Pauli limited d-wave superconductors: quantum breached pair phase and thermal transitions

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Abstract
We report a quantum phase transition in Pauli limited d-wave superconductors and give the mean field estimates of the associated quantum critical point. For a population imbalanced d-wave superconductor a stable ground state phase viz quantum breached pair phase has been identified which comprises of spatial coexistence of gapless superconductivity and nonzero magnetization. Based on the thermodynamic and quasiparticle indicators we for the first time analyze this phase, discuss the thermal behavior of Pauli limited d-wave superconductor, give accurate estimates of the thermal scales associated with such systems and map out the pseudogap regime. Our work shows that while the Pauli limited superconductors are known to exhibit exotic modulated superconducting phase at large imbalance of fermion populations; in the regime of weak imbalance an intriguing phase of competing orders is realized. We have established that rather than the superconducting pairing field, it is the average magnetization of the system that quantifies this quantum phase transition. Given that the existing Pauli limited superconductors possess unconventional pairing state symmetry of the superconducting order, our work promises to open up new avenues in the experimental research of these materials. We have also demonstrated an alternate scenario wherein the quantum breached pair phase is a natural outcome for a d-wave superconductor with unequal effective masses of the fermion species.

Keywords: superconductivity, Pauli paramagnetic superconductors, breached pair phase, pseudogap, quantum phase transition

(Some figures may appear in colour only in the online journal)

1. Introduction
Superconductivity, in competition or coexistence with magnetic correlations has been a primary area of research in condensed matter physics, over the past few decades. While magnetism is usually considered to be detrimental towards the existence of superconducting order, there are examples of materials where magnetic correlations reside proximate to or in coexistence with conventional [1–7] or unconventional [8–17] superconducting orders. The fascinating phenomena of coexisting orders as observed in these materials is dictated by the precise tuning of the energy landscape, often carried out via external control parameters such as, doping, pressure etc [8–10, 18, 19].

An equally intriguing but relatively less explored phenomenon of coexisting superconducting and magnetic correlations is observed in Pauli limited superconductors. The Pauli limited superconductors are characterized by their loss of superconducting order via Pauli paramagnetic pair breaking effect, which originates from the Zeeman splitting of the single electron energy levels [20, 21]. When a superconducting pair undergoes Pauli paramagnetic pair breaking it gives rise to unpaired fermions in the system. In the presence of such unpaired fermions an uniform (zero momen-
tum paired) superconducting state is no longer stable, rather the superconducting pair acquires a finite momentum which shows up as spatial modulation in the superconducting order. The unpaired fermions coexist with such spatially modulated superconducting state giving rise to what is now well known as the Fulde–Ferrell–Larkin–Ovchinnikov (FFLO) superconductivity [22, 23]. Pauli limited superconductivity has been realized both in solid state (e.g. CeCoIn5 [24–33], κ-BEDT [34–41], KFe2As2 [42–44] etc) as well as in ultracold atomic gas [45–48] systems. The central requirement for realizing Pauli limited superconductivity is the creation of an imbalance in the population of the fermionic species and thus a Fermi surface mismatch, via an applied Zeeman field in solid state systems or by loading different populations of the fermionic species in optical lattice in ultracold atomic gas set ups. While much attention has been paid to the FFLO phase over the past few years [24–44], another exotic phase of the Pauli limited superconductors exhibiting spatial coexistence of superconductivity and non zero magnetization, remains almost unexplored. The said phase is known as the ‘breached pair’ (BP) and corresponds to a situation where the imbalance in fermionic population is not strong enough to give rise to a FFLO phase but is sufficient to give rise to a Fermi surface mismatch [49–51]. The issue of the BP phase was first raised decades ago by Sarma [52] in his seminal work, where he discussed the possibility of self consistent mean field solution with gapless mode, in s-wave superconductors, in presence of an applied magnetic field. However, he found that such a phase if it exists would be energetically unfavorable as compared to the uniform superfluid (BCS) phase.

Advent of ultracold atomic gas experiments brought renewed interest in the physics of the BP phase. Through detailed analytic calculations it was demonstrated by Liu and Wilczek [53–55] that while for an imbalanced Fermi system the usual single band Hubbard model with on site interactions between the fermion species does not allow the BP phase to be a stable ground state, the same is indeed possible under non trivial circumstances such as, (i) imbalance in fermion effective masses in presence of contact interaction between them, (ii) momentum dependent interaction, (iii) same species repulsion etc [53–55]. It was further shown that for suitable choice of parameters a mass imbalanced s-wave superconductor hosts the BP phase as a stable ground state, which undergoes a second order quantum phase transition to the uniform superconducting phase as a function of decreasing Zeeman field [53]. This transition was said to belong to the class of topological Lifshitz transitions in the sense that the Fermi surface topology changes across this transition [56]. Note that this topological transition does not involve the change in any topological invariant. The fate of the BP phase in an imbalanced unconventional (non s-wave) superconductor however continues to remain an open question till date, in spite of almost all the known Pauli limited superconductors being unconventional in their pairing state symmetry.

A sufficient volume of literature has already been devoted to theoretically capture the physics of FFLO phase in the strong imbalance regime of Pauli limited nodal (d-wave) superconductors [57–64]. In the present paper we focus on the regime of weak population imbalance in such superconductors and for the first time demonstrate that the BP phase is a stable ground state over a significant regime of population imbalance in Pauli limited d-wave superconductors. We refer this ground state BP phase as the ‘quantum breached pair’ (QBP) phase and establish that this phase comprises of zero-momentum gapless superconductivity and nonzero magnetization, in coexistence. A second order quantum phase transition takes place between the QBP and unmagnetized d-wave superconductor (USC) phases, however, there is no explicit symmetry breaking across this phase transition. We emphasize that the superconducting pairing field is not a suitable order parameter when it comes to quantifying the phase transition between QBP and USC phases, as the pairing field remains unchanged across this transition. The phase transition between the QBP and USC phases is rather characterized by an alternative order parameter viz magnetization ($m_i$). As we demonstrate in the following sections, the ground state phases of the Pauli limited d-wave superconductor are categorized based on the, (i) superconducting pairing field ($\Delta_{ij}$), (ii) single particle density of states at the Fermi level ($N(0)$) and (iii) magnetization ($m_i$) as, (a) USC ($\Delta_{ij}(q = 0) \neq 0$, $N(0) = 0$, $m_i = 0$), (b) QBP ($\Delta_{ij}(q = 0) \neq 0$, $N(0) \neq 0$, $m_i \neq 0$), (c) FFLO ($\Delta_{ij}(q \neq 0) \neq 0$, $N(0) \neq 0$, $m_i \neq 0$) and (d) partially polarized Fermi liquid (PPLF) ($\Delta_{ij} = 0$, $N(0) \neq 0$, $m_i \neq 0$), where, $q$ corresponds to the superconducting pairing momentum.

Our real space approach to the problem enables us to identify and map out spatial coexistence of gapless d-wave superconducting pairing and nonzero magnetization, characteristic to the QBP phase. Apart from identifying the phase transitions at the ground state, the merit of this work rests in tracking the thermal evolution of these phases using a non perturbative numerical technique, mapping out the relevant thermal scales associated with the system and demonstrating that the QBP phase smoothly crosses over to its classical counterpart with increasing temperature. It must be noted that within the premises of lattice fermion models the existing works addressing the thermal physics of the Pauli limited d-wave superconductors are limited to mean field theory (MFT) [63, 64] which are known to significantly overestimate the thermal scales in the interaction regimes away from the weak coupling limit [49, 65]. The unconventional d-wave superconductors are established to be in the regime of intermediate coupling, which renders the MFT unsuitable to address the thermal behavior of these systems. Our technique takes into account the thermal (spatial) fluctuations of the pairing field at all orders and not just the saddle point fluctuations. Consequently, it is well suited to capture the thermal scales associated with the system accurately and gets progressively accurate with increasing temperature. As $T \rightarrow 0$, the thermal fluctuations die out and our approach becomes akin to the MFT at the ground state. In this spirit the quantum phase transition discussed in this work is basically the mean field estimate of the same. While we do
not expect any qualitative change in our ground state results via inclusion of quantum fluctuations, quantitative shifts in the ground state phase boundaries are possible.

While we discuss our results in the following sections, we highlight our principal observations here: (a) we for the first time demonstrate that the breached pair phase is a stable ground state of the Pauli limited d-wave superconductor. We refer to this ground state breached pair phase as QBP and show that it comprises of spatial coexistence of zero-momentum gapless superconducting order and nonzero magnetization. (b) By tuning the applied Zeeman field (or imbalance in the populations of the fermionic species) a second order quantum phase transition can be realized between the USC and QBP phases, quantified by the evolution of magnetization.

In this work, we give the mean field estimate of this quantum phase transition. (c) Based on the thermodynamic and quasiparticle signatures we track the thermal evolution of the ground state phases and map out the relevant thermal scales; we demonstrate that short range superconducting pair correlations survive up to temperatures $T \gg T_c$ and gives rise to the 'pseudogap' regime. (d) We show that for a d-wave superconductor with imbalance in the effective masses of the fermion species, a QBP phase is realized in the absence of any imbalance in population. The thermal phase diagram of such a system reveals the existence of ‘species dependent’ pseudogap scales which should be experimentally detectable.

The rest of the paper is organized as follows. In section 2 we discuss the model and the numerical technique used in this work, as well as the indicators used to characterize the phases, section 3 comprises of the main results of this work and their analysis. We discuss the mass imbalanced d-wave superconductors in section 4, and follow it up by drawing the conclusions of our work.

2. Model, method and indicators

In this section we sketch out the steps involved in studying the many body quantum Hamiltonian, discuss our choice of the parameters and the relevant indicators to characterize the phases of this system.

2.1. Model

Our starting Hamiltonian corresponds to a two-dimensional (2D) square lattice with nearest neighbor attractive interaction between the fermions, in presence of a Zeeman field, and reads as,

$$H = - \sum_{\langle ij \rangle, \sigma} t_{ij} \psi_i^\dagger \psi_j - U \sum_i n_i^\dagger n_i - \mu \sum_i n_i^\dagger n_i - h \sum_i \sigma_i \hat{n}_i$$

where, $t_{ij}$ corresponds to the hopping parameter such that $t_{ij} = t = 1$ for the nearest neighbors and is zero otherwise, $|U| > 0$ corresponds to the nearest neighbor attractive interaction between the fermions, the net number density of the fermions in the system is maintained through the chemical potential $\mu = (1/2)(\mu_\uparrow + \mu_\downarrow)$, while $h = (1/2)(\mu_\uparrow - \mu_\downarrow)$ corresponds to the effective Zeeman field.

2.2. Method

The partition function is a functional integral over the Grassman fields $\psi_{i\sigma}(\tau)$ and $\bar{\psi}_{i\sigma}(\tau)$

$$Z = \int D\psi D\bar{\psi} e^{-\frac{\beta}{\hbar} \int_0^\infty d\tau \mathcal{L}(\tau)}$$

$$\mathcal{L}(\tau) = \mathcal{L}_0(\tau) + \mathcal{L}_U(\tau)$$

$$\mathcal{L}_0(\tau) = \sum_{\langle ij \rangle, \sigma} \left\{ \bar{\psi}_{i\sigma} \left[ (\partial_\tau - \mu) \delta_{ij} + t_{ij} \right] \psi_{j\sigma} \right\}$$

$$\mathcal{L}_U(\tau) = -U \sum_{\langle ij \rangle, \sigma} \bar{\psi}_{i\sigma} \psi_{i\sigma} \bar{\psi}_{j\sigma} \psi_{j\sigma}$$

where, $\beta$ is the inverse temperature. Our strategy is to decompose the interaction in terms of the bosonic auxiliary d-wave pairing singlet $\Delta(\tau)$ using Hubbard–Stratonovich transformation [66, 67]. Here $\bar{i}$ and $\tau$ refers to the spatial and imaginary time dependence of the pairing field, respectively. In terms of the Matsubara frequency $\Omega_n = \frac{2\pi n}{T}$ the pairing field reads as, $\Delta_{\Omega_n}$, where $T$ is temperature. This leads to

$$Z = \int D\psi D\bar{\psi} D\Delta D\Delta^* e^{-\frac{\beta}{\hbar} \int_0^\infty d\tau \mathcal{L}(\tau)}$$

$$\mathcal{L}(\tau) = \mathcal{L}_0(\tau) + \mathcal{L}_U(\tau) + \mathcal{L}_{\Delta}(\tau)$$

$$\mathcal{L}_0(\tau) = \sum_{\langle ij \rangle, \sigma} \left\{ \bar{\psi}_{i\sigma} \left[ (\partial_\tau - \mu) \delta_{ij} + t_{ij} \right] \psi_{j\sigma} \right\}$$

$$\mathcal{L}_U(\tau) = -U \sum_{\langle i \neq j \rangle} \bar{\psi}_{i\sigma} \psi_{i\sigma} \bar{\psi}_{j\sigma} \psi_{j\sigma} + h.c.$$

$$\mathcal{L}_{\Delta}(\tau) = 4 \sum_{\langle i \neq j \rangle} \left| \frac{\Delta_{ij}^\dagger \Delta_{ij}}{|U|} \right|^2$$

Since the fermions are now quadratic, the $\int D\psi D\bar{\psi}$ integral can be performed to generate the effective action for the random background fields,

$$Z = \int D\Delta D\Delta^* e^{-S_{\text{eff}}[\Delta, \Delta^*]}$$

$$S_{\text{eff}} = \ln \text{Det}[\mathcal{G}^{-1} \{ \Delta, \Delta^* \}] + \int_0^\beta d\tau \mathcal{L}_{\Delta}(\tau)$$

where, $\mathcal{G}$ is the electronic Green’s function in the $\{ \Delta \}$ background. There are several options now, (i) quantum Monte Carlo retains the full ‘$i, \Omega_n$’ dependence of $\Delta$ computing $\ln \text{Det}[\mathcal{G}^{-1} \{ \Delta \}]$ iteratively for importance sampling. The approach is valid at all $T$, but does not readily yield real frequency spectra. (ii) Mean field theory (MFT) is time independent, neglects the phase fluctuations completely but can handle spatial inhomogeneity in amplitude of the pairing field. Thus, $\Delta_{\langle i \Omega_n \rangle} \rightarrow |\Delta_{\Omega_n}|$. When the mean field order parameter vanishes at high temperature the theory trivializes. (iii) Dynamical mean field theory (DMFT) retains the full dynamics but keeps $\Delta$ at effectively one site, i.e., $\Delta_{\langle i \Omega_n \rangle} \rightarrow \Delta(\Omega_n)$. This is exact when dimensionality $D \rightarrow \infty$. (iv) Static path approximation (SPA) approach retains the full spatial dependence in $\Delta$ but keeps only the $\Omega_n = 0$ mode,
i.e., $\Delta(\Omega_0) \rightarrow \Delta$. It thus includes classical fluctuations of arbitrary magnitude but no quantum ($\Omega_0 \neq 0$) fluctuations. One may consider different temperature regimes. (1) $T = 0$: since classical fluctuations die off at $T = 0$, SPA reduces to standard Bogoliubov–de-Gennes (BdG) MFT. (2) At $T \neq 0$ we consider not just the saddle-point configuration but all configurations. 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 $\Omega_0 = 0$ mode dominates the exact partition function, the SPA approach becomes exact as $T \rightarrow \infty$. Consequently, it is akin to the MFT only at $T = 0$ but captures the thermal physics of the system accurately.

We choose the last option (SPA) as our numerical technique. The resulting superconducting Hamiltonian reads as,

$$
H_{\text{SC}} = -\sum_{\langle ij \rangle, \sigma} t_{ij} \left( c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right) + \sum_{\langle ij \rangle} \Delta_{ij} \left( c_{i\uparrow}^\dagger c_{j\downarrow} + c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger \right) + \text{h.c.} - \mu \sum_{\langle ij \rangle} \hat{n}_{i\sigma} - h \sum_{\langle ij \rangle} \sigma_i \hat{n}_{i\sigma} + 4 \sum_{\langle ij \rangle} \left| \Delta_{ij} \right|^2 / |U| 
$$

(5)

where, the last term of $H_{\text{SC}}$ corresponds to the classical stiffness cost associated with the auxiliary field. Here, the $d$-wave singlet is defined as $\Delta_{ij} = (c_{i\uparrow} c_{j\downarrow} + c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger)$. It can further be expressed as $\Delta_{ij} = |\Delta_{ij}| e^{i\phi_{ij}}$, where $\phi_{ij} \in \{ \phi_{ij}, \phi_{ij}^\dagger \}$ is the direction dependent phase of the complex pairing field and $|\Delta_{ij}|$ is the pairing field amplitude, considered to be isotropic in the $xy$-plane. Note that in the usual mean field approach to $H_{\text{SC}}$ the superconducting gap function $\Delta_{ij}$ is assumed to be a real number, but here we retain the degrees of freedom associated with the pairing fields and amplitudes. The system can thus be envisioned as free fermions moving on a random background of $\Delta_{ij}$.

The background field $\Delta_{ij}$ obeys the Boltzmann distribution,

$$
P(\Delta_{ij}) \propto T_{\text{rel}} e^{-|\Delta_{ij}|} 
$$

(6)

which is connected to the free energy of the system. For large and random $\Delta_{ij}$ the trace is taken numerically. We generate the random background of $\{\Delta_{ij}\}$ by using Monte Carlo, diagonalizing $H_{\text{SC}}$ for each attempted update of $\Delta_{ij}$. The relevant fermionic correlators are computed on the optimized configurations at different temperatures. Evidently, the technique is computationally expensive. The computation cost is cut down by using a traveling cluster approximation (TCA), wherein instead of diagonalizing $H_{\text{SC}}$ for each attempted update of the auxiliary field, we diagonalize a smaller cluster surrounding the update site. Both SPA and TCA have been extensively benchmarked and used for several quantum many body systems. [49, 68–70].

**Variational ground state:**

Even for a selected interaction strength the ground state parameter space is huge in terms of $\mu - h$. In order to get a handle on this parameter space we first carry out a mean field variational calculation for the ground state. In the spirit of MFT we stripe the pairing (auxiliary) field $\Delta_{ij}$ off all fluctuations such that $|\Delta|$ is now a real number. For a selected $\mu - h$ cross section we fix the relative phase between the $x$- and $y$-components of the superconducting phase $\phi^{\text{rel}} = \phi_x - \phi_y$, such that $\phi^{\text{rel}}$ can take discrete values as, $0, \pi/4, \pi/2, \ldots, \pi$ etc. For each such choice of the relative phase, $|\Delta|$ is optimized so as to obtain the lowest energy configuration for the selected $\mu - h$ cross section. The process is carried out for different $\mu - h$ cross sections such that one obtains the optimized $|\Delta|$ and $\phi^{\text{rel}}$ corresponding to the minimum energy configuration. The optimized $\Delta \in \{ |\Delta|, \phi^{\text{rel}} \}$ configurations are then used to compute the magnetization of the system for the corresponding $\mu - h$ cross section. The ground state phase diagram is mapped out based on these quantities in the $\mu - h$ plane.

**Monte Carlo ground state:**

The ground state at different $\mu - h$ cross sections are verified by using Monte Carlo simulations and the results are found to be in excellent agreement with those obtained via the variational calculations. Within the framework of Monte Carlo protocol the system is cooled down from a random high temperature phase and is allowed to attain the lowest energy state at each temperature. Such unrestricted cooling allows us to retain the spatial fluctuations of all orders in the pairing field, which progressively dies out as the system approaches the ground state. For the Monte Carlo simulations the (a) average superconducting phase correlation ($\langle \phi_x^\sigma, \phi_y^\sigma \rangle$) and (b) the average magnetization ($m$) are used as suitable indicators to map out the ground state.

### 2.3. Parameters and indicators

In order to study the thermal behavior of the system we select a particular cross section of the ground state phase diagram, such that the net chemical potential is selected to be $\mu = -0.2t$ corresponding to a total fermionic number density of $n \approx 0.94$. The interaction is selected to be $|U| = 4t$ corresponding to the intermediate interaction regime, which is known to be suitable for realizing $d$-wave superconductivity [8, 71]. Note that since the system belongs to the intermediate regime of interaction ($|U| \gg t$) a perturbative approach (such as MFT) breaks down at finite temperatures and the fluctuations dominate. One thus need to resort to non perturbative techniques such as the one discussed in this paper to take into account the effects of fluctuations. Unlike the assumption of the MFT, superconductivity in this intermediate regime of interaction is lost at high temperatures via the loss of long range phase coherence of the superconducting pairing field rather than the suppression of the pairing field amplitude. The consequence are the pre-formed pairs at $T \neq 0$ leading to the pseudogap phase in the $d$-wave superconductors. Our estimates based on the variational as well as Monte Carlo calculations suggest a $d_{2\pm 2\pm}$ pairing state symmetry with the relative phase between the pairing field components being $\phi^{\text{rel}} = \pi$, in this parameter regime, in agreement with the existing literature [71]. The results presented in this paper correspond to a system size of $N = L \times L = 24 \times 24$, unless specified otherwise. The effect of the finite system size is

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discussed toward the end of the paper. We have analyzed our results based on the thermodynamic and quasiparticle indicators defined as below,

Site resolved and averaged magnetization:

\[ m_i = n_{\uparrow i} - n_{\downarrow i} \]

\[ m = \frac{1}{N} \sum_i (n_{\uparrow i} - n_{\downarrow i}) \]

Average phase correlation of pairing field:

\[ \phi^{xx} = \frac{1}{N} \sum_{i \neq j} \langle e^{i \omega_0}, e^{-i \omega_0} \rangle \]

\[ \phi^{xy} = \frac{1}{N} \sum_{i \neq j} \langle e^{i \omega_0}, e^{-i \omega_0} \rangle \]

Mixed phase correlation of pairing field:

\[ \phi^{xy} = \frac{1}{N} \sum_{i \neq j} \langle e^{i \omega_0}, e^{-i \omega_0} \rangle \]

Spin resolved single particle fermionic density of states (DOS):

\[ N_{\uparrow}(\omega) = \frac{1}{N} \sum_i |u_n^\uparrow|^2 \delta(\omega - E_n) \]

\[ N_{\downarrow}(\omega) = \frac{1}{N} \sum_i |v_n^\downarrow|^2 \delta(\omega + E_n) \]

Spectral lineshapes:

\[ A_\sigma(k, \omega) = -(1/\pi) \text{Im} G_\sigma(k, \omega) \]

Fermion occupation number:

\[ n_\sigma(k) = \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle \]

Distribution of pairing field amplitude:

\[ P(|\Delta_{ij}|) = \sum_{i \neq j} \delta(|\Delta| - |\Delta_{ij}|) \]

where, \( i \) and \( j \) correspond to two different sites on the lattice. \((\cdot, \cdot)\) correspond to thermal average and \( \sigma \) is the spin label. \( n_{\sigma} \) are the number of the individual fermionic species, while \( u_n^\sigma \) and \( v_n^\sigma \) are Bogoliubov eigenfunctions corresponding to the eigenvalue \( E_n \). \( n_\sigma(k) \) is the Fourier transform of the single particle Green’s function. \( G(k, \omega) = \lim_{\hbar \to 0} G(k, i\omega_n) \mid_{\omega_n = \omega + i\delta} \)

where \( G(k, i\omega_n) \) is the imaginary frequency transform of \( \langle c_k(\tau)c_{k}^\dagger(0) \rangle \).

3. Results

Figure 1 constitutes one of the main results of this work, wherein we show the magnetization–temperature \((m – T)\) phase diagram of Pauli limited d-wave superconductor. The highlight of this phase diagram is the \( T = 0 \) weak magnetization regime marked as the quantum breached pair (QBP) phase. Finite temperature leads the QBP phase to undergo smooth crossover to its classical counterpart and over a large part of the phase diagram the BP phase undergoes second order transition to partially polarized Fermi liquid (PPFL). The strong magnetization regime of the phase diagram belongs to the FFLO phase characterized by finite momentum superconducting pairing and first order thermal transition to PPFL phase. Sandwiched between the two is the unstable (phase separated) regime where the BP phase undergoes weak first order thermal transition to PPFL phase.

The phase diagram shows that the QBP phase undergoes a quantum phase transition (QPT) to the USC phase, as a function of decreasing magnetization. The mechanism which drives the QPT is the Pauli paramagnetic pair breaking and generation of low energy gapless excitation, which hosts unpaired fermions. For a population imbalanced s-wave superconductor the gapless superconducting state is realized beyond a critical Zeeman field \( h \geq h_{c2} \) (or population imbalance). Concomitant to this phenomena the system becomes unstable towards \( q = 0 \) superconducting pairing and undergoes transition to the FFLO phase. On the contrary, for a nodal d-wave superconductor, the critical field for paramagnetic pair breaking and generation of gapless superconducting states is different from the one \( (h_{c2}, \text{say}) \) at which the system undergoes transition to FFLO state. Over the regime \( h_{c1} \leq h \leq h_{c2} \) the system thus hosts a coexistent QBP phase comprising of ‘gapless’ \( q = 0 \) superconducting state and non zero magnetization. In what follows, we establish and analyze this phase diagram based on the thermodynamic and quasiparticle indicators.

3.1. Ground state

We begin our discussion of the ground state by showing the energy landscape of the system. Given the huge parameter space we are in the energy optimization process (via varia-
tional calculation) involves multiple steps which are summed up in figure 2 and are discussed below,

(a) As the first step we consider the population balanced system \((h = 0.0t)\) at a fixed \(\mu = -0.2t\) and optimize the energy at different interactions \(U/t\) over \(|\Delta|\) and \(\phi^{\text{rel}}\) (in the absence of fluctuations both these parameters are real numbers). The results obtained via this optimization is shown in figure 2(a) and we note that for weaker interactions the relative phase corresponding to the minimum energy is \(\pi\) showing a d\(_{2\_2\_2}\) pairing state symmetry of the superconducting state, in agreement with the existing literature \([71]\). Increasing \(U\) shifts the relative phase minima to a lower value such that for \(7t \leq U < 9t\) a d\(_{1\_2\_2}\) + id\(_{1\_2}\) pairing state with \(\phi^{\text{rel}} = 2\pi/3\) is stabilized. At still stronger interactions \(\phi^{\text{rel}}\) shifts to even lower values. The results discussed in this paper corresponds to \(|U| = 4t\) and our energy minimization suggests a d\(_{2\_2\_2}\) pairing state as the stable ground state at this interaction. For the minimum energy the corresponding value of \(|\Delta|\) (not shown in this figure) gives the pairing field amplitude. The inset of figure 2(a) sums up the change in \(\phi^{\text{rel}}\) w.r.t. \(U/t\).

(b) We next select the particular interaction \(|U| = 4t\), introduce population imbalance via the Zeeman field \(h/t\) and optimize the energy over \(|\Delta|, (\cos(qx))\) and \(\phi^{\text{rel}}\), where \(q\) corresponds to the pairing momentum; for the uniform d-wave superconductor \(q = 0\). Note that there are now three variational parameters as \(|\Delta|, \phi^{\text{rel}}\) and \(q\). This is to verify whether the pairing state undergoes a change (in terms of \(\phi^{\text{rel}}\)) with the imbalance. We show our results in figure 2(b) as the change in energy w.r.t. \(h/t\) for selected \(\phi^{\text{rel}}\). At all values of \(h/t\) the minimum energy configuration clearly corresponds to the the relative phase \(\phi^{\text{rel}} = \pi\), at this interaction, suggesting that the pairing state symmetry of the superconducting state remains unaltered with population imbalance. This narrows down the parameter space to \(|U| = 4t, \mu = -0.2t, \phi^{\text{rel}} = \pi\) at different \(h/t\). The remaining task is to determine how the pairing field amplitude \(|\Delta|\) varies with \(h/t\) for this choice of the parameters. This would enable us to determine the phase boundary between the superconducting and non superconducting phases at the ground state. Additionally, one needs to keep track of the pairing momentum \(q\) so as to be able to determine the phase boundary between the uniform and non uniform (FFLO) superconducting phases.

(c) The minimization over \(|\Delta|\) and \(q\) is carried out over different choices of spatial modulations such as, \(\Delta_x \sim |\Delta| \cos(qx), \Delta_y \sim |\Delta| \cos(qx + y), \Delta_x \sim |\Delta| \cos(qx + y)\) etc. Since we are not discussing the FFLO phase in detail in this paper, we show the energy landscape for one such choice of \(\Delta_x\) at different \(h/t\), in figure 2(c). Note that for weak imbalance the \(|\Delta|\) corresponding to the minimum energy state does not undergo significant change with \(h/t\), larger \(h/t\) leads to the development of a weak minimum at smaller \(|\Delta|\) value indicating that population imbalance leads to suppression in the pairing field amplitude. This is expected because with increasing imbalance there are now lesser number of fermions which can undergo pairing.

(d) Finally in figure 2(d) we show how the pairing momentum \(q = \sqrt{q_x^2 + q_y^2}\) varies with the population imbalance. For \(h \geq 0.9t\) we note that the pairing momentum \(q\) picks up a non zero value indicating an FFLO state. Figures 2(c) and (d) together gives the phase boundary between the uniform and FFLO superconducting states.

The energy minimization process is carried out over different \(\mu - h\) cross sections so as to map out the ground state phase diagram. By computing the magnetization over the optimized configurations one can demarcate the regimes of coexisting superconducting order and non zero magnetization. The ground state obtained from variational calculations is confirmed by Monte Carlo simulation, wherein fluctuations are taken into account in the pairing field amplitude and phase, i.e. \(|\Delta| \rightarrow \Delta_0|\) and \(\phi^{\text{rel}} = \phi_q^{\text{rel}} - \phi_p^{\text{rel}}\), respectively.

We next proceed to analyze the ground state thus obtained, in terms of different indicators. Figure 3(a) shows the ground state phase diagram of the system in the \(\mu - h\) plane, as determined through Monte Carlo simulation at a selected interaction strength of \(|U| = 4t\). In the \(\mu - h\) plane the system hosts four different phases as, (i) unmagnetized d-wave superconductor (USC), (ii) coexistence, (iii) Fulde–Ferrell–Larkin–Ovchinnikov (FFLO) and (iv) partially polarized Fermi liquid (PPFL). The phases are demarcated by critical magnetic fields \(h_c1, h_c2\) and \(h_c3\), corresponding to a
second order phase transition from the USC to coexistence phase at \( h_{c1} \sim 0.2t \), a first order transition of coexistence to FFLO at \( h_{c2} \sim 0.9t \) and a second order transition from FFLO to PPFL phase at \( h_{c3} \sim 1.25t \), respectively. We note that the order of phase transition from the FFLO to PPFL phase is in agreement with the existing results [63]. The phase transition between the USC and coexistence phase, discussed for the first time in this paper, is of second order, as expected [53].

The indicators used to demarcate these phases are the \( x \)-component of the average phase correlation \( \phi^{xx} \) (the \( y \)-component of the phase correlation behaves identically) and the average magnetization \( m \). These indicators however do not give any information regarding the spectral behavior of the underlying state. Consequently, based solely on these indicators a distinction between the superconducting state being gapped or gapless cannot be made. The regime \( h_{c1} < h \leq h_{c2} \) is thus shown as the ‘coexistence’ phase. While both the USC (\( 0 < h \leq h_{c1} \)) and coexistence (\( h_{c1} < h \leq h_{c2} \)) phases comprise of \( q = 0 \) d-wave pairing, the distinction between the gapped and gapless superconductivity can be made via the single particle DOS, which we discuss next. A (nodal) gapped superconductor with finite magnetization would correspond to a phase separated state, while a gapless superconductor with finite magnetization corresponds to a QBP phase. While our calculations are carried out in the grand canonical ensemble we recast the phase diagram in the \( n - m \)-plane in figure 3(b). The USC phase now collapses to the \( x \)-axis, while the coexistence, FFLO and PPFL phases are demarcated by \( m_{c1} \) and \( m_{c2} \) corresponding to the critical magnetization. We choose a particular cross section of this phase diagram at \( \mu = -0.2t \) (\( n \approx 0.94 \)) to understand the physics of the system both at the ground state as well as at the finite temperatures. We have verified that the qualitative behavior of the system is independent of the choice of \( \mu \) (or \( n \)), except for very small filling. The Zeeman field regime being probed is \( h = [0:1.4] \) where \( h = [0:0.9] \) correspond to the ‘notional’ weak imbalance regime, where the superconducting state has \( q = 0 \) pairing.

In order to characterize the underlying superconducting state we next show the spin resolved single particle DOS at different Zeeman field, in figure 4. In the absence of any population imbalance the DOS corresponding to the two spin species are identical and centered around the Fermi level \( (\omega = 0) \), giving rise to a nodal gap. The \( d_{x^2-y^2} \) character of the pairing field is evident with \( N(\omega) \propto \omega \) as \( \omega \to 0 \). Increasing imbalance shifts the spin resolved DOS away from \( \omega = 0 \) with them being now centered around the shifted Fermi level \( \omega = \pm h \). However, an interesting behavior is observed at \( \omega = 0 \) where there is now an accumulation of finite spectral weight leading to a gapless superconducting state. The behavior of the DOS is in dramatic contrast with that of imbalanced s-wave superconductors where even though the DOS corresponding to the different spin species are centered around the shifted Fermi levels, the spectrum remains gapped and there are no low energy states at \( \omega = 0 \), unless the system hits the FFLO phase [49]. The coexistence phase shown in figure 3 thus hosts a gapless \( q = 0 \) superconducting phase along with a nonzero magnetization, characteristic to the QBP phase. The transition from the gapped to gapless superconducting phases is the signature of the quantum phase transition between the USC and QBP phases.

The information obtained from the thermodynamic and quasiparticle signatures is summed up in figure 5 which shows the ground state phase diagram at \( \mu = -0.2t \) and \( |U| = 4t \). The phase diagram shows only the USC and QBP phases and for the time being we ignore the \( q \neq 0 \) pairing state. There are three indicators based on which the phases are demarcated, along with the \( x \)-component of the average phase correlation \( \phi^{xx} \) and the average magnetization \( m \) we now show the inverse of the DOS at the Fermi level \((1/N(0)) \) which gives a measure of the energy gap \( (E_g \sim 1/N(0)) \). As \( N(0) \to \infty, E_g \to 0 \), i.e. a large spectral weight at the Fermi level correspond to a gapped superconducting state. Based on this indicator we show that for \( h \leq 0.2t \) the system is a gapped superconductor with zero magnetization corresponding to the USC phase. In the regime \( 0.2t < h \leq 0.85t \), \( 1/N(0) \) vanishes indicating a gapless phase, simultaneous non zero \( \phi^{xx} \) and \( m \) qualifies the phase to be a QBP. For \( h \geq 0.85t \), \( \phi^{xx} \) collapses to zero while \( m \) remains finite, suggesting a non superconducting PPFL phase.

Having mapped out the ground state phase diagram we next move on to a deeper analysis of these phases. We begin with the spin resolved momentum occupation number \( n_s(k) \) as a function of increasing Zeeman field, shown in figure 6. The momentum occupation number, which is one of the standard indicators to map out the underlying Fermi surface of the superconducting state, is the Fourier transform of the single particle Green’s function [72]. In the regime of balanced \((h = 0t)\) or very weakly imbalanced population the momentum occupation number corresponding to the two spin species are identical, i.e. they exhibit the usual Fermi type distribution corresponding to the d-wave superconducting state. Increasing imbalance leads to mismatch in this distribution and accumulation (or depletion) of weight at isolated \( k \)-points, along the nodal directions \((\pm \pi/2, \pm \pi/2)\), of the Brillouin
Figure 4. Zeeman field dependence of spin resolved fermionic density of states ($N_{\sigma}(\omega)$), at $T = 0$. The black (red) curves correspond to $N_{\uparrow}(\omega)$ ($N_{\downarrow}(\omega)$), respectively. Note the accumulation of spectral weight at the Fermi level ($\omega = 0$) with increasing field.

Figure 5. Ground state phase diagram at $\mu = -0.2t$ and $|U| = 4t$ as determined based on the indicators, (i) $x$-component of average superconducting phase correlation ($\phi^{xx}$), (ii) average magnetization ($m$) and (iii) inverse of DOS at the Fermi level ($1/N(0)$) (see text).

Figure 6. Zeeman field dependence of spin resolved fermionic occupation number ($n_{\sigma}(k)$), at $T = 0$. The $x$ and $y$-axes of the panels correspond to $k_x$ and $k_y$, respectively and the intensity of color shows the magnitude of $n_{\sigma}(k)$. Note that the mismatch in the Fermi surface is restricted at the $\{\pm \pi/2, \pm \pi/2\}$-$k$-points.

zone. The $n_{\sigma}(k)$ is thus an important quantity which gives evidence of the change in the 'notional' Fermi surface topology with population imbalance. In that spirit, $n_{\sigma}(k)$ indicates a Lifshitz like transition between the USC to QBP phases. Along the nodal directions the Fermi surfaces changes from being identical to disparate with increasing imbalance across this transition, which can be considered as a signature of the Lifshitz like transition [53, 56].

Figure 7 shows the real space signatures of the QBP phase as the spatial maps for a typical Monte Carlo configuration of superconducting pairing field and magnetization at selected Zeeman field cross sections. The rows in the figure correspond to three different quantities viz (i) amplitude of superconducting pairing field ($|\Delta_{ij}|$), (ii) correlation of the $x$-component of superconducting phase between a reference site and other sites of the lattice ($\cos(\phi_0 - \phi_i)$) and (iii) site resolved magnetization ($m_i$). At the lowest field shown in the figure the superconducting state is robust with nearly uniform pairing field amplitude and (quasi) long range phase coherence. On the other hand, magnetization is very weak ($\sim 0.1$) in this regime. With increasing Zeeman field isolated islands of depleted superconductivity emerges in the system, as characterized by regions with suppressed pairing field amplitude and phase correlation. The islands grow in size and begin to merge with each other as the field is increased further. Increase in spatial inhomogeneity promotes spectral weight accumulation at the Fermi level i.e. a gapless superconducting state. Interestingly, at these regions of depleted superconductivity the magnetization begins to gain weight as shown in the bottom row of figure 7. The snapshots reveal that over a regime of Zeeman field gapless superconductivity coexists with nonzero magnetization, characteristic to the QBP phase.

After establishing the ground state behavior of the system we now focus on the thermal evolution of the various phases. At the onset, we note that the thermal transition discussed in this paper are basically Berezinsky–Kosterlitz–Thouless (BKT) transitions, corresponding to algebraic decay of quasi long range order in two-dimensions.

3.2. Finite temperature

We show thermal evolution of the global indicators viz average superconducting phase correlations and average magnetization in figure 8. In panels (a)–(c) we show the field dependence of the average phase correlation components $\phi^{xx}$, $\phi^{yy}$ and $\phi^{xy}$ corresponding to the d-wave superconducting pairing field, across the USC and QBP regime, as the system evolves in temperature. Note that the superconducting state is fairly robust in the field regime under consideration, with a nonzero (indicated by the point of inflection of the curves) $T_c$. The system loses the (quasi) long range phase coherence at $T_c$, which
Depletion at isolated regions in space while the emergence of magnetization complements this depletion. Zeeman fields are presented next in figure 9. For $T$ magnetization at large transfer of spectral weight away from the (shifted) Fermi level. Increasing temperature leads to piling up of spectral weight and progressive closure of these gaps. Simultaneously, the coherence peaks at the gap edges flatten out via large transfer of spectral weight away from the (shifted) Fermi level.

The spin resolved DOS at different temperatures, at selected Zeeman fields are presented next in figure 9. For $h > 0$ the DOS at the ground state exhibits nodal gap at the shifted Fermi levels, increasing temperature leads to piling up of spectral weight and progressive closure of these gaps. Simultaneously, the coherence peaks at the gap edges flatten out via large transfer of spectral weight away from the (shifted) Fermi level, indicating the loss of (quasi) long range phase coherence. While the depletion of spectral weight at the shifted Fermi level is observed even at high temperatures owing to the correlation effects, we note that beyond a temperature, $T_{pg}$, say, the behavior of the gap closure becomes non monotonic. The temperature range $T_c < T < T_{pg}$ corresponds to the regime where short range superconducting pair correlations survive in the system even after the loss of (quasi) long range phase coherence and gives rise to the pseudogap phase. The figure demonstrates how the pseudogap scale undergoes progressive suppression with increasing imbalance in population.

Thermal evolution of the momentum resolved spectral line-shapes are presented next in figure 10, for a selected Zeeman field of $h = 0.6t$, which corresponds to the QBP phase at the ground state. The figure shows the lineshape $A_\uparrow(k, \omega)$ for the momentum trajectory $(0,0) \rightarrow (\pi,0) \rightarrow (\pi,\pi) \rightarrow (0,0)$, across the Brillouin zone. We note that at the lowest temperature prominent gap opens up along $(\pi/2,0) \rightarrow (\pi,0) \rightarrow (\pi,\pi/2)$. Progressive increase in temperature suppresses the gap and finally leads to its closure at $T \geq 1.25T_c$, where $T_c \sim 0.08t$. The behavior of $A_\uparrow(k,\omega)$ (not shown here) is similar to $A_\uparrow(k,\omega)$. Overall, in the nodal direction ($\pm \pi/2, \pm \pi/2$) the lineshape is characterized by a single peak which is roughly immune to thermal evolution, while there is opening of gap in the antinodal direction which undergoes progressive closure with temperature.

The real space signature is demonstrated next in figure 11 via the spatial maps. Once again we use (i) $|\Delta_0|$, (ii) $\cos(\phi_0^x - \phi_0^y)$, and (iii) $m_i$, as our indicators and track them as they evolve in temperature at $h = 0.6t$. Apart from the complementary spatial realization of superconducting pairing field and magnetization characteristic to the QBP phase at the lowest temperature, we note enhancement in spatial fragmentation of $|\Delta_0|$ with increasing temperature. The observation sets the thermal transition scale of the system. In figure 8(d) we present the thermal evolution of average magnetization at different Zeeman field. Increasing temperature leads to thermal pair breaking and gives rise to unpaired fermions, consequently, magnetization is larger at high temperatures. For $h \geq 0.2t$ the system is in QBP phase as indicated by non zero magnetization at $T = 0$.

The spin resolved DOS at different temperatures, at selected Zeeman fields are presented next in figure 9. For $h > 0$ the DOS at the ground state exhibits nodal gap at the shifted Fermi levels, increasing temperature leads to piling up of spectral weight and progressive closure of these gaps. Simultaneously, the coherence peaks at the gap edges flatten out via large transfer of spectral weight away from the (shifted) Fermi level.

Thermal evolution of average phase correlation $\phi^x$, $\phi^y$, and (d) average magnetization ($m_i$), with Zeeman field. The point of inflection of the curves correspond to the $T_c$.

Thermal evolution of momentum resolved spectral line-shapes are presented next in figure 10, for a selected Zeeman field of $h = 0.6t$, which corresponds to the QBP phase at the ground state. The figure shows the lineshape $A_{\uparrow}(k, \omega)$ for the momentum trajectory $(0,0) \rightarrow (\pi,0) \rightarrow (\pi,\pi) \rightarrow (0,0)$, across the Brillouin zone. We note that at the lowest temperature prominent gap opens up along $(\pi/2,0) \rightarrow (\pi,0) \rightarrow (\pi,\pi/2)$. Progressive increase in temperature suppresses the gap and finally leads to its closure at $T \geq 1.25T_c$, where $T_c \sim 0.08t$. The behavior of $A_{\uparrow}(k,\omega)$ (not shown here) is similar to $A_\uparrow(k,\omega)$. Overall, in the nodal direction ($\pm \pi/2, \pm \pi/2$) the lineshape is characterized by a single peak which is roughly immune to thermal evolution, while there is opening of gap in the antinodal direction which undergoes progressive closure with temperature.

The real space signature is demonstrated next in figure 11 via the spatial maps. Once again we use (i) $|\Delta_0|$, (ii) $\cos(\phi_0^x - \phi_0^y)$, and (iii) $m_i$, as our indicators and track them as they evolve in temperature at $h = 0.6t$. Apart from the complementary spatial realization of superconducting pairing field and magnetization characteristic to the QBP phase at the lowest temperature, we note enhancement in spatial fragmentation of $|\Delta_0|$ with increasing temperature. The observation
Figure 9. Temperature dependence of the single particle DOS at the Fermi level corresponding to the up-spin (a)–(d) and down-spin (e)–(g) fermion species, at selected Zeeman fields.

Figure 10. Thermal evolution of the momentum resolved spectral lineshape ($A_{\uparrow}(k, \omega)$) across the (0,0) → ($\pi$,0) → ($\pi$, $\pi$) → (0,0) trajectory in the Brillouin zone, at $h = 0.6t$.

is validated by the phase coherence maps which demonstrates the increasing inhomogeneity and thus the loss of (quasi) long range phase coherence due to thermal fluctuations. The fragmentation and loss of phase coherence of superconducting pairing field is accompanied by emergence of regions of large magnetization, a signature of the ‘finite temperature BP phase’ [49]. This regime of phase uncorrelated superconducting islands (at $T > T_c$) is the visual realization of the pseudogap phase, and can be thought to be a system of phase uncorrelated Josephson junctions. As the isolated islands of superconducting pairing field progressively shrinks with temperature the system loses its superconducting order and undergoes transition to the PPFL phase.

Note that both the QBP and the finite temperature pseudogap phases are characterized by spatially inhomogeneous superconducting state and non zero spectral weight at the Fermi level of the quasiparticle spectra. The key distinction between these two phases is the presence (or absence) of (quasi) long range phase coherence of the superconducting pairing field (i.e. the superconducting phase stiffness). While the QBP phase is characterized by a finite superconducting phase stiffness, i.e. a quasi long range phase coherence between the fragmented superconducting islands, the said phase coherence is lost in the finite temperature pseudogap phase, indicating the loss of global superconducting order. Both the USC and QBP phases undergo smooth cross over to the finite temperature BP phase and then undergoes transition to the pseudogap phase with increasing temperature.

We now sum up the information gathered based on our analysis of thermodynamic and quasiparticle indicators and revise the thermal phase diagram shown in figure 1. The revised phase diagram in the $h – T$ plane is presented in figure 12. Along with the thermodynamic phases discussed earlier, the figure shows the pseudogap phase over a regime of temperature $T_c < T < T_{pg}$, and $T_{pg}$ undergoes progressive suppression with Zeeman field. The high field regime correspond to the FFLO phase and as shown in the phase diagram, is
Figure 11. Real space maps corresponding to the (a) pairing field amplitude $|\Delta_{ij}|$, (b) pairing field phase coherence $\cos(\phi_x^0 - \phi_x^i)$ and (c) magnetization $m_j$, as they evolve in temperature, at a selected Zeeman field of $h = 0.6t$. Increase in temperature leads to loss of phase coherence and eventual spatial fragmentation of the superconducting state.

Figure 12. Zeeman field-temperature ($h - T$) phase diagram of population imbalanced d-wave superconductor, showing the BP, QBP, FFLO, PPFL and pseudogap phases. The solid curve correspond to $T_c$, with the regime of second order transition shown by black curve while the red curve shows the regime of first order phase transition. The dashed curve correspond to $T_{pg}$ marking the crossover from the pseudogap to the PPFL phase.

characterized by large suppression in $T_c$, which makes its experimental realization, non trivial. Over a large part of the $h - T$ plane the system loses its global superconducting order via a second order thermal phase transition. The high field low temperature regime hosting the FFLO phase undergoes a first order thermal phase transition to lose its superconducting order. The order of these phase transitions are in agreement with the experimental observations of Pauli limited superconductors such as CeCoIn$_5$ [31].

Next, we take two temperature cross sections of this phase diagram to highlight the quasiparticle behavior as the system transits from BP to pseudogap to PPFL regimes, in figure 13. In panel (a) we show the up-spin DOS at $T = 0.05t$ as a function of increasing Zeeman field. For $h \lesssim 0.6t$ the prominent coherence peaks signify (quasi) long range phase coherence while the system is in the BP phase. At $h \sim 0.7t$ the system is at the verge of transition to the pseudogap phase as suggested by a large accumulation of spectral weight at the shifted Fermi level. The coherence peaks smear out considerably and transfers large spectral weight away from the shifted Fermi level. The DOS at $h = 0.8t$ and $0.9t$ are representative of the pseudogap regime. Note that the behavior of the DOS in this regime is different from that observed at $h = 0.7t$, owing to the finite temperature short range FFLO fluctuations at higher Zeeman fields. $h = t$ corresponds to the PPFL phase at $T = 0.05t$ and we find the DOS to be akin to the free electron tight binding spectra of a square lattice. All superconducting correlations have died out at this field.
Panel (b) shows the distribution of the superconducting pairing field amplitude across the \( h - T \) plane mentioned in panel (a). We note that for weak Zeeman fields the distribution remains unchanged from the one observed for a d-wave superconductor, at \( h = 0 \). The mean amplitude of the pairing field also remains roughly constant. Increasing field shifts most of the weight to low amplitude |\( \Delta_j \)|, indicating suppression of the pairing by Zeeman field. The distribution shows that as expected the FFLO phase comprises of superconducting pairing with suppressed amplitudes.

A high temperature scan at \( T = 0.15t > T_{c0} \) is shown in panel (c), where \( T_{c0} \) correspond to the \( T_c \) at \( h = 0 \). At all values of \( h \) we find that the magnitude of the coherence peak is reduced to almost half of what was observed at \( T = 0.05t \), as there are now only short range pair correlations surviving in the system without any (quasi) long range order. Consequently, the coherence peaks have smeared out as is expected from the pseudogap phase. The system transits to the PPFL phase at \( h \sim 0.7t \), indicated by the complete disappearance of the coherence peaks. The weak depletion in the DOS at the shifted Fermi level as observed for \( h \gtrsim 0.7t \) arises due to the strong correlation regime we are in, and continues to survive even at higher temperatures. The corresponding distribution of |\( \Delta_j \)| is shown in panel (d). We notice that the distribution is significantly broader due to thermal fluctuations and is roughly independent of the choice of \( h \) since the long range superconducting pair correlations have died out at this temperature, as compared to its \( T = 0.05t \) counterpart.

4. Discussion and conclusion

4.1. Imbalance in mass

In the earlier sections of this paper we have discussed about how a Pauli limited d-wave superconductor gives rise to a quantum breached pair phase with coexisting zero-momentum gapless superconducting order and nonzero magnetization. We demonstrated that due to the shift in the Fermi level of the individual fermion species there is a pile up of spectral weight at the ‘unshifted’ Fermi level as suggested by the spatial depletion of the superconducting order. The regions of depleted superconductivity serves as host to the unpaired fermions in the system which gives rise to nonzero magnetization.

In this section, we discuss an alternative scenario where similar physical phenomena plays out. At this end we consider a Fermi–Fermi mixture with fermion species having unequal effective masses. In the context of ultracold atomic gases such Fermi–Fermi mixtures have already been realized as, Li\(_6\)–K\(_{40}\) mixture [73–76], albeit with an isotropic s-wave symmetry of the pairing state. While superfluidity is yet to be achieved in such mixtures, the degenerate Fermi regime [73, 76], Fermi resonance between Li\(_6\)–K\(_{40}\) atoms [75–77] and formation of Li\(_6\)–K\(_{40}\) hetero molecules [74] are already a reality. Moreover, other Fermi–Fermi mixtures such as, Dy\(^{161}\), Dy\(^{163}\), Er\(^{167}\) etc are expected to be experimentally realizable in the near future [78, 79].

The theoretical efforts that have been put in to understand such hetero molecules are primarily concentrated on continuum models. Density functional theory combined with local density approximation [80], functional renormalization group analysis [81], mean field theory with Gaussian fluctuations [82, 83], T-matrix and extended T-matrix approaches [84–86] have been employed to understand the physics of Fermi–Fermi mixtures. Within the purview of lattice fermion models, quantum Monte Carlo study on one dimensional mass imbalanced system [87], non perturbative lattice Monte Carlo based analysis of two-dimensional system [88] and a recent static path approximation based Monte Carlo study [89] are some of the efforts worth mentioning.

In the present section we present a similar scenario with the pairing symmetry being non local, a target that can be achieved in experiments pertaining to ultracold atomic gases. In the context of solid state systems, materials with unequal masses of the fermions can be envisaged as different fermion species belonging to different electronic bands. Below we demonstrate that a quantum breached pair state and the associated phase transitions can be realized in such systems even without an imbalance in the fermionic populations.

The Fermi–Fermi mixture comprising of unequal mass fermion species subjected to a non local interaction can be depicted by the Hamiltonian,

\[
H_{\text{SC}} = - \sum_{\langle i,j \rangle, \alpha} t_{ij}^\alpha (c_{i\alpha}^\dagger c_{j\alpha} + \text{h.c.}) + \sum_{i \neq j} |\Delta_{ji}|^2 (c_{iL}^\dagger c_{jH} + c_{iH}^\dagger c_{jL}) + \text{h.c.}
\]

\[
- \mu \sum_{\alpha} \hat{n}_{\alpha} + 4 \sum_{i \neq j} \frac{|\Delta_{ji}|^2}{|U|}
\]

where, \( \alpha = L, H \) corresponds to the light and heavy fermion species, respectively. Note that the imbalance in mass is imibed in the hopping parameter \( t_{ij}^\alpha \), wherein, \( t_{ij} \sim 1/m_i \); \( m_H \) and \( m_L \) correspond to the masses of the heavy and light species, respectively. Once again we set the hopping to be nearest neighbor and the energy scales are measured in units of \( t_p \) which is set to unity. As our tuning parameter we define the ratio between the hopping parameters corresponding to the fermion species as, \( \eta = t_H/t_L = m_L/m_H \). Thus, \( \eta \geq 1 \) corresponds to the balanced (equal mass) limit of the system and \( \eta = 0 \) corresponds to maximum imbalance, wherein one of the fermion species is completely localized.

We show the thermodynamic behavior corresponding to this system in figure 14, in terms of the \( x \)-component of the average phase correlation \( \phi^{x*} \) and average magnetization \( m \), at different \( \eta \). We note that though the phase correlation gets progressively suppressed with increasing mass imbalance, over a regime of imbalance \( \eta \leq 0.4 \) the system hosts nonzero magnetization along with a finite phase correlation, at the ground state. In order to verify whether this coexistence phase is a QBP phase we have examined the single particle DOS and have found them to be gapless.

In the limit of mass balance (\( \eta = 1 \)) the DOS corresponding to the two species exhibit nodal gap at the Fermi level corresponding to an uniform d-wave superconductor. As the
imbalance increases one of the species gets semi-localized, as a result the gain in the condensation energy through pairing is less than that in case of the balanced mixture, i.e. not all the fermions get paired up. There is now accumulation of finite spectral weight at the Fermi level, the resulting gapless spectra accommodates the excess (unpaired) fermions and give rise to a coexistence phase characteristic to the QBP. For weaker interaction strength, gapless superconductivity is realized for smaller imbalance ($\eta < 0.4$) the $T = 0$ state shows coexisting superconducting order and non-zero magnetization.

In figure 15 we show the composite phase diagrams for the proposed scenario of Fermi–Fermi mixture, both at the ground state as well as at finite temperature. The ground state phase diagram is shown in panel (a). In the regime of $\eta \sim 0$ the system is a partially polarized Fermi liquid (PPFL) with $m \neq 0$ and $\phi^{xx} \neq 0$, with increasing $\eta$ the pairing field phase correlation $\phi^{xx}$ picks up weight and progressively increases as more fermions participate in the pairing. Simultaneously, the magnetization gets suppressed $m \rightarrow 0$ (due to decrease in the number of unpaired fermions) and eventually drops to zero at $\eta \sim 0.3$, beyond which the system is an un-magnetized d-wave superconductor. The regime with $m \neq 0$ and $\phi^{xx} \neq 0$ correspond to the QBP phase, in the phase diagram, $\eta \sim 0.3$ is thus the mean field estimate of the quantum critical point for the quantum phase transition between the USC and QBP phases, at the parameters under consideration. The average phase correlation ($\phi^{xx}$) continues to increase and becomes saturated for $\eta > 0.5$, to the magnitude expected from the balanced system.

In panel (b) we present the corresponding finite temperature behavior. The figure shows four distinct phases as, (i) superconductor (BP), (ii) PG-I, (iii) PG-II and (iv) PPFL; along with three important thermal scales as, (i) $T_c$, (ii) $T_{PB}^{pg}$ and (iii) $T_{PB}^{II}$. Before we characterize the phases individually we emphasize that unlike a system with imbalance in fermion populations, there are two pseudogap regimes for systems with mass imbalance, as shown in the figure. In one of the earlier works the author had carried out detail analysis of mass imbalanced Fermi–Fermi mixtures with on-site interaction [89], such as, Li$^6$–K$^{40}$. The analysis showed that since the two fermion species are being subjected to different ‘scaled’ temperatures, the regime over which the short range correlations survive in each of them are different. Consequently, while in the PG-I regime both the species are pseudogapped, in the PG-II regime it is only the lighter species which is pseudogapped while the heavier species is a partially polarized Fermi liquid. We do not expect any qualitative change from this picture when the pairing state symmetry is d-wave, as demonstrated in figure 15(b). As expected, the BP regime involves finite temperature coexistence of d-wave superconductivity and non-zero magnetization, while the PPFL phase is highly magnetized with vanishing superconducting correlations. The transitions from superconductor to PG-I, crossover from PG-I to PG-II and from PG-II to PPFL are marked by $T_c$, $T_{PB}^{pg}$ and $T_{PB}^{II}$ respectively. As $\eta = 1.0$ corresponds to balanced limit, the $T_c$ and $T_{PB}^{II}$ scales collapse to one at this point. The survival of the pseudogap regimes upto $T \gg T_c$ ensures that signatures of mass imbalance in such systems can be accessed through species resolved spectroscopic experiments, even when the superconducting transition scales are strongly suppressed due to imbalance.

In conclusion, in this paper we have carried out a systematic study of Pauli limited d-wave superconductors, within the purview of a lattice fermion model. Unlike the existing body of literature, we focus our analysis on the regime of population imbalance where it is not strong enough to give rise to the exotic FFLO phase, but at the same time is sufficient to give rise to Fermi surface mismatch and unpaired fermions. To the best of our knowledge, we for the first time demonstrate that in d-wave Pauli limited superconductors, imbalance in fermion populations give rise to a quantum phase transition from an uniform superconductor to a quantum breached phase pair. We give a mean field estimate of the quantum critical point of this transition. This quantum phase transition is quantified by the average magnetization of the system, rather than the superconducting pairing field. The merit of this work rests not just in establishing the quantum breached pair phase of the Pauli limited d-wave superconductors but also in accessing the thermal phases of such systems. While the existing literature on the Pauli limited d-wave superconductors seem to be restricted to studies based on the mean field theory,
we for the first time implement a non perturbative numerical technique which enables us to access the thermal scales accurately, owing to its inclusion of the spatial fluctuations of the superconducting pairing field. Apart from the population imbalanced d-wave superconductors we have discussed about an alternate scenario where a quantum breached pair phase can be realized, viz a mass imbalanced d-wave superconductor. We have mapped out the ground state and finite temperature phase diagrams for such systems and showed that while the ground state does host a quantum breached pair phase, the finite temperature phase comprises of species selective regimes for the survival of short range pair correlations, giving rise to two pseudogap phases.

While much attention has been paid to understand the FFLO physics of the Pauli limited d-wave superconductors, this is the first work which establishes the existence of a quantum breached pair state in these systems over a significant regime of imbalance. We have discussed several thermodynamic and quasiparticle indicators which should be accessible to the existing experimental probes. We believe that this work is likely to open up exciting new avenues for experimental research to observe quantum breached pair phase in solid state materials as well as in ultracold atomic gas setups.

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Appendix A.

A.1. Finite size effect

The results presented in the main text correspond to a particular lattice size of $L = 24$. Any lattice calculation is however likely to be plagued by finite size effect. In order to verify whether the quantum breached pair phase discussed in this paper is an artifact of finite lattice sizes we have carried out the simulations at different system sizes (upto $L = 40$). In figure A1 we show the thermal evolution of average of $x$-component of the superconducting phase correlation and average magnetization at $L = 36$ for different Zeeman field. As is evident from the figure, there is indeed nonzero magnetization at $T = 0$ for $h \gtrsim h_{c1} \sim 0.2$ suggesting that the quantum breached pair phase is robust and stable against finite lattice size effects.

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Figure A1. Thermal evolution of the $x$-component of average superconducting phase correlation (a) $\phi^{x}_{\text{ave}}$ and (b) average magnetization ($m$), with Zeeman field, for system size of $L = 36$. For $h \gtrsim h_{c1} \sim 0.2$ suggesting that the quantum breached pair phase is robust and stable against finite lattice size effects.
