Gapless Triplet Superconductivity in Magnetically Polarized Media

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We reveal that in a magnetically polarized medium, a specific triplet commensurate pair density wave superconducting (SC) state, the staggered d-wave II-triplet state, may coexist with homogeneous triplet SC states and even dominate eliminating them under generic conditions. When only this TPDW SC state is present, we have the remarkable phenomenon of gapless superconductivity. This may explain part of the difficulties in the realization of the engineered localized Majorana fermion modes for topological quantum computation. We point out qualitative characteristics of the tunneling density of states, specific heat and charge susceptibility that identify the accessible triplet SC regimes in a spinless medium.

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Singlet superconductivity (SC) and ferromagnetism (FM) are directly competing phenomena. The discovery of SC coexisting with FM in UGe$_2$ [1], and other bulk FM-SC [2, 3], in heterostructures where proximity of SC and FM is enforced [4,5] necessarily involves exotic spin-triplet SC states. Numerous theoretical models with homogeneous triplet SC states possibly odd in frequency have been proposed [7–13]. For the 2-D SC state that develops at the interfaces of some oxide insulators like LaAlO$_3$/SrTiO$_3$ [12] in the presence of FM [13] a modulated or Pair Density Wave (PDW) triplet state of FFLO type has also been suggested [14].

The observation of proximity induced SC in the half metallic (fully polarized) FM CrO$_2$ in contact with SC NbTiN [4] demonstrates that effectively spinless systems may exhibit SC as well. Triplet SC in spinless systems is of enormous interest because a spinless triplet SC wire can exhibit at its two edges localized Majorana fermion modes [14–16]. Such localized Majorana fermions [17] would allow for non-local quantum information storage avoiding local decoherence as well as for logical manipulations through braiding because of their non-abelian character [16]. The localization of these modes is a crucial requirement for quantum-bit realizations and braiding manipulations, and it can occur only if a finite SC gap is present [17].

In the present Letter, based on a systematic study of the interplay of all SC condensates allowed by symmetry in a fully spin-polarized medium, we show that under realistic generic conditions a triplet SC state exhibiting a commensurate density wave modulation of the superfluid density may coexist with, or even dominate eliminating it, the homogeneous (zero momentam) triplet SC. When this triplet commensurate pair density wave SC (TCPDWSC) state dominates we have robust gapless SC, a situation that would be catastrophic for the engineered topological quantum bits. We report phase transitions between the various types of accessible triplet SC states including transitions between gapped and gapless SC states, as well as qualitative physical characteristics in the density of states, specific heat and charge susceptibility that would allow to identify the type of triplet SC in which the system of interest is in.

A similar TCPDWSC state channel has been suggested to occur in the high field SC state of CeCoIn$_5$ coexisting with singlet SC and spin density waves [18, 19] explaining fascinating neutron scattering results [20]. There have also been studies of TCPDWSC in the singlet channel, also called η-pairing, [21, 23–27] mainly motivated by the extraordinary physics in the pseudogap and other stripe regimes of cuprates [28, 29] where extended FS in the SC state has been reported as well [22].

Our starting point is a BCS-type Hamiltonian with frozen spin: $H = \sum_k \xi_k c_k^\dagger c_k - \sum_k (\Delta^Q_k c_k^\dagger c_{-k}^\dagger + h.c) - \sum_k (\Pi^Q_k c_k^\dagger c_{-k}^\dagger + (k+Q) + h.c)$. The first term in describes a tight binding dispersion which generically can be written as a sum of particle-hole symmetric terms and particle-hole asymmetric terms: $\xi_k = \gamma_k + \delta_k$. When $\delta_k = 0$ there is particle-hole symmetry or perfect nesting while finite values of $\delta_k$ destroy the nesting conditions. The second term $\Delta^Q_k = \sum_{k'} V_{k,k'}^Q c_{-k'}^\dagger c_{k'} c_k$ represents unconventional SC with zero pair momentum, and the last term $\Pi^Q_k = \sum_{k,k'} V_{k,k'}^Q c_{-k'} c_{k'} c_k$ is the TCPDWSC or modulated SC state. Although our TCPDWSC bear some resemblance with the FFLO state [30] because Cooper pairs have finite total pair momentum and the the superfluid density is inhomogeneous, they are fundamentally different. In fact, our TCPDWSC is a spin-triplet state whereas the FFLO is a spin-singlet trying to survive the Zeeman field. The wavevector of the superfluid modulation in our TCPDWSC is the commensurate nesting vector $Q$. In the FFLO state instead, the wavevector of the superfluid modulation is variable scaling with the magnitude of the magnetic field.

The effective interactions of the itinerant quasiparticles $V_{k,k'}^Q, V_{k,k'}^Q$, may have a purely electronic origin in the case of FM superconductors. However, our approach is generic irrespective of the microscopic origin of the effective interactions, and the validity of our findings is generic as well. In the case of heterostructures, we assume within our approach that the effective potentials
incorporate the proximity effects as well. Naturally, we would expect in that case a real space dependence of the potentials, that we neglect here. We only focus on qualitative symmetry questions that would not be affected by a smooth space dependence. In fact, the modulation of the superfluid density in our TCPDWSC state has a wavelength negligible compared to the coherence length and the characteristic lengths of the heterostructure. We therefore expect our qualitative findings to hold for bulk materials and for nanostructures as well.

To treat both types of SC order parameters (OPs) in a compact manner we introduce a Nambu-type representation using the spinors \( \Psi^i_{\kappa} = (c^i_{\kappa}, \xi_{-\kappa}, c^i_{\kappa+Q}, \xi_{-\kappa-Q}) \), and we use the basis provided by the tensor products \( \hat{\rho}_i = (\hat{\sigma}_i \otimes 1_2) \) and \( \hat{\sigma}_i = (1_2 \otimes \hat{\sigma}_i) \), where \( \hat{\sigma}_i \) with \( i = 1, 2, 3 \) are the usual 2x2 Pauli matrices and \( 1_2 \) the unit 2x2 matrix. The absence of spin index in the hamiltonian affects the symmetry classification of the acceptable triplet SC states, for which we produced a systematic phase map. In fact, the OPs are normally classified by their behavior under inversion \((\hat{I}) \ k \rightarrow -k\), translation \((\hat{t}_Q) \ k \rightarrow k+Q\) and time reversal \((\hat{T})\).

Instead of the latter we may use complex conjugation \((\hat{K})\) which is related to time reversal via the relations \(\hat{T} = -\hat{K}(\Delta^0_k)\) and \(\hat{T} = i\hat{K}(\Delta^Q_k)\). Since the spins are frozen, the homogeneous \((q = 0)\) SC pair states may only have odd parity: \(\Delta^0_k = -\Delta^0_{-k}\). Under translation we have both signs \(\Delta^0_{k+Q} = \pm \Delta^0_{k}\) and under \(\hat{T}\) we get \(\hat{T}\Delta^0_k = -\Delta^0_{-k}\). TCPDWSC states may have both parities \(\Pi^Q_k = \pm \Pi^Q_k\) and both signs under translation since \(\Pi^Q_{k+Q} = -\Pi^Q_{-k} = \mp \Pi^Q_k\). Time reversal demands that \(\hat{T}\Pi^Q_k = \mp \Pi^Q_k\) implying the relation \(\hat{T} = i\hat{K}\) for the TCPDWSC states. The break of time reversal allows finally four possible SC OPs, two homogeneous SC states and two TCPDWSC states: \(\Delta^Q_k\), \(\Delta^Q_{-k}\), \(\pi \Pi^Q_k\), \(\pi \Pi^Q_{-k}\). Here the first index \(q = 0\) or \(q = Q\) indicates the total momentum of the pair (or the characteristic wavevector of the superfluid density), the second index \(R\) or \(I\) indicates whether the OP is real or imaginary, the third index \(\pm\) indicates parity under inversion \(\hat{I}\) and the last index denotes gap symmetry under \(\hat{t}_Q\). The symmetry properties of the OPs under inversion \(\hat{I}\) and translation \(\hat{t}_Q\) imply a specific structure in \(k\)-space. Every OP \(M_k\) is written in the form \(M_k = M_{fk}\) where the form factors \(f_k\) belong to the different irreducible representations of the point group.

According to the above symmetry classification there exist four possible pairs of competing homogeneous and modulated SC states. Using our formalism we calculate Greens functions and from them self-consistent systems of coupled gap equations for each case. The pairs \(\Delta^Q_k\) with \(\Pi^Q_{IR+}\) and \(\Delta^Q_{-k}\) with \(\Pi^Q_{-IR+}\) obey the system of coupled equations:

\[
\Delta_k = \sum_{k'} V_{k,k'} \Delta_{k'} \sum_{\pm} \frac{1}{\mp 2 \pi^2 (\pm \sqrt{\gamma_k^2 + \Delta^Q_{\pm k}^2})} \tanh \left( \frac{E_k(k')}{{\Delta}_k^Q} \right) \]

where \(E_k(k') = (\sqrt{\gamma_k^2 + \Delta^Q_{\pm k}^2})\) and \(\Delta^Q_k\) and the quasiparticle energies are \(E_k(k) = (\sqrt{\gamma_k^2 + \Delta^Q_{\pm k}^2})^2\). The remaining two cases, competition of \(\Delta^Q_k\) with \(\Pi^Q_{IR-}\) and \(\Delta^Q_{-k}\) with \(\Pi^Q_{-IR-}\), obey the following equations:

\[
\Delta_k = \sum_{k'} V_{k,k'} \Delta_{k'} \sum_{\pm} \frac{B_{k'} \mp \gamma_{k'}^2 + \Delta^Q_{\pm k} \Delta^Q_{\pm k'}}{E_k(k') \mp 2 \pi^2 (\Delta^Q_{\pm k})} \tan \left( \frac{E_k(k')}{{\Delta}_k^Q} \right) \]

and \(\Pi_k = \sum_{k'} V_{k,k'} \Pi_{k'} \sum_{\pm} \frac{B_{k'} \mp \gamma_{k'}^2 + \Delta^Q_{\pm k} \Delta^Q_{\pm k'}}{E_k(k') \mp 2 \pi^2 (\Delta^Q_{\pm k})} \tan \left( \frac{E_k(k')}{{\Delta}_k^Q} \right)\)

where \(B_{k'} \equiv \gamma_{k'}^2 + \Delta^Q_{\pm k} \Delta^Q_{\pm k'}\), and the dispersions are \(E_k(k) = [\Delta^Q_{\pm k} - \Delta^Q_{\pm k}^2 + (\pm \gamma_{k} \Pi^Q_k \Delta^Q_{\pm k}^2)]^{1/2}\).

The effective potentials \(V_{k,k'} = V_{kk'}/\Gamma\) (separable potentials). We have solved self consistently the above systems of equations on a square lattice with \(\gamma_k = -t_1 (\cos{k_x} + \cos{k_y})\) and \(\delta_k = -t_2 \cos{k_x} \cos{k_y}\) and \(Q = (\pi, \pi)\). The choice of a tetragonal dispersion is motivated by the fact that CrO\(_2\) as well as strong FM superconductors like UGe\(_2\) and URhGe exhibit all a tetragonal structure, however, our qualitative findings are generic. The corresponding form factors belong to irreducible representations of the tetragonal group \(D_{4h}\). Specifically: \(\Delta^Q_{IR-} \sim \sin{k_x} + \sin{k_y}\) (s-wave), \(\Delta^Q_{IR+, IR-} \sim \sin{k_x} \pm \sin{k_y}\) (p-wave) and \(\Pi^Q_{IR} \sim \cos{k_x} + \cos{k_y}\) (d-wave). For every competing pair we have performed a large number of self-consistent calculations varying pairing potentials in the two channels, temperatures and ratios \(t_2/t_1\).

The first important result is that the TCPDWSC \(\Pi^Q_{IR+}\) OP can never survive. Specifically, the \(\Pi^Q_{IR+}\) gap is zero regardless of the values of the pairing potentials and the particle-hole asymmetry \(t_2/t_1\) term. We conclude that although the state \(\Pi^Q_{IR+}\) is allowed by symmetry, it is never realized. Therefore, we only report results about the relevant competition of the remaining TCPDWSC OP \(\Pi^Q_{IR-}\) with both zero momentum SC states.

The phase sequences as \(t_2/t_1\) grows starting from zero and for various values of the pairing potentials for the competition \(\Delta^Q_k\) with \(\Pi^Q_{IR+}\) and \(\Delta^Q_{-k}\) with \(\Pi^Q_{-IR+}\) are shown in the respective panels of Fig. 1. Arrows in Fig. 1 indicate the cascade of phases observed when the ratio \(t_2/t_1\) grows starting from zero at each region of the map. The variation of \(t_2/t_1\) may simulate various effects such as chemical doping, or stress effects as well as proximity effects. Since we consider a spin-polarized background, all states reported coexist with FM, and the transitions to the FM state reported at high values of \(t_2/t_1\) has the meaning of a transition to a state that is only ferromagnetic with no SC OP present.

Both cases share the characteristic feature that the TCPDWSC state \(\Pi^Q_{IR-}\) is finite in the largest part of the maps of the pairing potentials. Thus, since we do not limit to a specific microscopic model that could correspond to a specific value for the pairing potentials, the existence of the modulated TCPDWSC phase
FIG. 1. Maps of the dependence of phase sequences on the effective interactions \( V^A \) and \( V^\Pi \) for low temperature. Arrows indicate the cascade of phases obtained when \( t_2/t_1 \) grows starting from zero. The black dots separate regions of different phase sequences under growing \( t_2/t_1 \). All phases coexist with ferromagnetism (FM). The phases indicated as FM only FM is present. Panel (a) depicts the interplay of \( \Pi^{QR+} \) with \( \Delta^{QI-} \) whereas panel (b) that of \( \Pi^{QR+} \) with \( \Delta^{QI+} \). The potentials are in units of \( t_1 \).

The lowest free energy is situated at the point \((\Delta, \Pi) = (0, 0.94t_1)\) where only \( \Pi^{QR+} \) is finite despite the fact that it exhibits gapless SC.

The stability of the solutions of the self consistent equations has been verified by free-energy calculations as well. The free-energy difference \( \Delta F \) between

\[ \Delta F = \frac{\Delta^2}{\beta^2} + \frac{\Pi^2}{\beta^2} - \frac{1}{\beta^2} \sum_k \sum_{j=\pm, i=\pm} \ln \left( \frac{1 + e^{-\beta \epsilon_j(k)}}{1 + e^{-\beta \epsilon_i(k)}} \right) \]

where \( E_{\pm}(k) \) the energy dispersions for each competing pair and \( \epsilon_{\pm}(k) \) the energy dispersions obtained when both gaps are zero. The safest way to ensure that the solutions of the coupled gap equations correspond to the minimum of the free-energy difference is to vary \( \Delta F \) with respect to the magnitudes of the gaps and verify that \( \Delta F \) attains its minimum for these values. We report in Fig. 2 the variations of the free-energy difference with \( \Delta^{QI-} \) and \( \Pi^{QR+} \) at low-T for \( t_2/t_1 = 0 \) and for \( V^A = V^\Pi = 3t_1 \) to illustrate the dominance of the TCPDWSC state. These values of the pairing potentials correspond to the cascade of transitions \( \Pi \rightarrow \Delta \rightarrow FM \) when \( t_2/t_1 \) grows (cf. Fig. 1b). It is clear that \( \Delta F \) attains its minimum value for \((\Delta, \Pi) = (0, 0.94t_1)\), thus the ground state consists solely of the TCPDWSC phase.

We report in Fig. 3 the dependence of the OPs on \( t_2/t_1 \) at low-T (Fig. 3a) and the phase diagram (Fig. 3b) obtained by the coupled-gap equations. We stress that at low-T for \( t_2/t_1 = 0 \) the values of the gaps are in full agreement with the \( \Delta F \) minimum requirement, i.e \((\Delta, \Pi) = (0, 0.94t_1)\). The \( t_2/t_1 \) transition from the modulated to the homogeneous SC state is first order, and we note that the TCPDWSC gap is significantly larger than the homogeneous SC gap despite the fact that the pairing potentials have the same magnitude (Fig. 3b). The phase diagram shows that the transition \( \Pi \rightarrow \Delta \) with \( t_2/t_1 \) is not limited to low-T. The modulated SC phase extends to higher temperatures (Fig. 3b) than the homogeneous SC phase. The boundary separating the two SC states remains first order and ends at a tricritical point. Decreasing the temperature moves the boundary
to lower $t_2/t_1$-values. This allows a first order transition with respect to temperature within the superconducting phase from the TCPDWSC to the homogeneous SC state. An example of such a transition realized for $t_2/t_1 = 2$ is shown in the inset of Fig. 3b.

A question that naturally arises is how the exotic TCPDWSC state $\Pi_k^{R+ -}$ can be identified experimentally. Quite remarkably, specific heat measurements at low-T may be sufficient. Specifically, isolated TCPDWSC states exhibit an extended FS whereas the FS is limited to two Fermi points in the coexistence phase $\Delta + \Pi$. Therefore a polynomial behavior of the specific heat at low-T is a signature of the coexistence phase. As particle-hole asymmetry $t_2/t_1$ grows for example with gate voltage, only the modulated SC state $\Pi_k^{Q R+ -}$ continues to exhibit extended FS whereas the zero momentum SC states as well as the coexistence phase present limited FS consisting of isolated Fermi points. We note that the extended FS is also a feature of the spin-singlet $\eta$-pairing [22].

Consequently the TCPDWSC state $\Pi_k^{Q R+ -}$ is the sole SC state that exhibits a linear low-T behavior of the specific heat and this is robust since it holds even for finite values of $t_2/t_1$. This is illustrated in Fig. 3 where the Fermi surface and the specific heat for $t_2/t_1 = 1.0$ in the TCPDWSC phase (red) and $t_2/t_1 = 2.5$ in the homogeneous SC phase (blue) of Fig. 3b are reported. We observe that in the $\Pi_k^{Q R+ -}$ phase the Fermi surface is extended imposing the linear behavior of the specific heat at low-T. On the other hand, in the $\Delta_k^{Q I+ -}$ phase we only have two Fermi points and the specific heat at low-T exhibits a polynomial behavior. This is also the case for the other homogeneous SC state $\Delta_k^{Q I+ -}$ as well as for the coexistence phase $\Delta + \Pi$. Therefore linear low-T specific heat in the SC state identifies the triplet TCPDWSC state.

The difference in the FS is reflected in the behavior of the electronic density of states (DOS) $N(\omega)$ accessible by tunneling. In our spinor formalism: $N(\omega) = -\frac{1}{2\pi} \text{Im} \sum_k \text{Tr} \{ G(k, \omega_n + \omega + i\eta) \}$. Performing the analytical continuation it can be shown to take the form: $N(\omega) = \sum_k \{ \delta(\omega + E_\pm(k)) + \delta(\omega - E_\pm(k)) \}$. As an example we present in Fig. 5 the DOS in the $\Pi_k^{Q R+ -}$, the $\Delta_k^{Q I+ -}$ state and the coexistence phase $\Delta + \Pi$ for $t_2/t_1 = 0$ (left) and $t_2/t_1 = 1$ (right). In each case the pairing potential is $3t_1$. The vanishing DOS at the Fermi level identifies the coexistence phase $\Delta + \Pi$ in the case of perfect nesting $t_2/t_1 = 0$, whereas the finite DOS for particle-hole asymmetry $t_2/t_1 \neq 0$ is a direct signature...
of the TCPDWSC state. We note that finite DOS at the Fermi level has also been reported in spin-singlet PDW states [21].

Finally, measurements related with the charge-charge correlation function $P(q, i\omega_n=0)$ for the lowest Matsubara frequency $\omega_n=0 = \pi T$ along the diagonal and the antidiagonal of the first Brillouin zone (FBZ) may provide the ultimate experimental strategy to distinguish the different accessible triplet SC states.

We illustrate this in Fig. 6 where $P(q, i\omega_n=0)$ is reported along the diagonal (left) and the antidiagonal (right) of the FBZ in the $\Pi_{k}^{Q R+}$ (red), the $\Delta_{k}^{Q I-}$ (green), the $\Delta_{k}^{Q I-}$ (blue) and the coexistence phase $\Delta + \Pi$ (magenta) at low-$T$ for $t_2/t_1 = 0$. The pairing potentials are $V_{\Delta, \Pi} = 3t_1$.

![Diagram](attachment:diagram.png)

**FIG. 6.** (Color online) Charge-charge correlation function $P(q, i\omega_n=0)$ along the diagonal (left) and the antidiagonal (right) of the FBZ in the $\Pi_{k}^{Q R+}$ (red), the $\Delta_{k}^{Q I-}$ (green), the $\Delta_{k}^{Q I-}$ (blue) and the coexistence phase $\Delta + \Pi$ (magenta) at low-$T$ for $t_2/t_1 = 0$. The pairing potentials are $V_{\Delta, \Pi} = 3t_1$.

In summary, within a generic microscopic mean field theory we explored systematically the interplay of all possible triplet SC states in an effectively spinless system. We find that the inhomogeneous TCPDWSC state $\Pi_{k}^{Q R+}$ having the p-wave symmetry can never survive the two allowed by symmetry homogeneous triplet SC states. However, the other TCPDWSC $\Pi_{k}^{Q R+}$ having d-wave symmetry may either appear alone or coexist with the homogeneous SC OPs driving the phenomenon of gapless SC over a wide parameter range. Our findings are universally applicable to any strongly ferromagnetic system that develops superconductivity including devices designed to host localized Majorana modes for topological quantum computation. Geometry and the presence of one-spin triplet SC does not guarantee the relevance of a device designed to host Majorana qubits, it should be tested against the eventual emergence of catastrophic gapless triplet SC and we have identified some experimental paths for such tests.

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