Realizing DIII Class Topological Superconductors using $d_{x^2-y^2}$-wave Superconductors

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In this work, we show that a quasi-one-dimensional $d_{x^2-y^2}$-wave superconductor with Rashba spin-orbit coupling is a topological superconductor (TS). This time-reversal invariant DIII class TS supports two topologically protected zero energy Majorana fermions at each end of the system. In contrast to proposals using $s$-wave superconductors in which a strong magnetic field and the fine tuning of the chemical potential are needed to create Majorana fermions, in our proposal, the topologically non-trivial regime can be reached in the absence of a magnetic field and in a wide range of chemical potential. Experimental signatures and realizations of the proposed superconducting state are discussed.

Introduction—A Majorana fermion is a real fermion which has only half the degrees of freedom of a usual Dirac fermion. It was first pointed out by Read and Green [1] that zero energy Majorana fermion modes exist at the vortex cores of a 2D $p_x + i p_y$ superconductor and these Majorana fermions are non-Abelian particles [2]. Soon after, Kitaev constructed a spinless fermion model and showed that a single Majorana fermion exists at each end of a $p$-wave superconducting wire [3]. Recently, several groups proposed that effective $p$-wave superconductors can be realized when an $s$-wave pairing is induced in systems with spin-orbit coupling [4][13].

particularly, the (quasi)-one-dimensional effective $p$-wave superconductors attracted much attention [6][15] due to the fact that Majorana fermion end states can exist in the absence of vortices and the energy separation between the Majorana zero energy mode and other finite energy fermionic modes is relatively large, on the order of the $p$-wave pairing gap [10].

The existence of Majorana fermions in the above mentioned systems is profound. It is related to the symmetry of the Hamiltonian which describes the system. According to symmetry classification of Hamiltonians [14][16], a BdG Hamiltonian with particle-hole symmetry, broken time-reversal symmetry and broken $SU(2)$ spin rotation symmetry, falls into the D class. In one spatial dimension, a D class Hamiltonian is classified by a $Z_2$ topological number. A system described by a BdG Hamiltonian with a non-trivial $Z_2$ topological number possesses Majorana end states.

To be in the proposed topologically non-trivial regime, it requires a Rashba spin-orbit coupling to break the spin degeneracy, a magnetic field to break the Kramers degeneracy at the Rashba-band crossing point (RCP), fine tuning the chemical potential to the RCP and finally induce an $s$-wave superconducting pairing at the Fermi energy. However, tuning the chemical potential to the RCP, which is near the electronic band bottom, reduces the electron density severely and electrons can be easily localized by disorder in this regime. The strong magnetic field required can also suppress superconductivity. A schematic picture of this proposal is shown in Fig.2a.

A DIII class Hamiltonian respects both time-reversal and particle-hole symmetry and breaks $SU(2)$ spin rotation symmetry [14][16]. In this Letter, we point out that a DIII class TS can be realized when electrons in a quasi-one-dimensional wire with spin-orbit coupling acquire a $d_{x^2-y^2}$-wave pairing. In the topologically non-trivial regime, two zero energy Majorana fermion modes appear at each end of the wire. In our proposal, Majorana fermions can be created in the absence of an external magnetic field and in a wide range of chemical potential, e.g. there is no need to tune the chemical potential to the RCP. In the presence of an external magnetic field, the system is in the D class and a single Majorana end state appears at each end of the wire. Experimental signatures and realizations of this DIII class TS will be discussed at the end.

Single-channel model—Before studying the more realistic quasi-one-dimensional quantum wires, in this section, we first consider a strictly one-dimensional DIII class Hamiltonian which supports double Majorana end states in the absence of an external magnetic field.

We construct the following model

$$H_{1D} = H_i + H_{SO} + H_{SC} + H_Z$$

$$H_i = \sum_{j,\alpha} \left( \frac{t}{2} (\psi_j^\dagger \sigma_\alpha \psi_{j+1} + h.c.) - \mu \psi_j^\dagger \sigma_\alpha \psi_j \right)$$

$$H_{SO} = \sum_{j,\alpha,\beta} -\frac{1}{2} \sigma_\alpha \psi_j^\dagger \psi_{j+1,\beta} \sigma_\beta \psi_{j+1} + h.c.$$ (1)

$$H_{SC} = \sum_{j} \frac{1}{2} \Delta_0 \left( \psi_j^\dagger \sigma_\alpha \psi_{j+1,\alpha} + \psi_j \sigma_\alpha \psi_{j+1,\beta} \right) + h.c.$$ (1)

$$H_Z = \sum_{j} V_j (\psi_j^\dagger \psi_{j+1} - \psi_j \psi_{j+1}^\dagger)$$

where $\psi_j$ is a fermion operator at site $j$, $\alpha$ and $\beta$ are the spin indices, $t$ is the hopping amplitude, $\alpha_R$ is the spin-orbit coupling strength, $\Delta_0$ is the superconducting pairing amplitude, and $\sigma_\alpha$ is a Pauli spin matrix. $V_j$ denotes the strength of the Zeeman term. Without the pairing terms, the above model describes a wire with spin-orbit coupling. If an $s$-wave (on-site superconducting) pairing is induced on the wire, as it is done in Ref., no Majorana fermions can be created without breaking time-reversal symmetry. In the following, we show that our model supports double Majorana end states in the presence of time-reversal symmetry.

The energy spectrum of $H_{1D}$ with $V_j = 0$ is shown in Fig.1a. Due to Krammers degeneracy, every energy level in Fig.1a is doubly degenerate. It is evident from the energy spectrum that zero energy modes exist when the chemical potential satisfies $|\mu| < |\alpha R|$. The sum of the two ground-state wavefunctions is shown in Fig.1b to confirm that the zero energy modes are end states.
In other words, there are two Majorana fermions at each end of the wire. In the topologically trivial regime where $|\mu| > \alpha_R$, the ground state wavefunctions are predominantly in the bulk as shown in FIG.1c.

To understand how the DIII topological superconducting state is achieved in our model, we note that a general criteria for realizing a one-dimensional DIII class TS is to have an odd number of negative pairing amplitudes at the Fermi points with Fermi momentum between 0 and $\pi$ \cite{17}. We show that this is indeed the case for $H_{1D}$.

In the momentum space, Hamiltonian $H_{1D}$ can be written as

$$H_{1D}(k) = \sum_k \Psi_k^\dagger \begin{pmatrix} -(t \cos k + \mu) + i \sigma_0 \sin k \sigma_y \Psi_k + \Delta_0 \cos k \Psi_k^\dagger \Psi_{-k}^\dagger + h.c. \end{pmatrix},$$

(2)

where $\Psi_k^\dagger = (\Psi_{kR}, \Psi_{kL})$. The Hamiltonian has spectrum $E(k) = \pm \sqrt{\left[(t \cos k - \mu) \pm \alpha_R \sin k \sigma_y \right]^2 + \left(\Delta_0 \cos k \right)^2}$ and it is generally gapped unless $|\mu| = \alpha_R$ at which points topological phase transitions take place. In the basis which diagonalize the Rashba term, the Hamiltonian can be written as

$$\tilde{H}_{1D}(k) = \sum_{k,a=\pm} \left[-(t \cos k + \mu) + a(\alpha_R \sin k \sigma_y)\tilde{\psi}_{ka}^\dagger \tilde{\psi}_{ka} + \text{sgn}(k)\Delta_0 \cos k \tilde{\psi}_{ka}^\dagger \tilde{\psi}_{-ka} + h.c.\right],$$

(3)

where $\tilde{\psi}_{ka}$ denotes a fermion in the new basis. When $|\mu| < \alpha_R$, there are two Fermi points $k_1, k_2$ with $0 < k_1, k_2 < \pi$. In this regime, it can be shown that one and only one of the pairing amplitudes of the two bands at the Fermi level $\Delta_0 \cos k_1$ and $\Delta_0 \cos k_2$ is always negative. Therefore, the superconductor is in the topologically non-trivial regime. A schematic picture is shown in FIG.2b. When $|\mu| > \alpha_R$, we have $\cos k_1 \cos k_2 > 0$ and the pairing amplitudes at the two Fermi points have the same sign and the system is in the topologically trivial regime.

In short, in order to reach the topologically non-trivial regime, we need to break the spin degeneracy by the Rashba term and induce a $k$-dependent pairing such that there can be an odd number of negative pairing amplitudes for positive $k$ at the Fermi energy. It is important to note that there is no need to tune the chemical potential to the RCP which is near the band bottom. If the induced pairing is $s$-wave \cite{6,13}, the topologically non-trivial phase is not accessible.

The topologically non-trivial state can be further verified by calculating the topological invariant of $H_{1D}(k)$ \cite{17}. The topological invariant can be written as

$$N_{DIII} = \frac{\text{Pf}[Tq(k = \pi)]}{\text{Pf}[Tq(k = 0)]} \exp\left\{-\frac{1}{2} \int_0^\pi dk \text{Tr}[q^\dagger(k)\partial_k q(k)]\right\},$$

(4)

where Pf denotes the Pfaffian, $T = i\sigma_y$ is the time-reversal operator, and $q(k) = \frac{1}{2}[e^{i\theta_+}(\sigma_0 - \sigma_y) + e^{i\theta_-}(\sigma_0 + \sigma_y)]$ which is an off-diagonal block of the flat-band Hamiltonian \cite{17,18} derived from $H_{1D}(k)$. Here, $e^{i\theta_\pm} = \frac{\pm \cos(k) - \mu \pm \alpha_R \sin k}{\sqrt{(-\cos(k) - \mu \pm \alpha_R \sin k)^2 + \Delta_0^2 \cos^2 k}}$. From Eq.4 the topological invariant number can be found to be trivial ($N_{DIII} = 1$) when $|\mu| > \alpha_R$ and non-trivial ($N_{DIII} = -1$) when $|\mu| < \alpha_R$.

Single-channel model with finite $V_z$. When $V_z$ is finite, the energy spectrum of $H_{1D}(k)$ becomes $E(k) = \pm \sqrt{F(k) \pm 2\sqrt{G(k)}}$, where $F(k) = (t^2 \cos k + \mu k^2 + \Delta_0^2 \sin^2 k + V_z^2)$ and $G(k) = (t^2 \cos k + \mu k^2)^2 V_z^2 + (t^2 \cos k + \mu k^2) \Delta_0^2 \sin^2 k + V_z^2 \Delta_0^2 \cos^2 k$. From the energy spectrum, we note that the energy gap closes when $(\mu \pm t)^2 = V_z^2 - \Delta_0^2$ and $|\mu| = \sqrt{V_z^2 + \Delta_0^2}$.

Moreover, the $V_z$ term breaks time-reversal symmetry and changes the Hamiltonian from DIII class to D class. It is known that a 1D Hamiltonian in D class
regions between a number of Z points. but there are no topological phase transitions at these points with chemical potential $\mu = \mp |\sqrt{V^2 - \Delta_0} - t|$ respectively. Double Majorana fermion end states exist when $\mu$ is between $c_1$ and $c_2$. Single Majorana fermion end states exist when $\mu$ is in the regions between $a_1$ and $c_1$, $c_2$ and $a_2$.

The energy eigenvalues of $H_{1D}$ versus the chemical potential are shown in Fig.3. In Fig.3, the region between $c_1$ and $c_2$ allows double Majorana fermions where $c_1$ and $c_2$ are points with $\mu = \mp |\sqrt{V^2 - \Delta_0} + t|$ respectively. When $|\mu| > |\sqrt{V^2 - \Delta_0} + t|$, the Hamiltonian is topologically trivial and the Majorana end states disappear. At points $b_1$ and $b_2$ where $\mu = \mp \sqrt{V^2 + \alpha_R^2}$, the energy gap closes but there are no topological phase transitions at these points.

The even and odd number of Majorana end states in Fig.3 can be verified by calculating the $Z_2$ Majorana number $\mathcal{M}$ of $H_{1D}(k)$. Following Refs [3, 11] the Majorana fermion number can be defined as

$$\mathcal{M} = \text{sgn}[\text{Pf}(B(0))] \text{sgn}[\text{Pf}(B(\pi))] = \pm 1.$$ (5)

The matrix $B(k)$ is defined as $B(k) = H_{1D}(k)(\sigma_x \otimes \sigma_0)$. $B(k)$ is anti-symmetric and its Pfaffian is well-defined. $\mathcal{M} = \pm 1$ indicates the even and odd number of Majorana fermions at one end of the wire respectively. In terms of the parameters of the Hamiltonian, the Majorana number can be written as

$$\text{sgn}[(t + \mu)^2 - (V^2 - \Delta_0^2)][(-t + \mu)^2 - (V^2 - \Delta_0^2)].$$ (6)

The Majorana numbers calculated according to Eq.6 are consistent with the results shown in Fig.3. The Majorana number is $\mathcal{M} = -1$ when $|\sqrt{V^2 - \Delta_0} - t| < |\mu| < |\sqrt{V^2 - \Delta_0} + t|$ and $\mathcal{M} = 1$ otherwise.

Multi-channel case—In realistic situations, multiple transverse sub-bands of a wire are occupied and it is important to show that Majorana fermions exist in this situation. In this section, we show that Majorana fermions exist in quasi-one-dimensional wires. Importantly, the quasi-one-dimensional model can be realized by inducing $d_{x^2-y^2}$-wave superconductivity on a wire with strong spin-orbit coupling.

In the quasi-one-dimensional case, the Hamiltonian can be written as:

$$H_{1D} = H_t + H_{SO} + H_{SC} + H_Z,$$
$$H_t = \sum_{R,i,a} \frac{1}{2} \left[ \langle \psi_R \mid d_i \psi_R \rangle - \langle \psi_R \mid d_i \psi_R \rangle \right] - \mu \psi_R \psi_R,$$
$$H_{SO} = \sum_{R,i,a,\beta} \frac{1}{2} \left[ \langle \psi_R \mid d_i \psi_R \rangle - \langle \psi_R \mid d_i \psi_R \rangle \right] \times \left[ \langle \beta \mid \psi_R \rangle \psi_R \right] + h.c.,$$
$$H_{SC} = \sum_{R,i} \frac{1}{2} \left[ \langle \psi_R \mid \psi_R \rangle - \langle \psi_R \mid \psi_R \rangle \right] - \Delta_0 \langle \psi_R \mid \psi_R \rangle + \Delta_0 \langle \psi_R \mid \psi_R \rangle + h.c.,$$
$$H_Z = \sum_{R,i} V_z \langle \psi_R \mid \psi_R \rangle.$$ (7)

Here, $R$ denotes the lattice sites, $d_i$ denotes the two unit vectors $d_x$ and $d_y$ which connects the nearest neighbor sites in the $x$ and $y$ directions respectively. This model is the same as the tight-binding model in Ref[12] except for the superconducting pairing terms. The pairing terms in $H_{1D}$ can be written as $\Delta_0[\cos(k_x) - \cos(k_y)]$ in the momentum space. Therefore, $H_{1D}$ describes a quantum wire with spin-orbit coupling and a $d_{x^2-y^2}$-wave superconducting pairing. A schematic picture of the experimental setup is shown in Fig.4.

FIG. 3: Excitation energy as a function of chemical potential. The parameters of $H_{1D}$ are: $t = 12$, $\Delta_0 = 1$, $\alpha_R = 4$ and $V_z = 10$. Points $a_1$, $b_1$ and $c_1$ (with $i = 1,2$) denote gap closing points with chemical potential $\mu = \mp |\sqrt{V^2 - \Delta_0} + t|$, $\mu = \mp |\sqrt{V^2 - \Delta_0} + t|$ and $\mu = \mp |\sqrt{V^2 - \Delta_0} - t|$ respectively. Double Majorana fermion end states exist when $\mu$ is between $c_1$ and $c_2$. Single Majorana fermion end states exist when $\mu$ is in the regions between $a_1$ and $c_1$, $c_2$ and $a_2$.

FIG. 4: A wire with strong spin-orbit coupling in proximity to a $d_{x^2-y^2}$-wave superconductor. Double Majorana end states may appear in the absence of an external magnetic field.
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perconducting states through Andreev reflection experi-
can be distinguished from each other and from trivial su-
zero bias conductance peak of $G \approx 2 \frac{e^2}{h}$ in An-
degree reflection experiments [21, 22] when a normal metal
lead couples to a Majorana end state. On the other hand,
the double Majorana end states in DIII class TS induce a
zero bias conductance peak of $G \approx 2 \frac{e^2}{h}$ instead.
Therefore, the two topological superconducting phases
can be distinguished from each other and from trivial su-
perconducting states through Andreev reflection experi-
ments.

**Discussion**—A few important comments follow. First,
the DIII class topological superconductor proposed in
this work is truly different from the time-reversal in-
variant superconducting state obtained by inducing an
s-wave or a d-wave pairing on the surface of a topological
insulator (TI) [25,27]. The TI surface state is described
by a single Dirac cone (in the simplest case). With only
a single species of fermion at the Fermi level, one cannot
create a superconducting wire with double Majorana end
states even though single Majorana fermions can be cre-
ated in the presence of an external magnetic field. Sato et
al. studied a d-wave superconductor with Rashba terms
in the presence of an external magnetic field but no DIII
class TS phase is reported [28].

Second, it is pointed out recently that single Majorana
fermion end states can be created at arbitrary chemical
potential if a magnetic field is applied along the wire in
the s-wave pairing case [20,27]. However, the magnetic
field $\vec{B}$ required to reach the topologically non-trivial
state is still strong comparing to the induced pairing gap
$\Delta_S$, namely, $\mu_0 |\vec{B}| > \Delta_S$ where $\mu_0$ is the effective
magnetic moment of electrons.

Third, for simplicity, we assumed that the wire is
aligned along the x-direction. Tilting the wire with re-
spect to the x-axis slightly has no major effect on the
Majorana end states since this kind of perturbation does
not change the symmetry class of the system.

Fourth, one possible realization of $H_{qLD}$ is by induc-
ing $d_{x^2−y^2}$-wave superconducting pairing on the Au (111)
surface state. It has been shown that the Au (111) sur-
face has a Rashba band with Rashba energy of about
60meV [29]. The proximity gap induced on Au by LSCO
can reach 10meV [30]. These large energy scales make Au
on LSCO a promising candidate of realizing topological
superconducting states. However, the induced proxim-
ity pairing shown in the recent experiment may not be
d-wave due to the presence of strong disorder in the Au
layer.

Another candidate material of a DIII class TS is a
layered heavy fermion superconductor CeCoIn$_5$. Bulk
CeCoIn$_5$ is a $d_{x^2−y^2}$-wave superconductor. Recently, su-
perconducting thin films of CeCoIn$_5$ with only several
atomic layers thick can be fabricated [31]. Suppose we
have a thin film of CeCoIn$_5$, due to the strong spin-orbit
coupling and the broken of inversion symmetry on the
surface, the top layer of CeCoIn$_5$ acquires a Rashba term
[32]. Therefore, the top layer of CeCoIn$_5$ can be de-
scribed by $H_{qLD}$. In a separate work, we show in detail
that a thin film of CeCoIn$_5$ is a DIII class TS.

**Conclusion**—We show that a quasi-one-dimensional
$d_{x^2−y^2}$-wave superconductor with Rashba spin-orbit cou-
ting terms is a DIII class TS which supports double Ma-
ajorana end states. In the presence of a magnetic field, sin-
gle Majorana end states appear. These two topological
superconducting states can be probed using Andreev re-
fection experiments. We suggest that Au wires on LSCO
and thin films of CeCoIn$_5$ are candidate materials of this
new topological superconducting state.

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zero modes are robust against disorder even when $V_z$ is finite. However, this is truly only for the strictly one-dimensional case.

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