, \( \alpha = h_{c2}^{orb} / h_{c2}^{P} \), 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 \( \sim 10^5 \) due to Fermi liquid corrections, (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 fermion CeCoIn$_5$, the \( \kappa \)-BEDT based layered superconductors, and population imbalanced cold Fermi gases make the Pauli limit relevant.

Early extensions of \( \kappa \) 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 (FF) and Larkin and Ovchinnikov (LO). There is no longer a first order transition between the uniform SC and the normal state.

Direct evidence for a modulated state conforming to FFLO predictions remains elusive. However, in CeCoIn$_5$ there are measurements of the specific heat, magnetic torque, muon spin relaxation, NMR, and in particular magnetic neutron scattering that suggest the presence of some state with magnetic modulations. Similarly, in the \( \kappa \)-BEDT based organics there is indirect evidence for a modulated state at large in plane fields. For cold atomic gases, fermionic superfluidity has been explored mainly in the continuum situation and the effect of imbalance has been probed in detail with the Fermi gas tuned to unitarity.

The microscopic models for superconductivity (or superfluidity) is these systems are widely different but they all 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 at a coupling regime well beyond the reach of ‘BCS’ mean field theory (at least for the heavy fermions and the atomic gases).

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, equivalent to the unitary point in the continuum, and crucially involves amplitude and phase fluctuations in describing the thermal physics.

Our main results, from a recently developed Monte Carlo approach, are the following: (i) We discover that fluctuation effects suppress \( T_c \) scales by a factor of more than 4 compared to widely used mean field theory. (ii) Intermediate fields allow for a temperature window over which the superfluid supports significant magnetization which, although homogeneous on the average, shows noticeable configurational fluctuation. (iii) 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. (iv) Larger fields lead to a relatively low \( T_c \) striped FFLO ground state.

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

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:

\[
H = H_0 - h \sum_i \sigma_{iz} - |U| \sum_{ij} n_{i\uparrow} n_{i\downarrow}
\]

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. \( \sigma_{iz} = (1/2)(n_{i\uparrow} - n_{i\downarrow}) \). We will set \( t = 1 \) as the reference energy scale. \( \mu \) is the chemical potential and \( h \) is the applied magnetic field in the \( \hat{z} \) 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, as seems to be appropriate to many of the current superconductors. This requires retaining fluctuations well beyond 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 \( \Delta_i = |\Delta_i|e^{i\phi_i} \). In the static limit of the auxiliary field, this leads to the effective Hamiltonian:

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

where \( H_{cl} = \sum_i |\Delta_i|^2 \) is the stiffness cost associated with the auxiliary field. The Boltzmann weight for the occurrence of a particular configuration \( \{\Delta_i\} \) is,

\[
P\{\Delta_i\} \propto Tr e^{\beta H_{\text{eff}}}
\]

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

B. Numerical method: Monte Carlo and variational calculation

Mean field theory (MFT) 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. In the present work thermal fluctuations are incorporated via a static auxiliary field (SAF) technique which, implemented via Monte Carlo, can access system sizes larger than typical quantum Monte Carlo (QMC) calculations. This helps in accessing relatively long wavelength spatially modulated (FFLO) paired states. Our approach also allows calculation of dynamical properties without 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. The approximation has been extensively bench marked, and used successfully in the zero field case\cite{footnote}. We will discuss the limitations of the SAF approach and cluster based update at the end of the paper.

The zero temperature limit within the SAF scheme is equivalent to unrestricted Hartree-Fock-Bogolyubov theory, where the ground state 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 kind of periodic configurations: (i) ‘axial stripes’: \( \Delta_i \sim \Delta_0 \cos(qx_i) \), and diagonal stripes \( \Delta_i \sim \Delta_0 \cos(q(x_i + y_i)) \) and (ii) two dimensional modulations, \( \Delta_i \sim \Delta_0(\cos(qx_i) + \cos(qy_i)) \), 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).

We will discuss calculations in the FFLO regime in detail elsewhere. For completeness we just mention here that for a \( L \times L \) lattice, with periodic boundary conditions, the possible FFLO wave vectors are dictated by the lattice size. A smaller size of the lattice would thus be incapable of capturing the expected continuous variation of the FFLO wave vector with magnetic field. The constraint imposed by the lattice size becomes more serious at weaker \( U/t \). As a result, even though the choice of \( L = 24 \) was sufficient to capture the modulated
ground state at $U/t = 4.0$, a much larger lattice was required to capture the same at $U/t = 2.0$.

C. Parameter regime and indicators

Any real space numerical calculation is required to have $L \gg \xi_0$, 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 $U/t = 4$, both within Monte Carlo and the variational scheme. We have also explored $U/t = 2$ 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 had 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 physics seems similar so this paper focuses on a single $\mu$. The density at this point is $n \sim 0.94$, and does not significantly depend on $h$ or $T$. We have studied the temperature dependence at a large number of fields in the window $h/t \sim [0 : 1.5]$. 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 (a) $|\Delta_i|$, (b) phase correlation $\cos(\theta_i - \theta_j)$ 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 (d) 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:

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

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

where, $N = L^2$.

(iii) We monitor the bulk magnetization and the SC order parameter, $S(q = 0; T, h)$. Finally, (iv) we compute the momentum occupation number $\langle \langle n_{kr} \rangle \rangle$ that carries the signature of imbalance and FFLO modulation. We also compute the fermionic density of states (DOS) and the detailed momentum resolved spectral functions but these aspects are not discussed in the present paper.

III. RESULTS

Our presentation of the results is organized as follows. We first highlight the huge difference between the mean field results and that of our Monte Carlo approach due to the importance of thermal amplitude and phase 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 noticeable 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 the mean field approach (which seems to be the standard tool in imbalanced fermion studies) 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 breached pair (BP) and FFLO character. A much more detailed phase diagram will be shown in Fig.4. The mean field approach makes the assumption of a constant $\Delta_i$ throughout the system. While
this is reasonable at low $T$, and can cover the finite $T$ window also when $U/t \ll 1$, it badly fails in our coupling regime.

Fig.1.(b) presents 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. This phase diagram is roughly the lattice version of the continuum phase diagram experimentally established for imbalanced fermions at unitarity. We will discuss the parallel with experiments in much greater detail later.

### A. Ground state

Within our ‘static’ framework the ground state of the system can be determined by using a variational technique, where one computes the energy for a family of trial configurations $\{\Delta_i\}$. These correspond to different modulation vectors $q$ as described in the earlier section. The variational approach to determine the ground state configuration has been carried out in the same spirit as Cheisa et al., wherein spiral, uniaxial and checkerboard type modulations were compared to determine the stable ground state in a lattice model.

In Fig.2.(a) and Fig.2.(b) we have shown the dependence of the energy on the ‘magnitude’ $\Delta_0$, 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 $h = 0.95$ shows an absolute minimum at $q = (0, \pi/3)$.

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 and Larkin and Ovchinnikov, and confirmed by several later studies, we find that a $\Delta_i$ 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 $\mu$ as the fermion density increases from zero towards half filling. In the PPFL, as the name suggests, there are still minority carriers. The detailed nature of the LO phases will be discussed elsewhere.
B. Overview of thermal phase diagram

Mean field theory for $s$-wave superconductors in a magnetic field indicate that (in the continuum case) the SC to normal 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.\(^{38,39}\) 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 the continuum limit. Additionally, the specific prediction of $T_c$, etc, is valid only in the weak coupling limit where fluctuation effects beyond mean field are weak.

In the presence of an underlying lattice, even mean field theory suggests that there is 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.

As already discussed in the context of Fig.1, the Monte Carlo phase diagram shows that fluctuation effects significantly suppress $T_c$. The heating and cooling runs in Fig.4 indicate that apart from $T_c$ suppression the MC also reveals the presence of deep metastable LO phases (where the true ground state is at $q = (0, 0)$), and the state that one ends up with is path dependent.

Fig.4 shows the $h−T$ phase diagrams as evolved through a heating and a cooling cycle. The thermal transition from the SC to normal state is second order upto a field $h$, say, beyond which it becomes first order (with the ordered state still being at $q = (0, 0)$).

Over the regime of second order transition, heating the system from a variationally determined USF state leads to gradual loss of order, and slowly increasing magnetization, and a transition at a scale $T_c(h)$. We can call this an USF to BP crossover and then a transition to the disordered PPFL phase. In this field regime, when the system is subjected to cooling from a random high temperature state it shows a second order transition from PPFL to BP and then heads towards the USF state as $T \rightarrow 0$.

In the first order transition window, $h_1 < h < h_2$, 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. 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. As can be seen from the figure, at low and intermediate magnetic fields the heating and cooling cycles do not show a path dependence and an USF ground state is recovered on cooling. In the first order transition region, however, the USF ground state is not recovered on cooling and a finite magnetization ground state is seen.

2. Fluctuations

While the actual order in our lattice model 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 $\approx 1.5$.

In what follows we provide a detailed description of the thermal response of the imbalanced superconductor for three typical field regimes.
C. Low field response: the unpolarised superfluid

We begin the characterization with the low magnetic field regime ($0 < h < 0.3$) where the $q = 0$ superfluid state is realized as the stable ground state. Over most of the $T < T_c$ window the magnetization is negligible. As a representative of this regime we select $h = 0.10$. In Fig.6 we present (a) the superfluid structure factor $S_\Delta(q)$ and the (b) magnetic structure factor $S_m(q)$. At this field the SC structure factor loses its peaked feature as $T$ increases but the $q = (0, 0)$ peak in the magnetic structure factor remains $\lesssim 10^{-5}$ even at $T_c$. There are no finite $q$ features in the magnetic structure factor. The thermal transition is reversible and no thermal history effects show up.
D. Intermediate field: breached pair state

Next we consider the intermediate magnetic field regime of 0.3 < h < 0.7 by highlighting the response at h = 0.5. The ground state is still a homogeneous USF but now increase in T leads quickly to development of finite magnetization, and the up and down spin Fermi surfaces are no longer equal. ‘Unpaired’ fermions coexist with a q = (0, 0) condensate. This is a breached pair state.

We characterize this phase through its thermal evolution according to the various indicators, as depicted in Fig.7, where we have tracked MC snapshots of (a) the pairing amplitude $|\Delta(x,y)|$, (b) phase correlation $\cos(\theta_x - \theta_{x,y})$, (c) superfluid structure factor $S_\Delta(q)$, (d) magnetization $n(x,y)$, (e) magnetic structure factor $S_m(q)$, and (f) number density $n(x,y)$.

With the increase in temperature MC snapshots indicate that the $|\Delta(x,y)|$ becomes inhomogeneous (although a thermal average would be homogeneous again), and the phases begin to decohere. The first row shows the behavior of $|\Delta|$ the second row shows the phase correlations, and the third the SC structure factor. These are by themselves not very different from what one observes at weak field. It is row 4 that shows the new feature where between $T = 0.08t$ and $0.15t$ one observes the emergence of significant magnetization in 'clumps'. The magnetization, crudely, follows a pattern that is spatially complementary to the SC order. The local magnetization can reach a value $\sim 0.4$ even for $T < T_c$ (the system average however is much smaller). The 5th row shows the magnetic structure factor, essentially a diffuse peak around $q = (0,0)$, while the last row shows the density profile (almost homogeneous).

We have calculate the momentum occupation number $n_\sigma(k) = \langle c_{\sigma k}^{\dagger} c_{\sigma k} \rangle$. In Fig.8 we have shown $n_{\uparrow}(k)$ and $n_{\downarrow}(k)$ at $h = 0.50$ 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. At $T \sim 0.13t \sim T_c$ (not shown here) we note a visible difference between the two Fermi surfaces.

E. High field: appearance of metastable FFLO states

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

In Fig.9 we have plotted the superfluid and magnetic structure factors pertaining to the heating and the cooling cycles at different temperatures. During the heating cycle the system evolves from a $q = (0,0)$ USF state at $T = 0$ to a finite $T$ BP state, but on first order transition to the normal state it shows prominent fluctuations at finite $q!$

This peak in the superfluid structure factor at $T$ just above $T_c$ is suggestive of a metastable LO state. At higher $T$ this finite $q$ feature is replaced by a diffuse peak around the origin. The magnetic structure factor is dominated by the $q = (0,0)$ feature (i.e the finite magnetization) and additional finite $q$ features are hard to resolve.

The situation is dramatically different when one cools down the system from high temperature. The system encounters similar $q \neq 0$ fluctuations but instead of transitioning 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. The magnetic structure factor also demonstrates weak subsidiary peaks at $q \neq 0$ along with the prominent $q = 0$ peak at the lowest temperature probed. We show the real space pattern corresponding to this state later.

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 size mismatch between the up and down Fermi surfaces with temperature one can also see the modification in the Fermi surface shape at the low temperature at the end of the cooling cycle. An ideal LO ground state with uniaxial modulation leads to a Fermi surface that is anisotropic and we will compare our MC based Fermi surface to that generated from such an ideal state.

In Fig.10 we present the $T$ dependence of $n_\sigma(k)$. The cooling cycle shows signature of the weak metastable LO phase at the low temperature. It can be seen that at the lowest temperature where a modulated superfluid state is realized, the corresponding Fermi surfaces show directional anisotropy. The rise in temperature wipes out this anisotropy.

What does this metastable LO state look like in real space?

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**Fig. 8.** Color online: Thermal evolution of the momentum occupation number $n_\sigma(k)$ at $h = 0.50$.  

**Fig. 9.** The new feature where between $T = 0.08t$ and $0.15t$ one observes the emergence of significant magnetization in 'clumps'. The magnetization, crudely, follows a pattern that is spatially complementary to the SC order. The local magnetization can reach a value $\sim 0.4$ even for $T < T_c$ (the system average however is much smaller). The 5th row shows the magnetic structure factor, essentially a diffuse peak around $q = (0,0)$, while the last row shows the density profile (almost homogeneous).
FIG. 9. Color online: Thermal evolution of the superfluid ($S_{\Delta}(q)$) and magnetic ($S_m(q)$) structure factor at $h = 0.80$, through the heating and cooling cycles.

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 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. Thus, a node in the superfluid order parameter correspond to a peak in the magnetic order parameter in this system.

Before we end this section we show the momentum occupation number $n_\sigma(k)$ in presence of an ideal, axially modulated LO state. An weaker variant of the same has been observed and presented in Fig.10. Fig.12 shows the anisotropic deformation of the Fermi surfaces in presence of an underlying modulated superfluid state, even more prominently.

IV. DISCUSSION

Having finished the presentation of our results we need to touch upon the following topics, notably, the reliability/limitations of our results, a conceptual framework for understanding the numerical data, the relevance of these ‘strong coupling’ results to experiments, and the wider possibilities of our method in exploring imbalanced superfluids in other situations.

A. Numerical method: limitations and benchmarks

The primary numerical technique we use is a Monte Carlo implementation of a ‘single field’ static auxiliary field decomposition of the A2DHM. The ‘single field’ and ‘static’ aspects bring in certain limitations, while size limitations of the MC introduce another source of error. We comment on these successively.

(i) The single field decomposition of the attractive Hubbard model using a pairing field is exact, as long as both spatial and temporal (quantum) fluctuations of this field are retained. Since we have dropped the time dependence our results in principle could be inaccurate at low temperature - where quantum rather than thermal fluctuations are more important. Thankfully, over the field regime that we have explored the system has simple $q = (0, 0)$ order so the quali-
FIG. 10. Color online: Momentum occupation numbers $n_\sigma(k)$ at different temperatures through the heating and the cooling cycle computed at $\hbar = 0.80$.

FIG. 11. Color online: Spatial maps characterizing the metastable LO state through (a) Order parameter amplitude, (b) Phase correlation, (c) Magnetization and (d) Number density distribution.

The tentative nature of our results should be valid even at low $T$. At high $T$, the method should anyway work well since the finite Matsubara modes $\Omega_m$ are well separated from the $\Omega_m = 0$ (static) mode that we retain.

(ii) A single field decomposition that is static cannot in general capture all possible mean field states. In particular when the FFLO state becomes relevant both the magnetic and density channels become relevant. We find that even in the FFLO window the density is almost homogeneous so an auxiliary density field is superfluous. The presence of an additional magnetic channel may make a quantitative difference to our results but should leave the primary features unaffected.

(iii) The MC implementation using the Bogolyubov-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 $T$ studies to mean field theory. We can access much larger size (upto $40 \times 40$, 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

FIG. 12. Color online: Momentum occupation function representative of an ideal striped LO state.
MC in the $h = 0$ problem earlier by comparing to full QMC\textsuperscript{58}.

(iv) For the variational calculations we have gone upto size $48 \times 48$ but found it difficult to access FFLO phases when $U \lesssim 2t$. Mostly we have used $L = 24$ variational minima as the starting point for MC heating and these states have consistently been energetically better than what we could obtain by MC cooling. However it is possible that ‘multimode’ FFLO solutions may have even lower energies but we have seen no trace of such phases from the MC.

B. Landau-Ginzburg framework

While our MC results indicate that MFT makes a poor prediction of the $T_c$ in the strong coupling problem, and would miss issues of metastability, it is still useful to put up a Landau framework for qualitatively understanding our results. In the weak coupling limit the Landau-Ginzburg theory could have been systematically derived\textsuperscript{58,59}, here they serve as a phenomenological construct.

The weak coupling form suggested by Casalbuoni \textit{et al.}\textsuperscript{59} for the superfluid in the presence of a magnetic field, is:

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

This complicated form of the functional, 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 standard functional involving only $\alpha$, $\beta$ and $\epsilon$, we have $\beta > 0$ and 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\textsuperscript{58,59}. 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 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 phase fluctuations.

This phenomenology by itself does not indicate the regime over which a metastable LO state may exist. We plan to map that out from the numerics and suggest a more comprehensive Landau framework in the near future.

C. Connection with experiments

The possibility of an unusual superconducting state is suggested from thermodynamic properties viz. the specific heat\textsuperscript{20} and magnetization measurements\textsuperscript{10,19} in CeCoIn$_5$. The specific heat measurements revealed the occurrence of a second thermal transition at low $T$, speculated to lead to a finite momentum superfluid phase. Similar results have been seen also in the $C_V$ of the organic superconductor $\kappa$-(BEDT-TTF)$_2$Cu(NCS)$_2$\textsuperscript{58}. Our $h - T$ phase diagram is more akin to what one observes in the 115 family when the magnetic field is applied perpendicular to the $ab$ plane. While we have direct signatures of the magnetic character and superfluidity we plan to compute the $C_V(T,h)$ as well to compare with these experiments in the ‘BP window’.

Nuclear magnetic resonance (NMR) studies have argued that significant difference between the relaxation rate in the normal state, the ‘BCS state’ and the unusual phase suggests that the unusual state indeed has FFLO modulation\textsuperscript{58}. Moreover, Knight shift measurements carried out on CeCoIn$_5$ reveal the existence of additional peak like features in the NMR spectrum in the high magnetic field regime and at low temperature\textsuperscript{23}. It is suggested that these additional peaks are a consequence of the spatially modulated nature of the underlying superfluid state\textsuperscript{58}. Since the NMR relaxation rate can be related to the fermion DOS we can compare the predictions based on our ongoing spectral calculations to the measured rates.

A key experimental probe to understand the magnetic character of the superfluid is neutron scattering. Measurements\textsuperscript{16,20} on the 115 compound suggest a finite momentum magnetic order in the superfluid state. Our computation, in the cooling run at $h = 0.8$ finds similar signatures, arising from a metastable LO state. We will establish a quantitative connection between the local magnetisation and the local $\Delta$, in forthcoming papers.

Finally, a few comments about possible signatures of amplitude and phase fluctuations in the strong coupling system and their impact on field dependent spectral properties. An important prediction in this regard is the existence of pseudogap in the normal state of the system. Since, CeCoIn$_5$ and unitary cold atomic gas are both at strong coupling it would be very interesting to explore the presence of a pseudogap in these systems, and the field dependence of the same. Experimentally, the presence of pseudogap has been realized in cold atomic systems\textsuperscript{61}. Moreover, it has also been suggested that in presence of an imbalance the pseudogap undergoes progressive suppression with increasing magnetic field\textsuperscript{62,63}. We can readily access dynamical properties in the normal state and are working to establish the field dependence of the pseudogap in our model.

D. 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
Finally, cold Fermi gases involve a trapping potential and a non trivial spatial dependence of the region where the field 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.

A natural extension of the present method, involving a 'two field' decomposition, can handle the effect of disorder on the FFLO state, including the thermal effects which are in general difficult to access.

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V. CONCLUSION

We have used a real space numerical technique to study the behavior of a Pauli limited superconductor in the coupling regime corresponding to the peak $T_c$ in the BCS to BEC crossover window, in the presence of a Zeeman field. The normal Fermi system undergoes a second order phase transition to a homogeneous superfluid at moderate fields, but the state has strong spontaneous fluctuations of the local magnetization and superconducting order parameter. At stronger fields the thermal transition changes to first order and while the true ordered state should be the $q = 0$ superconductor we see signatures of a deep metastable FFLO state in which the system gets trapped. At even higher fields a genuine FFLO ground state is obtained. We provide detailed spatial maps of the system, the neutron measurable structure factor and momentum distribution functions.

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