Majorana corner flat bands in two-dimensional second-order topological superconductors

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In this paper we find that confining a topological superconductor with a harmonic potential leads to a proliferation of Majorana corner modes. As a consequence, this results in the formation of Majorana corner flat bands which have a fundamentally different origin from that of the conventional mechanism. This is due to the fact that they arise solely from the one-dimensional gapped boundary states of the hybrid system that become gapless without the bulk gap closing under the increase of the trapping potential. The Majorana corner states are found to be robust against the strength of the harmonic trap and the transition from Majorana corner states to Majorana flat bands is merely a smooth crossover. As harmonic traps can be realized in cold atom experiments or heterostructures, this proposal paves a way to observe these Majorana corner flat bands in an experimental context.

Introduction: Topological insulators (TIs) and superconductors (TSCs) have opened a new avenue for topology in both condensed matter and high-energy physics [1–11]. These topological materials have a bulk-boundary correspondence: there are gapped bulk states characterized by a topological invariant and topologically protected gapless states localized on boundaries.

Recently, a new concept of topological materials, so-called higher-order TSCs and TIs, have attracted much attention [12–20]. In terms of the conventional understanding of the bulk-boundary correspondence, these materials are topologically trivial, since both bulk and boundary states are gapped. However, there are robust gapless states on the “edge” of the boundary of these materials. In $d$-spatial dimensions, $n$-th order topological insulators and superconductors have $(d−n)$-dimensional gapless localized modes. Therefore, higher-order TSCs are good candidate systems for finding Majorana zero modes (MZMs) because they are localized as $(d−n)$-dimensional bound states. The MZMs are their own antiparticles and obey non-Abelian statistics [21–24]. Conventional TIs and TSCs are understood as examples of first order topological materials.

In second-order TSCs these MZMs have been studied at the corners of a two-dimensional (2D) system and hinges of a three-dimensional (3D) system where neighboring hinges have different chiralities [25, 26]. These zero-energy corner modes are known as Majorana corner states (MCSs) which have been studied in various kinds of system such as high-temperature superconductors (SCs) [27–31], $s$-wave superfluid [26, 32] systems with an external magnetic field [33, 34], and 2D and 3D second-order TSCs [35].

An important issue is to both find and determine the robustness of the MCSs. As shown in Ref. [29], the MCSs are robust in a 2D TI, also known as the quantum spin Hall insulator, in proximity with cuprate-based [36–38], or iron-based [39–42] high-temperature SCs, as shown schematically in Fig. 1. In this system, modest edge imperfections do not affect the MCSs while big edge imperfections just create new corners that host their own MCSs. This study suggests that the shape of the system is important for MCSs.

In this paper, we consider the harmonic potential (HP) as an example of a gradual confining potential. The HP is defined as $V_i = v_{\text{trap}} \{(i_x - i_x^c)^2 + (i_y - i_y^c)^2\}$ where $v_{\text{trap}}$ is the potential amplitude, and $i^c = (i_x^c, i_y^c)$ is the coordinate of the central site of the square lattice which we take as the origin. There is no well-defined edge associated with a gradual confining potential and near a MCS,
there is no additional corner where additional MCSs can appear. In the limit of a HP whose amplitude is much larger than the insulating gap, the region near the four corners of 2D TI in proximity with a d-wave SC becomes the location for unconventional superconductivity. It should be pointed out that in the homogeneous system by increasing the chemical potential there is a topological phase transition with bulk gap closing. Moreover, a time-reversal invariant (TRI) d-wave SC with [110] surface, has zero energy flat dispersion due to a nontrivial one-dimensional (1D) winding number at large enough chemical potential [8, 43–45]. Therefore, there might be a transition from MCSs to Majorana flat bands (MFBs) in a nonhomogeneous system with increasing the HP amplitude. The question arises: to what degree can the number of MCSs be varied as we change the amplitude of a confining potential? Will a topological phase transition occur as the bulk gap closes, or will there be a crossover as the bulk gap continues to decrease without closing?

In this work, we show that in a second-order TSCs with a confining HP the MCSs-MFBs transition is merely a crossover: the number of the MZMs gradually increases while there is no 2D bulk gap closing as the HP amplitude increases. We find that the increase of the number of MZMs indicates the appearance of new Majorana states, i.e., the increase in the number of MZMs originates from the fact that only gapped 1D boundary modes become gapless without closing the bulk gap. This eventually leads to a new kind of MFBs which we call Majorana corner flat bands (MCFBs).

This paper is organized as follows. We introduce the model of a two-dimensional TI with a proximity-induced d-wave superconducting gap, as shown schematically in Fig. 1. This system hosts the MCSs when the chemical potential is smaller than the insulating gap. After introducing our model, it will be shown that the MCSs-MFBs transition in OBCs system is a crossover and there is no bulk gap closing as the HP amplitude increases. Then, it will be proposed that this kind of MFB is new and different from the conventional one, which has already been reported along the [110] surface of a TRI 2D nodal d-wave SC, in the sense that they only originate from MCSs or 1D gapped boundary states as illustrated in Fig. 2. Finally, we propose an experimental realization for observing this kind of MFB.

FIG. 2. (Color online) A schematic picture of the procedure by which MCSs become MFBs. (Left panel) There is no HP. The system has topologically distinct 1D gapped modes on the adjacent boundaries which leads to gapless MCSs at the intersection of two different boundaries, i.e., corners. (Right panel) After including the HP, the gapless MCSs remain gapless. However, the 1D gapped boundary modes convert to gapless modes as MCFBs.

Formalism: The Bogoliubov-de Gennes (BdG) Hamiltonian of a 2D TI in proximity with a SC is given by,

\[ H = \frac{1}{2} \sum_{ij} \psi_i^\dagger \begin{pmatrix} \hat{H}_{ij}^N & \hat{\Delta}_{ij} \\ \hat{\Delta}_{ij}^\dagger & -\hat{H}_{ij}^N \end{pmatrix} \psi_j, \]

with \( \psi_i = (c_i^{\uparrow}, c_i^{\downarrow}, \sigma^x c_i^{\uparrow}, \sigma^y c_i^{\downarrow}, \sigma^z c_i^{\uparrow}, \sigma^z c_i^{\downarrow}) \).

Here, \( c_i^{\alpha,\beta}(c_i^{\alpha,\beta}) \) denotes the creation (annihilation) operator of an electron at site \( i = (ix, iy) \), in orbital \( \alpha = a \) or \( b \), with spin \( \beta = \uparrow \) or \( \downarrow \). The normal state and superconducting parts of the Hamiltonian are given by \( \hat{H}_{ij}^N = m_{ij} \sigma_x s_0 + A_{ij}^x \sigma_x s_z + A_{ij}^y \sigma_y s_0 - \delta_{ij} (\mu - V_i) \sigma_0 s_0 \), and \( \hat{\Delta}_{ij} = -i\Delta_{ij} \sigma_y s_0 \), respectively. The mass term is \( m_{ij} = m_0 \delta_{ij} - (t/2) (\delta_{i,i+z} + \delta_{i,i-z} + \delta_{i,i+y} + \delta_{i,i-y}) \) where \( m_0 \) is on-site orbital-dependent energy, and \( t \) is the intra-orbital nearest neighbor hopping amplitude along the \( x \) and \( y \) directions with unit vectors \( \hat{x} \) and \( \hat{y} \). The \( \sigma_{x,y,z} \) and \( s_{x,y,z} \) are Pauli matrices acting on orbital and spin degree of freedoms, respectively, and \( \sigma_0 \) and \( s_0 \) are \( 2 \times 2 \) unit matrices. Moreover, \( A_{ij}^x = (-i\lambda/2)(\delta_{i,i+z} - \delta_{i,i-z}) \), \( A_{ij}^y = (i\lambda/2)(\delta_{i,i+y} - \delta_{i,i-y}) \) are the spin-orbit coupling terms with amplitude \( \lambda \), where the symbol i denoting \( \sqrt{-1} \) should not be confused with the site-index that generally occurs subscripted. The chemical potential is given by \( \mu \) and \( V_i \) is the 2D single particle potential amplitude at site \( i \). The d-wave superconductivity order parameter with \( d_{x^2-y^2} \) symmetry is expressed as \( \Delta_{ij} = (\Delta_d/2)(\delta_{i,i+z} + \delta_{i,i-z} - \delta_{i,i+y} - \delta_{i,i-y}) \).

In the absence of any single particle potential \( V_i = 0 \), the corresponding BdG Hamiltonian in momentum space can be written as \( \mathcal{H} = \sum_k \Psi_k^\dagger \mathcal{H}_{\text{BdG}} \Psi_k / 2 \) where \( \Psi_k^\dagger = \sum_i \psi_i \mathcal{D}^{\dagger}_{ij} \mathcal{D}_{ij} \)}

\[ \mathcal{D}^{\dagger}_{ij} \mathcal{D}_{ij} \]
$E(k) = \pm \sqrt{m^2(k) + x^2 \sin^2 k_x + y^2 \sin^2 k_y} + \mu,$  

so, the insulating gap as an important quantity in our analysis, is given by $|m(k = 0)| = |m_0 - 2t|$. Through this work, we set $m_0 = 1.5$, $t = \lambda = 1$, and $\Delta_d = 0.5$.

Robustness of MCSs, crossover with MFBs and Majorana corner flat bands: In a TRI system, MCSs manifest themselves as Majorana Kramers pairs which are protected zero-energy modes localized at the four corners of the 2D TI in proximity with a $d$-wave. By adding proximity-induced $d$-wave superconductivity, the helical gapless boundary modes of the 2D TI become gapped, so in our system as a 2D square sample, there are 1D gapped localized modes along the four boundaries when the chemical potential is smaller than the insulating gap. By constructing the low-energy Hamiltonian and through the use of localized modes, we can define the topological invariant, which depends on the direction of a boundary [29]. Since the 1D effective systems along the vertical and horizontal boundaries have different topological invariant or Dirac mass, there should be gapless zero modes at four intersections or corners of the 2D TI known as MCSs.

We argue that in a second-order TSC, the MCSs-MFBs transition is actually a crossover in the OBCs system with increasing the HP amplitude: the number of MZMs gradually increases while there is no bulk gap closing as is illustrated in Fig. 3. It can be seen that there are branches of eigenvalues whose values decrease from 0.5 with increasing the HP amplitude although the bulk gap remains open. We find that the proliferation of the MZMs originate from the fact that only gapped 1D boundary modes becomes gapless without the 2D bulk gap closing.

In contrast, in the PBCs system with an increasing HP amplitude, the 2D bulk gap is closed if the potential amplitude at the four corners ($v_{\text{trap}}(r_c)$) of the 2D TI becomes larger than the insulating gap ($v_{\text{trap}}(r_c) > 1$) as shown in Fig. 4. In this case, by increasing the HP amplitude there are no MZMs because there are no 1D gapped boundary modes to become gapless. We confirm that, using sharp potentials such as circular potential, the 2D bulk gap is closed in both OBCs and PBCs systems. Moreover, we have verified that the same behavior persists for larger systems [46].

To see the MCSs-MFBs transition in more detail, we show the real space dependence of the zero-energy local density of states in Fig. 5. In the region outside the black circles of the two lower middle panels of this figure, the HP amplitude is larger than the insulating gap locally, so Fig. 5(b),(e), and (h) indicate that MCSs are robust
consider. Moreover, in Eq. 6, $q_{\parallel}$ zero-energy modes at a surface parallel to $k_{\parallel}$ has a finite winding number, there are sizes the chiral symmetry operator such that $\det(q_{\parallel})$ where $k_{\parallel}$ is independent of $k_{\perp}$. Figure 5 shows the BdG Hamiltonian, (d,e,f) two-dimension harmonic potential, and (g,h,i) zero-energy local density of states for a $51 \times 51$ square lattice with OBCs in the presence of three different HP amplitudes $v_{\text{trap}}(r_c) = 0.4$ (a,d,g), 1.4 (b,e,h), and 2.2 (c,f,i) for $\mu = 0$. Outside the two black circles $v_{\text{trap}} > |m(k = 0)|$ i.e. the HP amplitude is larger than the insulating gap locally. The unit of eigenvalues is $|m(k = 0)|$. The smearing factor in the local density of states is 0.005.

FIG. 5. (Color online) (a,b,c) Eigenvalues of the BdG Hamiltonian, (d,e,f) two-dimension harmonic potential, and (g,h,i) zero-energy local density of states for a $51 \times 51$ square lattice with OBCs in the presence of three different HP amplitudes $v_{\text{trap}}(r_c) = 0.4$ (a,d,g), 1.4 (b,e,h), and 2.2 (c,f,i) for $\mu = 0$. Outside the two black circles $v_{\text{trap}} > |m(k = 0)|$ i.e. the HP amplitude is larger than the insulating gap locally. The unit of eigenvalues is $|m(k = 0)|$. The smearing factor in the local density of states is 0.005.

even outside this circle. Moreover, the region outside the circles can host MFBs, and the additional MZMs originate from only gapped 1D boundary modes that become gapless [46].

**MFBs & MCFBs:** Let us discuss the difference between conventional MFBs in a $d$-wave SC and MCFBs in our system. In a SC with order parameter symmetry $d_{2−2}$, it is well known that there are Andreev flat bound states, which appear at the [110] surface. On the other hand, there is no zero energy bound state at the [100] and [010] surfaces [47, 48]. For this nodal SC, it is possible to define a 1D partial Brillouin zone by fixing the $(d−1)$-dimensional momentum $k_{\parallel}$ at a certain point [43, 47, 49, 50]. As long as the pair potential in such a partial Brillouin zone (BZ) is fully gapped, we can define the one dimensional winding number as the topological invariant of a nodal TSC:

$$W(k_{\parallel}) = \frac{1}{2\pi} \text{Im} \int dk_{\perp} \partial_{k_{\perp}} \ln \det(q),$$

where $k_{\perp}$ is the momentum in a one-dimensional BZ, and $k_{\parallel}$ is the momentum parallel to the surface that we consider. Moreover, in Eq. 6, $q(k)$ is the off-diagonal block of the BdG Hamiltonian in the basis that diagonalizes the chiral symmetry operator such that $\det(q(k)) = \{m^2(k) + (\Delta(k) + i\mu)^2 + \lambda^2 \sin^2 k_x + \lambda^2 \sin^2 k_y\}^2$. For a finite winding number, there are $|W(k_{\parallel})|$-fold degenerate zero-energy modes at a surface parallel to $k_{\parallel}$. Such highly degenerate surface bound-states are known as Majorana flat bands (MFBs) because the energy dispersion is independent of $k_{\parallel}$ [51].

A 2D homogeneous TI in proximity with a $d$-wave SC becomes SC with increasing chemical potential. This transition is a topological phase transition with bulk gap closing since a $d$-wave SC order parameter has line nodes. In this homogeneous system with large enough chemical potential, there are MFBs at the [110] surface because of nontrivial value of winding number. The origin of these MFBs are Andreev bound states. However, here we find that in the case of MCFBs not only there is no 2D bulk gap closing in the OBCs system with increasing harmonic potential amplitude, but also the number of MZMs increases only because of the reduction of the energy of the 1D boundary gapped modes. In addition, MCFBs cannot be characterized with winding number.

**Discussion** It should be added that although MCFBs consist of a lot of very spatially close MZMs, they cannot hybridize and become gapped out. This is in contrast to the fact that MCSs hybridize and annihilate if they are brought close together. The reason for the weak hybridization is naturally explained with the use of the 1D boundary modes and a crossover behavior as follows. We consider $|\text{MCS}(v_{\text{trap}})|$ and $|\text{1DM}(v_{\text{trap}})|$ as the wave functions of the MCSs and 1D gapped modes in the presence of a HP with amplitude $v_{\text{trap}}$, respectively. Without a confining potential ($v_{\text{trap}} = 0$), MCSs at corners and 1D gapped modes localized on boundaries are orthogonal, $\langle \text{MCS}(0)|\text{1DM}(0)\rangle = 0$, because these are eigenvectors of the BdG Hamiltonian with different energies. Since there is no bulk gap closing, the wave functions gradually change with changing the HP amplitude and remain orthogonal i.e. $\langle \text{MCS}(v_{\text{trap}})|\text{1DM}(v_{\text{trap}})\rangle \sim 0$. Therefore, the crossover makes the MFCBs stable by preserving the orthogonality of these wave functions.

**Summary & Experiment:** It has been recently proposed that a second-order TSC hosts Majorana corner states (MCSs) localized at the four corners of a 2D TI in proximity with some unconventional high-temperature SCs. Second-order TSCs always have $(d−1)$-dimensional gapped boundary modes and $(d−2)$-dimensional gapless modes. This work provides the theoretical framework to make the 1D gapped modes gapless in second-order TSCs. Our result suggest that increasing the gradual potential amplitude increases the number of MCSs by making only $(d−1)$-dimensional gapped boundary modes gapless. This finally leads to a new kind of MFB, namely Majorana corner flat bands (MCFBs), which cannot be characterized by 1D winding number and only originate from 1D gapped boundary modes that become gapless without closing the bulk gap. It also has been shown that the MCSs-MFBs crossover prevent from hybridizing MCSs.

In experiment, if one can observe the MCSs in second-order TSCs, such as a hybrid structure of TI and un-
conventional SC or even cold atom systems, one can also observe the MCFS-MFBs crossover and MFCBs with adding a gradual potential such as HP. In order to realize MCFS experimentally, we propose utilizing a harmonic trap potential in cold atoms or heterostructures. This work might open up new prospects for realizing MZMs and its applications in quantum computation and information, which will be left for future investigations.

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This supplemental material consists of the following four sections to provide more details about some arguments in the main text.

1. HAMILTONIAN SYMMETRIES

The Bogoliubov-de Gennes (BdG) Hamiltonian in momentum space,

\[ H_{\text{BdG}} = m(k) \sigma_z s_0 \tau_z + \lambda \sin k_x \sigma_x s_τ \tau_0 + \lambda \sin k_y \sigma_y s_0 \tau_z + \Delta(k) \sigma_0 \tau_y - \mu \sigma_0 s_0 \tau_z, \]  

(S1)

 possesses both particle-hole symmetry and time-reversal symmetry,

\[ \mathcal{T} H_{\text{BdG}}(k) \mathcal{T}^{-1} = H_{\text{BdG}}(-k), \]  

(S2)

\[ \mathcal{P} H_{\text{BdG}}(k) \mathcal{P}^{-1} = -H_{\text{BdG}}(-k), \]  

(S3)

where \( \mathcal{T} = i \sigma_0 s_0 \tau_0 \) and \( \mathcal{P} = \sigma_0 s_0 \tau_z \). The combination of these two symmetries can give rise to a chiral symmetry,

\[ \mathcal{S} H_{\text{BdG}}(k) \mathcal{S}^{-1} = -H_{\text{BdG}}(k), \]  

(S4)

where \( \mathcal{S} = -i \mathcal{P} \mathcal{T} \). Therefore, in the basis that diagonalizes chiral symmetry, the BdG Hamiltonian gets the following off-diagonal block form,

\[ \tilde{H}_{\text{BdG}} = \begin{pmatrix} 0 & q(k) \\ \tilde{q}^\dagger(k) & 0 \end{pmatrix}, \]  

(S5)

where \( q(k) \) is a 4 \times 4 square matrix. It can be shown that the determinant of \( q(k) \) is given by \( \det q(k) = \{m^2(k) + (\Delta(k) + i \mu)^2 + \lambda^2 \sin^2 k_x + \lambda^2 \sin^2 k_y\}^2 \) where

\[ \Delta(k) = \Delta_d (\cos k_x - \cos k_y), \]  

(S6)

\[ m(k) = m_0 - t(\cos k_x + \cos k_y). \]  

(S7)

2. FINITE SIZE EFFECTS

A two-dimensional (2D) topological insulator (TI) is a metal if the chemical potential is larger than the insulating gap, so the bulk gap should be closed at \( \mu \geq |m(k = 0)| \) with periodic boundary conditions (PBCs).
defined where $\mu$ is the chemical potential, and $V_i$ is the amplitude of the potential at site $i$. Using a harmonic potential (HP) as a single particle potential, the $V_i$ gets its maximum value at the four corners of a 2D TI, which we denote here by $v_{\text{trap}}(r_c)$. Therefore, for $\mu = 0$ and $v_{\text{trap}}(r_c) > |m(k = 0)|$, the $\tilde{\mu}_i$ is larger than the insulating gap at some sites close to the four corners. The number of these sites increases as we increase the HP amplitude. Moreover, for a given value of $v_{\text{trap}}(r_c)$, as we increase the system size, the HP becomes a smoother potential. Therefore, we anticipate that the bulk gap closes at a point closer to the insulating gap value as we increase the size of the system. In Fig. S1 and Fig. S2, we used two different lattice sizes to illustrate this. It should be added that in PBCs there are no boundary states. However, this is not the case for the open boundary conditions (OBCs) case. As shown in Fig. S3 and Fig. S4, increasing system size can only increase the number of boundary states and cannot close the bulk gap at smaller value of $v_{\text{trap}}(r_c)$. As shown in Fig. S5, there are no Majorana corner states and there is no crossover in the PBCs case.

3. THE ORIGIN OF MAJORANA CORNER FLAT BANDS

Majorana corner flat bands (MCFBs) originate from only gapped states localized at one-dimensional (1D) boundaries. In Fig. S6, the square of the wave function's amplitude associated with only blue points are plotted. As we increase the HP amplitude, the energy corresponding to these 1D boundary states become smaller, and they become more localized around the corners. By increasing the HP amplitude, more and more 1D gapped modes become gapless.
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FIG. S6. (Color online) Eigenvalues of the BdG Hamiltonian and the square of the wave function’s amplitude for different values of $v_{\text{trap}}(r_c)$ and for a $51 \times 51$ square lattice with OBCs. The square of the wave function’s amplitude are plotted only for the eigenvalues that are denoted with blue color. They are gapped boundary states that become gapless by increasing the HP amplitude. We take $m_0 = 1.5$, $\mu = 0$, $t = \lambda = 1$, $\Delta_d = 0.5$.

4. CIRCULAR POTENTIAL

Let us define the circular potential as $V_i = v_{\text{circ}}$ for $(i_x-i_c^x)^2+(i_y-i_c^y)^2 > R^2$ where $v_{\text{circ}}$ is the strength of the circular potential, and $i^c = (i_c^x, i_c^y)$ is the coordinate of the central site of a 2D sample. Here, we take $R = N_x/2$ where $N_x$ is the number of sites along $x$-axis direction. As shown in Fig. S7 and Fig. S8, the bulk gap closes in both OBCs and PBCs for a circular potential, so there is no crossover and no MCFBs in the presence of a circular potential which is not the case for HP.

FIG. S7. (Color online) a) Density of states, and b) eigenvalues of the BdG Hamiltonian as a function of $v_{\text{circ}}$ for a $51 \times 51$ square lattice with OBCs. The unit of all values is $|m(k=0)|$. We take $m_0 = 1.5$, $\mu = 0$, $t = \lambda = 1$, $\Delta_d = 0.5$.

FIG. S8. (Color online) a) Density of states, and b) eigenvalues of the BdG Hamiltonian as a function of $v_{\text{circ}}$ for a $51 \times 51$ square lattice with PBCs. The unit of all values is $|m(k=0)|$. We take $m_0 = 1.5$, $\mu = 0$, $t = \lambda = 1$, $\Delta_d = 0.5$. 