Topological massive Dirac edge modes and long-range superconducting Hamiltonians

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We discover novel topological effects in the one-dimensional Kitaev chain modified by long-range Hamiltonian deformations in the hopping and pairing terms. This class of models display symmetry-protected topological order measured by the Berry/Zak phase of the lower-band eigenvector and the winding number of the Hamiltonians. For exponentially decaying hopping amplitudes, the topological sector can be significantly augmented as the penetration length increases, something experimentally achievable. For power-law decaying superconducting pairings, the massless Majorana modes at the edges get paired together into a massive nonlocal Dirac fermion localized at both edges of the chain: a new topological quasiparticle that we call topological massive Dirac fermion. This topological phase has fractional topological numbers as a consequence of the long-range couplings. Possible applications to current experimental setups and topological quantum computation are also discussed.

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I. INTRODUCTION

The quest for the experimental realization of topological superconductors has turned out to be far more elusive than for their insulating counterparts. Simple models for topological superconductors have been proposed [1,2], but yet their unambiguous implementation is challenging in condensed matter or with quantum simulations. Here we address the issue as to whether those simple models [3,4] are in fact very specific in hosting their long sought-after topological properties. Quite on the contrary, we find that these properties can not only be generic with respect to natural extensions of the model-Hamiltonian terms, but also that Hamiltonian deformations can give rise to unconventional topological edge-mode physics that is novel *per se* and for applications in topological quantum computation.

The appearance of topological superconductors is having a strong impact [5–10] in condensed matter physics and quantum simulators. A tremendous effort is now directed at the experimental demonstration of existing topological models and at the development of new ones that may be easier to realize. What makes a topological superconductor interesting is the presence of Majorana modes as zero-energy localized modes at the edges or boundaries of the material. These modes lie within the superconducting gap and are rather exotic since Majorana fermions are their own antiparticles (holes). Standard (nontopological) superconductors do not exhibit such modes in their energy spectrum. Thus, topological superconductors represent new physics: Majorana modes are topologically protected against local perturbations disturbing the system and cannot be removed unless a topological phase transition occurs. This robustness makes them useful for storing and manipulating quantum information in a topological quantum computer.

In this paper we focus on the Kitaev chain model and propose novel modifications of the basic Hamiltonian, in order to enrich the appearance of Majorana physics (see Fig. 1) and even new topological excitations (see Fig. 2, Fig. 3). These modifications come in two ways: (i) exponentially decaying kinetic terms and (ii) long-range (LR) interaction terms. They produce novel beneficial topological effects and new unconventional topological physics, respectively. In case (ii), we propose a hopping deformation that allows us to significantly increase the region in the phase diagram where Majorana zero modes (MZMs) are present. Interestingly enough, this modification may result in a realistic description for cold atoms in optical lattices. In case (ii), we study the topological properties of another complementary modification of the Kitaev model based on long-range pairing terms decaying algebraically with a certain exponent α. We discover novel topological effects not found in any simple model before (see Fig. 2): for $\alpha < 1$ the model suffers a major qualitative change manifested in the absence of MZMs that are transmuted onto Dirac modes, which are massive nonlocal edge states. These new edge states are topologically protected against perturbations that do not break fermion parity nor particle-hole symmetry. These modes appear as midgap superconducting states that cannot be absorbed into bulk states. These topological massive Dirac edge states are new physical quasiparticles that are absent in the standard Kitaev model. They represent a new unconventional topological phase.

II. LONG-RANGE DEFORMATIONS OF SUPERCONDUCTING HAMILTONIANS

We consider a model of spinless fermions on an L-site one-dimensional chain, with p-wave superconducting pairing and a hopping term. The Hamiltonian of the system is

$$H = \sum_{j=1}^{L}\left(-J\sum_{l=1}^{L-1}\frac{1}{r_{l,\xi}}a_j^\dagger a_{j+l} + M\sum_{l=1}^{L-1}\frac{1}{R_{l\alpha}}a_j a_{j+l} - \frac{\mu}{2}\left(a_j^\dagger a_j - \frac{1}{2}\right) + \text{H.c.}\right), \quad (1)$$

where μ is the chemical potential, $J > 0$ is the hopping amplitude, the absolute value of $M = |M|e^{i\Theta}$ stands for the superconducting gap, $a_j(a_j^\dagger)$ are annihilation (creation) fermionic operators. The Hamiltonian deformations are $r_{l,\xi}, R_{l,\alpha}$. They are generic functions of an integer distance l, and parameters ξ and α, respectively. The total number of fermions modulo 2 is called the fermion parity and it is a conserved quantity for all

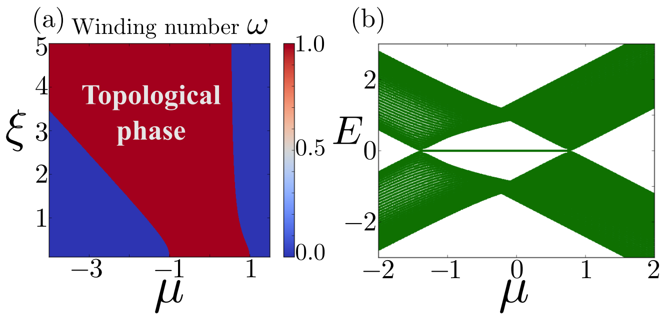

FIG. 1. (a) Topological phase diagram for the Kitaev chain with exponentially decaying hopping. As the penetration length ξ increases, the topological phase ($\Phi_{\rm B} = \pi\omega = \pi$) gets enlarged. For $\xi \to 0$ we recover the well-known Majorana chain with nearest-neighbour hopping only. (b) Energy spectrum for $\xi = 0.8$. The region with MZMs $\mu \in (-1,1)$ in the original model has been augmented in one to one correspondence with a nontrivial Berry phase and winding number.

models in (1). Considering only nearest-neighbors hopping and pairing, we recover the famous model introduced by Kitaev [4]. This model is topological displaying MZMs at the edges like in Fig. 2(a). In the topological phase, the ground state of the Kitaev model is twofold degenerate: a bulk of with even fermion parity, while populating the two Majorana modes at the edges amounts to a single ordinary fermion and odd parity. The conservation of fermion parity and the nonlocal character of the unpaired Majoranas at the edges make the system an ideal candidate for a topological qubit out of the twofold degenerate ground state [11,12].

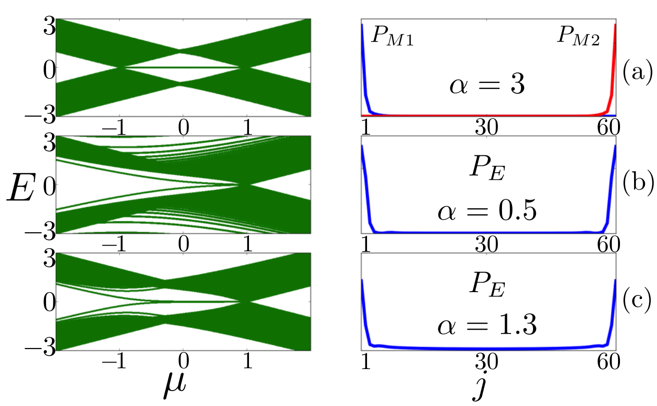

FIG. 2. Left: We plot the spectrum for the Kitaev chain with long-range decaying pairing, for $L = 60$ sites. On the right-hand side we show the probability distribution P_E of the edge modes for different topological phases. (a) Majorana sector with $\alpha = 3$. We can see MZMs for $\mu \in [-1,1]$ localised at the edges of the chain, as plotted on the right-hand side for $\mu = -0.5$ (P_{M1} and P_{M2}). Notice that each Majorana mode is decoupled, represented with different colors. (b) Massive Dirac sector with $\alpha = 0.5$. Within the new topological phase ($\mu < 1$), there are topological massive Dirac fermions localised at both edges at the same time, as shown on the right-hand side for $\mu = -1.5$. (c) Crossover sector with $\alpha = 1.3$. There are both MZMs and massive Dirac fermions depending on the value of μ. We plot the probability for a massive Dirac fermion at $\mu = -1.2$.

Without loss of generality, we may fix the pairing amplitude to be real and $M = J = \frac{1}{2}$. Assuming periodic boundary conditions, we can diagonalize the Hamiltonian deformations (1) in Fourier space and in the Nambu-spinor basis representing paired fermions [13]: $H = \frac{1}{2}\sum_k \Psi_k^\dagger H_k \Psi_k$, where $\Psi_k = (a_k, a_{-k}^\dagger)^{\rm t}$ and H_k is of the form $H_k = E_k \boldsymbol{n}_k \cdot \boldsymbol{\sigma}$. The energy dispersion relation is given by E_k, $\boldsymbol{\sigma}$ is the Pauli matrix vector and $\boldsymbol{n}_k$ is a unit vector called winding vector. Explicitly,

$$\boldsymbol{n}_k = -\frac{1}{E_k}(0, f_\alpha(k), \mu + g_\beta(k)),$$
$$E_k = \sqrt{(\mu + g_\xi(k))^2 + f_\alpha^2(k)}, \quad (2)$$

with

$$g_\xi(k) = \sum_{l=1}^{L-1} \frac{\cos(k \cdot l)}{r_{l,\xi}} \text{ and } f_\alpha(k) = \sum_{l=1}^{L-1} \frac{\sin(k \cdot l)}{R_{l,\alpha}}. \quad (3)$$

Particular instances of the functions $r_{l,\xi}$ and $R_{l,\alpha}$ have been considered in Refs. [14,15], where long-range deformations of the Kitaev chain were first considered.

These models (2) belong to the BDI symmetry class of topological insulators and superconductors [16,17], with particle-hole, time-reversal, and chiral symmetry. The inclusion of long-range effects do not break these symmetries, nor the conservation of fermion parity. This is an important condition for the topological character of the original short-range model to be preserved. These symmetries impose a restriction on the movement of the winding vector $\boldsymbol{n}_k$ from the sphere S^2 to the circle S^1 on the yz plane. Thus, we have a mapping from the reduced Hamiltonians H_k on the Brillouin zone $k \in S^1$ onto the winding vectors $\boldsymbol{n}_k \in S^1$. This mapping $S^1 \longrightarrow S^1$ is characterized by a winding number ω, a topological invariant defined as the angle swept by $\boldsymbol{n}_k$ when the crystalline momentum k is varied across the whole Brillouin zone (BZ) from $-\pi$ to $+\pi$,

$$\omega := \frac{1}{2\pi}\oint d\theta = \frac{1}{2\pi}\oint \left(\frac{\partial_k n_k^z}{n_k^y}\right) dk, \quad (4)$$

where we have used that $\theta := \arctan(n_k^z/n_k^y)$.

As a complementary tool in 1D systems, we can use the Berry/Zak phase [18–20] to characterize topological order. When the system is adiabatically transported from a certain crystalline momentum k_0 up to $k_0 + G$, where G is a reciprocal lattice vector, the eigenstate of the lower band of the system $|u_k^-\rangle$ picks up a topological Berry phase given by

$$\Phi_{\rm B} = \oint A_{\rm B}(k) dk. \quad (5)$$

The Berry connection $A_{\rm B}(k) = {\rm i}\langle u_k^- | \partial_k u_k^- \rangle$ connects by means of a parallel transport two infinitesimally close points on the manifold defined by $|u_k^-\rangle$ in k space. For the standard Kitaev chain [4], the resulting gauge-invariant phase Φ_B is quantized (0 or π) due to the particle-hole symmetry that characterizes distinct topological phases in one-to-one correspondence with the winding number [21].

III. AUGMENTED TOPOLOGICAL PHASES INDUCED BY EXPONENTIALLY DECAYING HOPPINGS

This remarkable effect is obtained choosing nearest-neighbor pairing, i.e., $R_{1,\alpha} = 1$ and $R_{l>1,\alpha} = \infty$ and $r_{l,\xi} = e^{\frac{(l-1)}{\xi}}$, where ξ is the penetration length of the exponentially decaying hopping terms. This Hamiltonian may be realizable in simulations of topological superconductors using cold atoms in optical lattices [22–24], where the exponential decay of the hopping terms with distance can be tuned, e.g., by varying the depth of the lattice potentials [25].

In Fig. 1 we plot the complete phase diagram by computing the winding number and the topological Berry phase from Eqs. (4) and (5). For $\xi \to 0$ we recover the usual Kitaev chain. The system is topological for $\mu \in [-1,1]$, displaying MZMs at the edges. Interestingly enough, when we increase the penetration length ξ, the region where we observe MZMs is augmented. In fact, this widening effect is purely due to the hopping deformation since we find that including an exponentially decaying pairing deformation does not change the topological phases. In the thermodynamic limit $L \to \infty$, the phase separation between the trivial and nontrivial topological phases can be computed analytically from Eq. (2), obtaining

$$\mu_{c1} = \frac{e^{\frac{1}{\xi}}}{1 + e^{\frac{1}{\xi}}}, \quad \mu_{c2} = \frac{e^{\frac{1}{\xi}}}{1 - e^{\frac{1}{\xi}}}. \qquad (6)$$

Thus, increasing the penetration length of the deformed hopping, we can arbitrarily enlarge the topologically nontrivial sector (see Fig. 1). Although symmetry-protected topological order is usually associated with local interactions, we have shown that nonlocal terms can favor the formation of a topological phase. Related studies for the Kitaev chain with long-distance hopping were carried out [26] and qualitatively similar effects have been recently observed in Ref. [27] for the spin-1 long-range Haldane model [28].

IV. UNCONVENTIONAL TOPOLOGICAL SUPERCONDUCTIVITY WITH DIRAC TOPOLOGICAL MASSIVE STATES

Long-range deformations may not only enlarge topological phases but also produce new types of topological phases. To this end, let us now consider pairing terms that decay algebraically with a power-law exponent α, and no deformation of the hopping terms. That is, $r_{1,\xi} = 1, r_{l>1,\xi} = \infty$ and $R_{\alpha,l} = l^{\alpha}$.

In the thermodynamic limit $L \to \infty$, the function $f_\alpha(k)$ in Eq. (3) is divergent at $k = 0$ for $\alpha < 1$. This function defines the long-range pairing and appears in the energy dispersion relation and the winding vector of Eq. (2). Thus, the dispersion relation and the group velocity also become divergent at $k = 0$ if $\alpha < 1$. Nevertheless, ω [Eq. (4)] and Φ_B [Eq. (5)] are still integrable. Moreover, it is not possible to gauge away the divergence from $k = 0$ by means of a gauge transformation, as in the ordinary Kitaev chain. Therefore, the divergence behaves as a topological singularity. A detailed discussion of this effect at $k = 0$ on the topological indicators is carried out in Sec. I of the Supplemental Material [29]. According to the behavior of $f_\alpha(k)$ at $k = 0$, we find three different topological sectors depending on the exponent α:

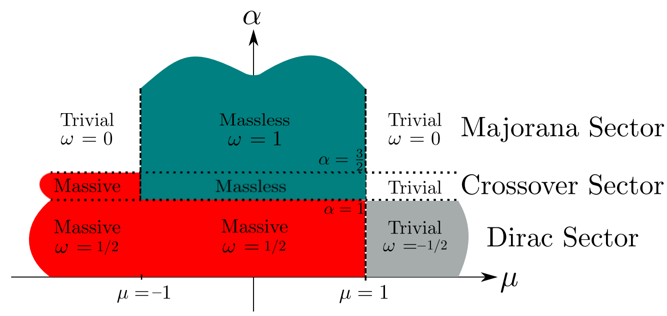

FIG. 3. Topological phase diagram for the Kitaev chain with long-range pairing. The wavy lines at the border of certain phases indicate that they extend endlessly. Fractional topological numbers highlight the appearance of an unconventional topological phase with massive nonlocal Dirac edge states. The topological characterisation of the crossover sector is discussed in the main text and the Supplemental Material [29].

(i) Majorana sector [$\alpha > 3/2$]

This sector is topologically equivalent to the one of the short-range Kitaev chain [4]: For $|\mu| > 1$, the phase is topologically trivial and we do not find MZMs. In the region $\mu \in (-1,1)$, we find that MZMs are always present [see Fig. 2(a)]. The function $f_\alpha(k)$ is not divergent and we can compute the winding number ω of Eq. (4) and the Berry phase Φ_B of Eq. (5) obtaining $\Phi_B = \pi\omega = \pi$. The lower-band eigenvector $|u_k^-\rangle$, thus, shows a $U(1)$ phase discontinuity at $k = 0$. The corresponding topological phase is depicted in blue in the phase diagram of Fig. 3.

(ii) Massive Dirac sector [$\alpha < 1$]

An unconventional topological phase appears for sufficiently slow decaying pairing. As an example, in Fig. 2(b) we see for $\alpha = 1/2$ two clearly different phases as a function of μ. For $\mu > 1$ the system is in a trivial phase, with no edge states. However, for $\mu < 1$ the system has a topological massive Dirac fermion at the edges, as shown in the wave function plot in Fig. 2(b). The two Majorana modes at the two distant edges have paired up onto a single massive Dirac fermion. Notice that the fermion is highly nonlocal and its nature is deeply rooted in the long-range/nonlocal character of the pairing term (see Sec. III of the Supplemental Material [29] for details). We notice that if we had considered imaginary pairing amplitudes within D symmetry class (particle-hole symmetric), the nonlocal massive Dirac fermions would persist. This topological quasiparticle is still protected by fermion parity: the ground state has still even parity, whereas the first excited state populates this nonlocal massive fermion and has odd parity. One cannot induce a transition between these two states without violating the fermion parity conservation of the Hamiltonian, and applying a nonlocal operation is needed. Moreover, the subspace of these two edge states is still protected by the bulk gap from bulk excitations. The conservation of fermion parity and the nonlocal character of the massive Dirac fermion make these two states ideal to define a topological qubit using two copies of the Kitaev chain [30–33]. Further details are detoured to Sec.V of the Supplemental Material. Additionally, in Sec. II of the Supplemental Material [29], by means of finite-size scaling we show that the mass of the Dirac fermion stays finite in the thermodynamic limit for $\mu < 1$ and $\alpha < 1$. This way we can prove that the effect is purely topological and caused by the long-range deformation.

When we close the chain, the edge states disappear as we may expect for a topological effect. Despite the long-range pairing coupling, the system still belongs to the BDI symmetry class [16,17], since no discrete symmetry has been broken. The winding number ω can still be formally defined using Eq. (4). However, the topological singularity at $k = 0$ deeply modifies the value of ω. For the trivial phase $\mu > 1$, the winding number is $\omega = -1/2$, whereas for the new unconventional topological phase is $\omega = +1/2$ if $\mu < 1$. The semi-integer character of ω is associated to the integrable divergence at $k = 0$, which modifies the continuous mapping $S^1 \longrightarrow S^1$. Notwithstanding, in this region there is still a jump of one unit between the two topologically different phases, $\Delta\omega = \omega_{\text{top}} - \omega_{\text{trivial}} = 1$ (see Fig. 3). Moreover, the topological indicators take on the same value within the whole phase until the bulk gap closes at $\mu = 1$, giving rise to a topological phase transition, and the new massive topological edge states disappear. Therefore, we can still establish a bulk-edge correspondence.

There is a novelty in this case regarding the parallel transport for the Berry phase. Namely, at $k = 0$ the adiabatic condition breaks down since both the energy dispersion relation E_k and the quasiparticle group velocity $\partial_k E_k$ diverge. Moreover, the singularity at $k = 0$ of the lower-band eigenvector $|u_k^-\rangle$, cannot be removed by a simple gauge transformation as it is not just a $U(1)$ phase difference, but a phase shift unitary jump,

$$|u^-_{k\to 0^+}\rangle = e^{i\pi P_\pm}|u^-_{k\to 0^-}\rangle, \tag{7}$$

where $P_\pm = \frac{1}{2}(\mathbb{1} \pm \sigma_z)$. More explicitly,

$$e^{i\pi P_-} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi} \end{pmatrix}, \quad e^{i\pi P_+} = \begin{pmatrix} e^{i\pi} & 0 \\ 0 & 1 \end{pmatrix}. \tag{8}$$

The difference in sign $\pm$ of the projector $P_\pm$ depends on the topological regime. For $\mu > 1$, the system is in a trivial phase with no edge states and the long-range singularity of $|u_k^-\rangle$ at $k = 0$ is given by $e^{i\pi P_-}$. On the other hand for $\mu < 1$, the system is in a topological phase with massive and nonlocal edge states. The singularity of $|u_k^-\rangle$ at $k = 0$ in that case is given by $e^{i\pi P_+}$.

(iii) Crossover sector [$\alpha \in (1,3/2)$]

This is a crossover region between sectors (i) and (ii). Within this sector, there are massless Majorana edge states for $-1 < \mu < 1$ like in sector (i), but for $\mu < -1$ the edge states become massive like in sector (ii). This is shown through finite-size scaling in Sec. II and III of the Supplemental Material [29]. The intuition behind this result is that the gap closes in the thermodynamic limit at $\mu = -1$ also for $\alpha \in (1, \frac{3}{2})$. The dispersion relation E_k is no longer divergent, however its derivative $\partial_k E_k$ (the group velocity) is still singular at $k = 0$ and the structure of the topological singularity changes accordingly. The winding number is not able to capture the mixed character of this sector. However, as detailed in Sec. I of the Supplemental Material [29], we can clearly see that the behavior of the winding vector and the lower-band eigenstate is different from the other two sectors.

In Fig. 3, we present a complete phase diagram summarizing the different topological phases of the model as a function of μ and α.

V. OUTLOOK AND CONCLUSIONS

We have found that finite-range and long-range extensions of the one-dimensional Kitaev chain can be used as a resource for enhancing existing topological properties and for unveiling new topological effects. In particular, for long-range pairing deformations, we observe nonlocal massive Dirac fermions characterized by fractional topological numbers. Hamiltonians with long-range pairing and hopping may be realized in Shiba chains as recently proposed in Refs. [34,35], where edge states can be detected, e.g., by scanning tunneling spectroscopy [36]. Alternatively, next-nearest neighbor hopping may be harnessed in atomic and molecular setups [23], where massive edge modes should be observable via a combination of spectroscopic techniques and single-site addressing [37,38]. The extension of existing models for qubits, constructed by topologically protected gapped modes, may boost the search for long-range deformations in more complicated topological models with symmetry-protected or even intrinsic topological order.

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[29] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.94.125121 for details on the winding vector, the analytical structure of the edge states, the finite-size scaling of the edge mass gap, the robustness of the massive Dirac edge states against disorder, and the construction of a topological qubit within the massive Dirac phase.
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