Coexistence of topological charge density waves and superconductivity in a two-dimensional topological superconductor

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Abstract. We perform microscopic mean-field studies of topological order in a two-dimensional s-wave topological superconductor with Rashba spin-orbit coupling and Zeeman field by solving the Bogoliubov-de Gennes equations. By solving for the spin-dependent Hartree potential self-consistently along with the superconducting order parameter, we show that topological charge density waves (TCDW) can coexist with topological superconductivity (TSC) at half filling just as in a conventional s-wave superconductor. Furthermore, we examine the effects of nonmagnetic impurities – which tend to create spin-polarised midgap excitation and pin the phase of charge density modulations – on possible interplay of TCDW and TSC.

1. Introduction

Whether charge density waves (CDW) compete or cooperate with superconductivity has been debated intensely for the last several decades, especially for unconventional superconductors such as high-$T_c$ cuprates in recent years. It is a topic of great interest to pursue in the new and rapidly growing field of topological superconductivity [1, 2]. In particular, the two-dimensional (2D) s-wave TSC model with Rashba spin-orbit (SO) coupling and Zeeman field [3, 4, 5] is one of the most promising models for platforms that can lead to realisation of fault-tolerant topological quantum computation [1, 5, 6]. There has been recent progress on the material side towards realising 2D s-wave TSC [7, 8, 9].

2. Model

We use the tight-binding model of Sato, Takahashi, and Fujimoto for 2D s-wave TSC with Rashba SO coupling and Zeeman field [3, 4]. Our mean-field Hamiltonian is given by [10]

$$
\mathcal{H} = \sum_{(ij)} \sum_{\sigma=\uparrow,\downarrow} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_i \sum_{\sigma=\uparrow,\downarrow} (\epsilon_i - \tilde{\mu} + \tilde{V}_{i\sigma}^{(H)} - \tilde{V}_{\sigma}^{(H)}) c_{i\sigma}^\dagger c_{i\sigma} + \frac{\alpha}{2} \left[ \sum_i (c_{i-x\uparrow}^\dagger c_{i\uparrow} - c_{i+x\uparrow}^\dagger c_{i\uparrow}) + i(c_{i-y\downarrow}^\dagger c_{i\downarrow} - c_{i+y\downarrow}^\dagger c_{i\downarrow}) + \text{H.c.} \right]
$$

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\[ + \sum_i (\Delta_i c^\dagger_i c^\dagger_i + \text{H.c.}) \]  

Here \( c^\dagger_i \) and \( c_{i\sigma} \) creates and annihilates, respectively, the electron at lattice site \( i \) with spin \( \sigma \), \( \hbar_{i\sigma} = -\hbar ( + \hbar ) \) for \( \sigma = \uparrow (\sigma = \downarrow) \), and we have defined

\[
\tilde{\mu} = \mu - \frac{\tilde{V}^{(H)}_{\uparrow} + \tilde{V}^{(H)}_{\downarrow}}{2}, \quad \tilde{h} = h + \frac{\tilde{V}^{(H)}_{\uparrow} - \tilde{V}^{(H)}_{\downarrow}}{2},
\]

with the bare chemical potential \( \mu \), the Zeeman energy \( -\hbar ( + \hbar ) \) for \( \sigma = \uparrow (\sigma = \downarrow) \), and the average Hartree potential for each spin component:

\[
\tilde{V}^{(H)}_{\sigma} = \frac{1}{N} \sum_i \tilde{V}^{(H)}_{i\sigma},
\]

where \( N \) is the total number of lattice sites. We assume an intrinsic \( s \)-wave pairing interaction \( U_i \equiv U < 0 \) that is uniform and results in the superconducting order parameter \( \Delta_i = U \langle c_{i\uparrow} c_{i\downarrow} \rangle \) and the Hartree potential \( V^{(H)}_{i\sigma} = U \langle c^\dagger_{i\sigma} c_{i\sigma} \rangle \), which is the average potential created by the electrons with spin \( \sigma \) and felt by those with the opposite spin \( \sigma \) at site \( i \). In the Hamiltonian (1), we consider hopping among nearest-neighbour sites \( \langle ij \rangle \) only with the probability amplitude \( t_{ij} \equiv t, \epsilon_i \) is the single-particle potential due to a nonmagnetic impurity at site \( i \), \( \alpha > 0 \) is the Rashba SO coupling strength, \( \hat{x} \) and \( \hat{y} \) are the unit vectors in the \( x \) and \( y \) directions, and H.c. stands for the Hermitian conjugate. Length and energy are measured in units of the lattice constant and \( t \), respectively.

An effective coupling constant \( U \) that is the same for the Hartree potential and the superconducting order parameter can be generated, for example, via the \( s \)-wave Feshbach resonance in a superfluid Fermi gas [11]. For \( h > 0 \), typically there are more spin-up electrons than spin-down electrons and the Hartree potential effectively reduces the Zeeman field. Intuitively, the average energy gain by the pairing interaction with spin-up electrons makes the electron to have its spin down less costly in terms of the Zeeman energy.

When the system has translational symmetry, \( V^{(H)}_{i\sigma} = \tilde{V}^{(H)}_{\sigma} \); \( \forall i \), and the Hamiltonian (1) can be expressed in momentum space as \( \hat{\mathcal{H}} = \frac{1}{2} \sum_k \hat{\Psi}_k^\dagger \hat{\mathcal{H}}(k) \hat{\Psi}_k \), where \( \hat{\Psi}_k = (c_{k\uparrow}^\dagger | c_{k\downarrow}^\dagger | c_{-k\uparrow}^\dagger | c_{-k\downarrow}^\dagger)^T \) and

\[
\hat{\mathcal{H}}(k) = \begin{pmatrix}
    \epsilon(k) - \hbar \sigma_x + \alpha \mathcal{L}(k) \cdot \sigma & i \Delta(k) \sigma_y \\
    -i \Delta(k)^* \sigma_y & \epsilon(k) + \hbar \sigma_z + \alpha \mathcal{L}(k) \cdot \sigma^*
\end{pmatrix},
\]

with \( \epsilon(k) = -2t (\cos k_x + \cos k_y) - \tilde{\mu} \) and \( \mathcal{L}(k) \equiv \mathcal{L}_x i \mathcal{L}_y = (\sin k_y, -\sin k_x) \). \( c^\dagger_{k\sigma} \) and \( c_{k\sigma} \) are the creation and annihilation operators of the electron with momentum \( k = (k_x, k_y) \) and spin \( \sigma \), and \( \sigma \equiv (\sigma_x, \sigma_y) \) and \( \sigma_z \) are the Pauli matrices. \( \hat{\mathcal{H}}(k) \) above reduces to the momentum-space Hamiltonian given in Ref. [4] when the Hartree potential is neglected, with \( \tilde{\mu} \equiv \mu \) and \( \tilde{h} \equiv h \).

Thus, various topological phases as classified in Ref. [4] according to the first Chern number or the Thouless-Kohmoto-Nightingale-Nijs (TKNN) number [12] can be achieved by replacing the chemical potential and Zeeman field by \( \tilde{\mu} \) and \( \tilde{h} \), respectively, when the Hartree potential is taken into account. Depending on the values of \( \tilde{\mu}, \tilde{h}, \alpha \), and the bulk order parameter, this model allows non-Abelian and Abelian phases with the TKNN number \( \nu = \pm 1 \) and \( \nu = -2 \), respectively, in addition to trivial phase with \( \nu = 0 \). Furthermore, topological density wave states such as spin density waves (TSDW) and charge density waves (TCDW) are also possible in Abelian phase [4].

In this 2D \( s \)-wave TSC model, there are two underlying chiralities, \( \eta_\pm \equiv -(\mathcal{L}_x \pm i \mathcal{L}_y)/\sqrt{\mathcal{L}_x^2 + \mathcal{L}_y^2} = \pm i(\sin k_x \pm \sin k_y)/\sqrt{\sin^2 k_x + \sin^2 k_y} \) [13, 14], which are analogous to the
two chiralities \( p_x \pm ip_y \) present in the nontrivial (non-Abelian) phase of the continuum model [15, 16, 17]. While in non-Abelian phase with a single Fermi surface, one chirality can be dominant over the other [4, 18, 19], the two chiralities \( \eta \pm \) associated with the two Fermi surfaces are always mixed in Abelian phase.

We solve the Bogoliubov-de Gennes (BdG) equations [20] on the effective Hamiltonian in Eq. (1) self-consistently for not only the superconducting order parameter, but also each spin component of the Hartree potential. We utilise numerically efficient algorithms for solving for the mean fields [21, 22] and for obtaining excitation spectrum and quasiparticle wavefunctions [23, 24], in both cases circumventing the high numerical demand of diagonalizing the BdG matrix. Self-consistent iterations are performed up to the \( l \)-th iteration step, where, e.g., the order parameter as a complex vector \( \vec{\Delta} \) of length \( N \) satisfies

\[
\frac{\|\vec{\Delta}^{(l)} - \vec{\Delta}^{(l-1)}\|}{\|\vec{\Delta}^{(l-1)}\|} < 10^{-6}
\]

and similarly for each spin component of the Hartree potential that can be regarded as a real vector of length \( N \). All the calculation presented below has been performed for zero temperature.

Table 1. Converged order parameters and the ground-state energy per electron for each of the three degenerate TSC, TCDW, and TSC+TCDW states in a homogeneous 64×64-site lattice with \( \tilde{\mu} = 0 \), \( U = -4t \), \( h = 1.5t \) and \( \alpha = t \) with PBC. The Zeeman field is effectively reduced to \( \tilde{h} = 0.9613t \).

| State    | \( \Delta_0 \) [\( t \)] | \( \Delta_C \) [\( t \)] | \( E/N_e \) [\( t \)] |
|----------|----------------|----------------|-----------------|
| SC       | 0.675          | 0.000          | -1.100          |
| CDW      | 0.000          | 0.675          | -1.100          |
| SC+CDW   | 0.422          | 0.527          | -1.100          |

3. Results

It has been shown by solving for the superconducting order parameter and each spin component of the Hartree potential self-consistently [10] that \( \tilde{\mu} = 0 \) corresponds to exactly half filling (i.e., one electron per site on average) and that uniform TSC and TCDW states – the latter with wave vector \((\pm \pi, \pm \pi)\) – are degenerate ground states at half filling, just as in the attractive Hubbard model for conventional s-wave superconductivity for uniform superconducting and CDW states [25]. Therefore, any linear superposition of the TSC and TCDW states is also a ground state and thus the two kinds of order can coexist for \( \tilde{\mu} = 0 \), where the system is in Abelian phase. In Table 1 we summarise an example of degenerate TSC, TCDW, and a mixed TSC+TCDW states for \( \tilde{\mu} = 0 \), \( U = -4t \), \( h = 1.5t \), and \( \alpha = t \) on a square lattice with 64×64 sites with the periodic boundary condition (PBC) and no impurity. Not only the ground-state energy, but also the excitation spectrum is identical among degenerate states, and in case of pure TSC and CDW states, the order parameter (superconducting or CDW) is also the same. When there are surface edges, there are two zero-energy bound states on each surface – as guaranteed by the bulk-edge correspondence to the topological invariant \( \nu = -2 \), but they are not Majorana fermions whenever there is nonzero CDW order parameter [4, 10].

It is known for conventional s-wave superconductivity that the presence of a nonmagnetic impurity, which tends to pin the phase of CDW, lifts the degeneracy in favour of CDW [25].
Due to the two underlying chiralities $\eta_{\pm}$ present in the system, it is an intriguing question as to what happens to degenerate TSC and TCDW states if a nonmagnetic impurity is deposited. While a single nonmagnetic impurity does not result in any quasiparticle bound state in a conventional $s$-wave superconductor [26], a nonmagnetic impurity can create spin-polarised, midgap quasiparticle excitation and can cause the spin of the midgap state to flip [10]. In this 2D $s$-wave TSC system, a nonmagnetic impurity can even bind a quasiparticle, leading to a phase transition of the ground state [10], and hence act exactly like a magnetic impurity (classical spin) in a conventional $s$-wave superconductor [27, 28, 29].

In Fig. 1 we show the real (a) and imaginary (b) parts of the superconducting order parameter $\Delta_i \equiv \Delta(x,y)$ in units of $t$ and the average number of electrons with spin up (c) and spin down (d) in the TSC state for $\bar{\mu} = 0$, $U = -4t$, $h = 1.5t$ and $\alpha = t$, with two nonmagnetic impurities with potential $V_{\text{imp}} = -t$ placed diagonally at the centre of a 64×64-site lattice, for $22 \leq x, y \leq 44$. Although the self-consistent calculation is started with uniform superconducting order parameter and Hartree potential, we can see in Fig. 1(c) and (d) that CDW with wave vector $(\pm \pi, \pm \pi)$ are induced by the two nonmagnetic impurities at the centre of the lattice. CDW extends over the entire lattice, albeit with nonuniform CDW order parameter: charge density modulations are most enhanced relatively close to the impurities. The superconducting order parameter is suppressed at the impurity sites and oscillates around them in its real part. Moreover, a small, oscillatory imaginary part is induced around the impurities, indicating the occurrence of spontaneous supercurrent: this is reminiscent of the influence of nonmagnetic impurities in a spin-triplet chiral $p$-wave superconductor [30].

Figure 2 illustrates the effects of four nonmagnetic impurities with potential $\epsilon_i \equiv V_{\text{imp}} = -0.5t$ placed at the centre of the lattice, $(x,y) = (32,32)$, $(33,32)$, $(32,33)$, and $(33,33)$ in a 64×64-site system with PBC, for $\bar{\mu} = 0$, $U = -4t$, $h = 1.5t$, and $\alpha = 2.5t$. The average number of electrons is shown for spin up (a) and down (b) in the TSC state, and for spin up (c) and down (d) in the pure TCDW state. Although the electron density is peaked at the impurity sites for both spin up and down, there is no impurity bound state in the TSC state for this potential strength.
Figure 2. Average number of electrons with spin up [(a) and (c)] and spin down [(b) and (d)] in the TSC [(a) and (b)] and pure TCDW [(c) and (d)] states for $\tilde{\mu} = 0$, $U = -4t$, $h = 1.5t$ and $\alpha = 2.5t$, with four nonmagnetic impurities with potential $V_{\text{imp}} = -0.5t$ placed at the centre of a $64 \times 64$-site lattice, for $22 \leq x, y \leq 44$.

Figure 3. LDOS for spin up at one of the impurity site $(x, y) = (33, 33)$ with $V_{\text{imp}} = -t$ in the pure TCDW state for $\tilde{\mu} = 0$, $U = -4t$, $h = 1.5t$, and $\alpha = 2.5t$ in a $64 \times 64$-site lattice.

Figure 4. LDOS for spin down at one of the impurity site $(x, y) = (33, 33)$ with $V_{\text{imp}} = -t$ in the pure TCDW state for $\tilde{\mu} = 0$, $U = -4t$, $h = 1.5t$, and $\alpha = 2.5t$ in a $64 \times 64$-site lattice.

In contrast, there are two particle and two hole bound states close to the gap edge in the pure TCDW state. In inhomogeneous states with impurities, $\tilde{\mu} = 0$ does not necessarily correspond to the exact half filling. For the states presented in Fig. 2, the TCDW state corresponds to half filling within the accuracy of the mean fields, while the TSC state deviates from half filling by one order of magnitude larger than the convergence of the mean fields. The energy per electron is $E/N_e = -1.9687t$ and $-1.9685t$ for the TCDW and TSC states, respectively.

The presence of impurity bound states is illustrated in terms of the local density of states (LDOS) at site $(x, y) = (33, 33)$ in Figs. 3 and 4 for spin up and down, respectively, for the
TCDW state in the same system as shown in Fig. 2 – except that \( V_{\text{imp}} = -t \), which yields two particle bound states with energy 0.1702\( t \) and 0.1997\( t \). The LDOS in Figs. 3 and 4 prominently shows the bound state at energy 0.1702\( t \) and the fact that its spin is mostly polarised to be down. Impurity bound states can also occur in TSC states for stronger potential strength.

4. Conclusions
By solving the BdG equations self-consistently, we have demonstrated the coexistence of superconductivity and CDW in Abelian phase of a 2D \( s \)-wave topological superconductor, and have found that CDW can be induced in TSC states by nonmagnetic impurities. Further studies as to how nonmagnetic impurities lift the degeneracy of TSC and TCDW states and can lead to possible interplay of the two states will be presented in a future publication.

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