Topological qubits in graphenelike systems

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The fermion-doubling problem can be an obstacle to getting half a qubit in two-dimensional fermionic tight-binding models in the form of Majorana zero modes bound to the core of superconducting vortices. We argue that the number of such Majorana zero modes is determined by a $\mathbb{Z}_2 \times \mathbb{Z}_2$ topological charge for a family of two-dimensional fermionic tight-binding models ranging from noncentrosymmetric materials to graphene. This charge depends on the dimension of the representation (i.e., the number of species of Dirac fermions—where the doubling problem enters) and the parity of the Chern number induced by breaking time-reversal symmetry. We show that in graphene there are as many as ten order parameters that can be used in groups of four to change the topological number from even to odd.

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I. INTRODUCTION

A major hurdle in the realization of quantum computers is the problem of decoherence. Qubits generically do not last long in the presence of the environment. Overcoming decoherence is possible if the qubit is stored nonlocally using a many-body state, in such a way that the reservoir, which only couples locally to the system, is unable to damage the quantum information.¹ An implementation of this scheme can be achieved if the many-body ground state supports excitations obeying non-Abelian braiding statistics. Non-Abelian braiding statistics that departs from the Bose-Einstein or Fermi-Dirac statistics can only be realized in effectively two-dimensional (2D) systems, such as the $\nu=5/2$ fractional quantum Hall state on the one hand,² or in chiral $p_x \pm ip_y$ 2D superconductors where a half vortex binds a zero-energy midgap state on the other hand.^{3,4} In the latter example, due to particle-hole symmetry (PHS), this zero mode is a Majorana fermion. A two-state system—a qubit—can be assembled from one complex fermion made up of a pair of such Majorana fermions sitting at far away vortices. The splitting of the energies from exactly zero is exponentially small in the separation between the vortices and thus the time to degrade a quantum superposition is exponentially large in the distance between the vortices.

Majorana fermions bound to the core of vortices in a superconductor were discovered by Jackiw and Rossi.⁵ There is a single zero-energy midgap state when the vorticity is $n = \pm 1$ (there are generically $|n|$ zero modes). However, these results are obtained for the case of the minimal representation of Dirac fermions whose support in space is the 2D continuum. The fermion-doubling problem, discovered in the context of lattice-gauge theory,⁶ prevents importing these results of Jackiw and Rossi to condensed-matter systems, which are models defined on lattices. In graphene, for instance, one does have the Majorana fermions from which it is possible to assemble the qubits, as shown by Ghaemi and Wilczek.⁷ However, there are four of them in each vortex because there are two Dirac cones for each spin polarization

in graphene. Even numbers of Majorana fermions are not stable, as local perturbations can move them away from zero energy.

One can get much insight into the problem of how many Majorana fermions can be realized in effectively 2D tight-binding models if one looks into ideas for addressing the fermion-doubling problem in lattice-gauge theories. There is the original proposal due to Wilson, which is achieved by adding perturbations (Wilson masses) to a lattice Hamiltonian that opens gaps at undesirable duplicate Dirac points.⁸ However, from the point of view of a lattice-gauge regularization of quantum chromodynamics, this option has the undesirable property of breaking the chiral symmetry. Alternatively, the idea that the fermion doubling can be overcome by considering an n -dimensional system as a boundary of a $(n+1)$ -dimensional one was put forth by Callan and Harvey in Ref. 9 (see also Refs. 10 and 11). In fact, it is the Callan-Harvey effect that is at work in the remarkable results obtained by Fu and Kane:¹² (i) surface states in three-dimensional (3D) topological insulators with time-reversal symmetry (TRS) realize an odd number of Dirac fermions in the minimal representation of the Clifford algebra. (ii) They can be used to achieve an odd number of Majorana fermions bound to vortex cores induced by the proximity to a type-II superconductor.

We argue in this paper that the Wilson prescription is a route to attain an odd number of Majorana fermions in effectively 2D condensed-matter systems. The chief reason is that one is not constrained to impose chiral symmetry as in lattice-gauge theory. However, not any Wilson mass can be used for this purpose, only those that break TRS. This approach naturally leads to a $\mathbb{Z}_2 \times \mathbb{Z}_2$ topological charge that discerns whether the system has an even or odd number of Majorana fermions attached to a superconducting (SC) vortex. In essence, the parity of the number of zero modes is determined by the number of Dirac points which have not been knocked out by changing the Chern number via the TRS-breaking Wilson mass. For systems where the number of species is odd, like in the case of surface states of TRS topological insulators, odd numbers of zero modes occur

without breaking TRS (odd $\times$ even case). In the case of graphene, which is one focus of this paper and where there is an even number of Dirac cones, TRS must be broken so as to obtain an odd Chern number and, in turn, an odd number of Majorana fermions (even $\times$ odd case). In all other cases, including graphene when TRS is unbroken (even $\times$ even case) and surface states of topological insulators with large enough magnetic field (odd $\times$ odd case), there are even numbers of Majorana fermions. Notice that, according to this $\mathbb{Z}_2 \times \mathbb{Z}_2$ classification, systems defined on 2D lattices must have both SC pairing correlations and a nonzero Chern number that accounts for a *thermal* Hall effect in order to have non-Abelian quasiparticles. This is “the poor cousin,” i.e., the mean-field version, of the $\nu=5/2$ quantum Hall state.

II. TUNING THE NUMBER OF MAJORANA FERMIONS

To illustrate how it is possible to use a Wilson mass prescription to change at will the number of Majorana fermions in a 2D tight-binding model, we begin with the pure Rashba kinetic energy

$$H_\alpha := \sum_{\mathbf{r}} \sum_{\hat{n}=\hat{x},\hat{y}} (i\alpha c_{\mathbf{r}+\hat{n}}^\dagger \sigma_{\hat{n}} c_{\mathbf{r}} + \text{H.c.}) \quad (1)$$

that we define on a square lattice with sites denoted by $\mathbf{r} = m\hat{x} + n\hat{y}$, where m and n are integers. Here, $c_{\mathbf{r}}^\dagger = (c_{\mathbf{r},s}^\dagger)$ is a doublet that creates on site $\mathbf{r}$ an electron with the spin projection $s = \uparrow, \downarrow$ along the quantization axis, $\sigma_{\hat{x}} \equiv \sigma_x \equiv \sigma_1$ and $\sigma_{\hat{y}} \equiv \sigma_y \equiv \sigma_2$ are the first two Pauli matrices while the third Pauli matrix σ_3 defines the quantization axis in spin space, and the real-valued number α sets the energy scale for the Rashba hopping. At half filling, i.e., at vanishing chemical potential, the Fermi surface collapses to the four nonequivalent Fermi points

$$\mathbf{p}_F = (0,0), (0,\pi), (\pi,0), (\pi,\pi). \quad (2)$$

These Fermi points are TRS in that they change by a reciprocal wave vector under the inversion $\mathbf{p} \rightarrow -\mathbf{p}$. Linearization of the energy spectrum of H_α in the vicinity of these four Fermi points yields an 8×8 massless Dirac Hamiltonian, i.e., a reducible representation of the Clifford algebra four times larger than the minimal one in 2D continuum space. This is a manifestation of the fermion doubling. Hamiltonian (1) preserves TRS but breaks completely SU(2) spin-rotation symmetry (SRS).

We now introduce the same spectral gap at all the Fermi points, Eq. (2). We achieve this with the help of a singlet SC order parameter parametrized by a complex-valued Δ ,

$$H_\Delta := \sum_{\mathbf{r}} [\Delta c_{\mathbf{r}}^\dagger (i\sigma_{\hat{y}}) c_{\mathbf{r}}^\dagger + \text{H.c.}], \quad (3)$$

that we add to Hamiltonian (1),

$$H_\alpha \rightarrow H_\alpha + H_\Delta. \quad (4)$$

This 2D tight-binding Hamiltonian is the relative to a non-centrosymmetric superconductor in the Rashba-Dirac limit and with singlet SC pairing studied in Ref. 13. A TRS-breaking vortex

FIG. 1. (Color online) Energy levels for the lattice Hamiltonian (8) as a function of $h_3 \equiv h_z$ for $h_1 \equiv h_x = 0.55h_3$, $h_2 \equiv h_y = 0.45h_3$, and $\alpha = \Delta(r=\infty) = 1$. Although finite-size effects prevent the closing of the bulk gap, the vanishing curvature of the gap in the bulk is a footprint of each thermodynamic transition as a function of h_z . In region IV, there are $8(=4 \times 2)$ midgap states, four bound to the vortex and four bound to the antivortex. Their degeneracy is lifted by the combined effects of intravortex-level or intervortex-level repulsion. There are $6(=3 \times 2)$, $4(=2 \times 2)$, and $2(=1 \times 2)$ midgap states in regions III, II, and I, respectively. In the limit in which the vortex and antivortex separation goes to infinity, the intervortex-level repulsion is exponentially suppressed and midgap states can be converted to Majorana fermions. Thus, an odd number of Majorana fermions attached to an isolated vortex are found in regions III and I.

$$\Delta \rightarrow \Delta(r) \exp(i\theta) \quad (5)$$

with the profile $\Delta(r)$, where r and θ are polar coordinates, binds four Majorana fermions at the Fermi energy via the Jackiw-Rossi solutions.¹³

Finally, we define the three independent TRS-breaking Wilson masses

$$H_h := \sum_{\mathbf{r}} \left(\sum_{\hat{n}=\hat{x},\hat{y}} h_{\hat{n}} c_{\mathbf{r}+\hat{n}}^\dagger \sigma_3 c_{\mathbf{r}} + \text{H.c.} + 2h_3 c_{\mathbf{r}}^\dagger \sigma_3 c_{\mathbf{r}} \right) \quad (6)$$

parametrized by the triplet of energy scales,

$$\mathbf{h} = (h_1, h_2, h_3) \equiv (h_x, h_y, h_z) \equiv (h_x, h_y, h_z). \quad (7)$$

Each Wilson mass breaks TRS and breaks SU(2) SRS down to U(1).

We are going to show numerically on the lattice and analytically in the continuum limit that the Wilson masses $\mathbf{h}$ can be used to change the number of Majorana fermions bound to the core of the vortex, Eq. (5), in

$$H := H_\alpha + H_\Delta + H_h \quad (8)$$

one by one from four to zero.

Figure 1 displays the energy spectrum of Hamiltonian (8) obtained from numerical diagonalization on a square lattice made of 39×39 sites. Periodic boundary conditions are imposed in the presence of a vortex and an antivortex with winding numbers ± 1 , respectively, that are as far apart as possible. A continuum of energy eigenstates is visible as are bulk-gap-closing transitions as a function of $h_3 \equiv h_z$. Midgap states are also visible although they are not located at the

Fermi energy because of level repulsion for states attached to the same defect and because of the finite separation between the two defects. Starting from four midgap states per isolated vortex in the thermodynamic limit, increasing h_3 decreases their number by one after each bulk-gap-closing transition.

The same results follow analytically after linearization of the spectrum around the Fermi points, Eq. (2). Indeed, linearization of Hamiltonian (8) yields, in the Bogoliubov-de-Gennes single-particle representation, the 16×16 -dimensional block-diagonal Hermitian matrix,

$$\mathcal{H} := \text{diag}(\mathcal{H}_1, \mathcal{H}_2, \mathcal{H}_3, \mathcal{H}_4) \quad (9a)$$

with the 4×4 Hermitian blocks

$$\mathcal{H}_j = \begin{pmatrix} -\eta_j & p & \delta_j & 0 \\ \bar{p} & \eta_j & 0 & \delta_j \\ \bar{\delta}_j & 0 & -\eta_j & -p \\ 0 & \bar{\delta}_j & -\bar{p} & \eta_j \end{pmatrix}, \quad (9b)$$

whereby the units $\hbar = v_F = 1$ have been chosen, the complex notation $p \equiv p_1 + ip_2$ is used for the momenta whereby $\bar{x}$ denotes the complex conjugate of x , and

$$\delta_1 = \delta_2 \equiv \Delta, \quad \delta_3 = \delta_4 \equiv \bar{\Delta}, \quad (9c)$$

$$\eta_1 \equiv \eta_{(0,0)} = 2(h_3 + h_1 + h_2), \quad (9d)$$

$$\eta_2 \equiv \eta_{(0,\pi)} = -2(h_3 + h_1 - h_2), \quad (9e)$$

$$\eta_3 \equiv \eta_{(\pi,\pi)} = 2(h_3 - h_1 - h_2), \quad (9f)$$

$$\eta_4 \equiv \eta_{(\pi,0)} = -2(h_3 - h_1 + h_2). \quad (9g)$$

The mathematical form of any of the four matrices $\mathcal{H}_j$ is the same as that studied in Ref. 14, provided the SC order parameter Δ and each η_j are identified, respectively, with the Kekulé and Haldane masses in Ref. 14. Thus, we can immediately borrow and tailor some of the results from Ref. 14 to the present case.

If all the η_j 's are zero and the SC order parameter has a single vortex with unit winding number, there are four Majorana fermions bound to it. As the magnitudes of the $|\eta_j|$'s increase, there will be a phase transition every time that $|\eta_j| = |\Delta(r=\infty)|$. Any such transition is characterized by a decrease in the number of Majorana fermions by one unit and a corresponding change in the value of the Chern number by ± 1 , depending on the sign of η_j . Therefore, by changing the Chern number of the system by ± 1 each time, one can knock out the Majorana fermions one by one.

Alternatively, one could start from the dominant Haldane masses limit defined by $|\eta_j| > |\Delta(r=\infty)|$ with $j=1, 2, 3, 4$. In this limit, the system sustains the thermal integer quantum Hall effect (IQHE) and supports four chiral Majorana fermions.^{15,16} One can then change $\mathbf{h}$ so as to cross successive quantum phase transitions at which any one of the $\eta_1, \dots, \eta_4$ equals in magnitude the spectral gap controlled by $|\Delta(r=\infty)|$. As before, each time we cross a phase transition, the Chern number and hence the number of Majorana fermions at a SC vortex core changes.

We note that the presence of a nearest-neighbor-hopping dispersion

$$\epsilon(\mathbf{p}) = -2t(\cos p_x + \cos p_y) \quad (10)$$

with $t \ll \alpha$ is equivalent to adding a constant chemical potential

$$\mu_j \equiv \epsilon(\mathbf{p}_j) \quad (11)$$

for each one of the four Fermi momenta, Eq. (2). The effect of this term is to shift the gap closing condition to

$$|\eta_j| = \sqrt{|\Delta|^2 + \mu_j^2}, \quad (12)$$

i.e., our results can be generalized to systems with quadratic dispersions and naturally explain the results found in Ref. 17.

III. TUNING THE NUMBER OF MAJORANA FERMIONS IN GRAPHENE

We are now going to demonstrate that the very same control on the number of Majorana fermions achieved with Hamiltonian (9) is also possible in graphene. We recall that in graphene, electrons with spin $s = \uparrow, \downarrow$ hop on a honeycomb lattice that is made of two triangular sublattices A and B. The conduction and valence bands touch at the two nonequivalent points $\mathbf{K}_{\pm}$ located at the opposite corners in the hexagonal first Brillouin zone (see Ref. 18 for a review). Finally, to account for the possibility of a SC instability, Nambu doublets are introduced with the index p and h to distinguish particles from their charge conjugate (holes). Hence, after linearization of the spectrum about the Fermi points $\mathbf{K}_{\pm}$, this leads to a single-particle kinetic energy represented by a 16×16 -dimensional matrix

$$\mathcal{H}_D := \alpha_1 p_1 + \alpha_2 p_2. \quad (13)$$

Here, α_1 and α_2 are two 16×16 -dimensional Dirac matrices.

It was shown in Ref. 14 that there exists 36 distinct order parameters such that any one, when added to $\mathcal{H}_D$, opens a spectral gap. These order parameters are identified by seeking all 16×16 matrices from the Clifford algebra that anticommute with $\mathcal{H}_D$. One complex-valued order parameter is that for singlet superconductivity. We shall denote the two corresponding 16×16 matrices from the Clifford algebra by $M_{\text{Re SSC}}$ and $M_{\text{Im SSC}}$ and define the perturbation

$$\mathcal{H}_{\Delta} := \Delta_1 M_{\text{Re SSC}} + \Delta_2 M_{\text{Im SSC}} \quad (14)$$

that opens the spectral gap $2|\Delta|$ with the complex valued

$$\Delta \equiv \Delta_1 + i\Delta_2 \quad (15)$$

parametrized by the real-valued Δ_1 and Δ_2 when added to $\mathcal{H}_D$. Next, we seek all 16×16 matrices from the Clifford algebra that (i) anticommute with $\mathcal{H}_D$ and (ii) commute with $\mathcal{H}_{\Delta}$. In this way, we find all ten TRS-breaking order parameters listed in Table I that alone would open a gap in the Dirac spectrum if not for their competition with the gap induced by singlet superconductivity. Within this set of ten matrices one can form groups of at most four matrices that are mutually commuting and therefore can be simultaneously diagonalized. Here, we choose the four-tuplet

TABLE I. The ten mass matrices with PHS that anticommute with α_1 and α_2 and commute with the singlet SC masses $M_{\text{Re SSC}}$ and $M_{\text{Im SSC}}$. Each mass matrix can be assigned an order parameter for the underlying microscopic model. The latin subindex of the order parameter's name corresponds to the preferred quantization axis in SU(2) spin space. Each mass matrix either preserves or breaks TRS, SRS, and sublattice symmetry (SLS). Each mass matrix can be written as a tensor product $X_{\mu_1\mu_2\mu_3\mu_4} \equiv \rho_{\mu_1} \otimes s_{\mu_2} \otimes \sigma_{\mu_3} \otimes \tau_{\mu_4}$, where ρ_{μ_1} , s_{μ_2} , σ_{μ_3} , and τ_{μ_4} correspond to unit 2×2 and Pauli matrices that act on particle-hole, spin-1/2, valley, and sublattice indices, respectively.

Order parameter	TRS	SRS	SLS	Here	$X_{\mu_1\mu_2\mu_3\mu_4}$
IQHE	False	True	False	M_{IQHE}	X_{3003}
Re VBS _x	False	False	True	$M_{\text{Re VBS}_x}$	X_{3110}
Re VBS _y	False	False	True	$M_{\text{Re VBS}_y}$	X_{0210}
Re VBS _z	False	False	True	$M_{\text{Re VBS}_z}$	X_{3310}
Im VBS _x	False	False	True	$M_{\text{Im VBS}_x}$	X_{0120}
Im VBS _y	False	False	True	$M_{\text{Im VBS}_y}$	X_{3220}
Im VBS _z	False	False	True	$M_{\text{Im VBS}_z}$	X_{0320}
Néel _x	False	False	False	$M_{\text{Néel}_x}$	X_{3133}
Néel _y	False	False	False	$M_{\text{Néel}_y}$	X_{0233}
Néel _z	False	False	False	$M_{\text{Néel}_z}$	X_{3333}

$\{\text{Re VBS}_x, \text{Im VBS}_y, \text{Néel}_z, \text{IQHE}\}$ for concreteness but the results hereafter apply to any other such four-tuplet of commuting mass matrices among the set of ten. Our main result regarding graphene is the fact that

$$\mathcal{H} = \mathbf{p} \cdot \boldsymbol{\alpha} + \Delta_1 M_{\text{Re SSC}} + \Delta_2 M_{\text{Im SSC}} + m_1 M_{\text{Re VBS}_x} + m_2 M_{\text{Im VBS}_y} + m_3 M_{\text{Néel}_z} + \eta M_{\text{IQHE}} \quad (16a)$$

is unitarily similar to Eqs. (9a) and (9b) with

$$\delta_{1,2,3,4} \equiv \Delta, \quad (16b)$$

$$\eta_1 \equiv -m_1 + m_2 + m_3 + \eta, \quad (16c)$$

$$\eta_2 \equiv m_1 - m_2 + m_3 + \eta, \quad (16d)$$

$$\eta_3 \equiv m_1 + m_2 - m_3 + \eta, \quad (16e)$$

$$\eta_4 \equiv -m_1 - m_2 - m_3 + \eta. \quad (16f)$$

The phase diagram in Fig. 2 follows.

There is a total of four SC pair potentials that open a uniform gap at $\mathbf{K}_{\pm}$ in graphene.¹⁴ One is the singlet SC pair potential, which we have discussed so far and the remaining three are all triplet SC pair potentials. For each such triplet SC mass, as in the singlet SC, there are four competing orders that commute pairwise and can be used, in principle, to knock out one by one Majorana fermions bound to the cores of isolated vortices.

IV. CONCLUSIONS

In summary, we have identified a mechanism to overcome the fermion-doubling barrier that can prevent the attachment of an odd number of Majorana fermions to the core of SC

vortices in graphenelike tight-binding models. This mechanism relies on a $\mathbb{Z}_2 \times \mathbb{Z}_2$ topological charge that measures the parity in the number of Majorana fermions attached to an isolated vortex and the use of TRS-breaking order parameters that compete with each other and with the SC order parameter to knock out one by one the Majorana fermions. In this surgical way, an odd number of Majorana fermions can be made to bind the vortices in a singlet SC order parameter, whereas this could only be achieved for the more elusive triplet SC order parameter in Refs. 3, 4, and 19. This mechanism applies to graphene with superconductivity induced by

FIG. 2. Schematic phase diagram of the competition between the singlet SC (Δ), thermal IQH (η), magnetic bond ($m_{1,2}$), and Néel (m_3) orders near the Dirac point in graphene. Here, $m_{1,2,3}$ are fixed while $|\eta|$ and $|\Delta|$ vary. When $m_{1,2,3}=0$, there are three phases (two large $|\eta|$ phases with $\eta > 0$ and $\eta < 0$ and one large $|\Delta|$ phase, according to Ref. 14). If we choose $m_{1,2,3}$ in such a way that $m_1 + m_2 + m_3$, $m_1 + m_2 - m_3$, $-m_1 + m_2 - m_3$, and $-m_1 - m_2 + m_3$ are all different, there are 15 phases as we change η and Δ . Shaded (non-shaded) regions represent a phase with the odd (even) Chern number (proportional to the thermal Hall conductivity divided by temperature). In phases that are adiabatically connected to a nonsuperconducting state (the horizontal axis $|\Delta|=0$), one can switch off the pairing without closing the gap. In these phases, the number of Majorana fermions is thus even.

the proximity effect, provided a way can be found to also induce and select from the remarkably large variety of coexisting and competing order parameters that graphene supports those with odd $\mathbb{Z}_2 \times \mathbb{Z}_2$ topological charge and thus odd number of Majorana fermions attached to isolated vortices.

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