Jan. 12th, 2024

Re: BJR1430
Superconducting triangular islands as a platform for manipulating Majorana zero modes

We thank both referees for their careful evaluation of our work and for the suggestions and comments that helped us further improve our paper. Both referees consider our work positively. Specifically, Referee #1 thinks that our paper could be published as a Letter once the suggested improvements have been made. Referee #2 believes that our central idea is novel in its "use of triangular structure that could allow to move the Majorana zero-modes by controlling which segments of the triangle are topological", and that it is "potentially interesting and could be of interest to the specialized research community." They nonetheless have some reservations regarding whether our paper has reached the bar of PRB Letter format.

In our detailed response attached below we have thoroughly addressed the questions and critiques of both referees, including elaboration on why our paper goes beyond the former developments in using vector potential to manipulate MZM and is in the same league as the other excellent Letters published in PRB. We hope the improved manuscript can now be recommended by the referees for publication in PRB as a Letter.

Summary of major changes in the revision:

1. A schematic drawing of a finite-width ribbon is added as an inset to Fig. 3 (a). The color coding of the topological phase diagrams is also revised according to Referee #2's suggestion.
2. Fig. 4 is updated with two new panels (b), (d) and an inset in (a). The complete evolution of the MZM in $\varphi \in [0, \frac{\pi}{3})$ is shown as an animation file included in the supplemental material.
3. A new Sec. 1 is added to the supplemental material with more analytic results of the 3-site Kitaev triangle.
4. The main text is revised to put more emphasis on manipulating the MZM according to Referee #1's suggestion.
5. A few new references have been added.

Report of the First Referee -- BJR1430/Winblad

Comment: *The paper BJR1430 studies models with Majorana zero modes (MZM) which have triangular structures. The models are based on Kitaev chain and the appearance of MZMs are tuned by vector potential. I think the paper could be considered for publication in Physical Review B as a Regular Article. To be published as a Letter, however, some changes/discussions are needed which are detailed below.*

Reply: We thank the referee for their positive assessment of our work and have made the suggested changes from the referee as detailed below.

Question #1: *The paper starts with a toy model "Kitaev triangle" which is a fine-tuned model of three sites but with superconducting coupling between sites. From my perspective, the first issue that needed justification is the superconducting coupling between sites, because superconductivity is a many-body effect but the model only contains three sites. Secondly, it is unclear to me why in equation (1) the potential theta is the "polar angle".*

Reply: We thank the referee for this question. Firstly, we agree with the referee that superconductivity is a many-body effect, and its thermodynamic stability is inseparable from the macroscopically many electrons in a bulk superconductor. However, the minimal model considered here should not be understood as a standalone, pristine superconductor, but an effective description of the low-energy physics of certain mesoscopic superconducting devices. The origin of the superconducting coupling between sites in the minimal model, which the referee questioned, can be due to a coherent mesoscopic superconducting sample, to which the three fermion sites are coupled. This is the same idea as the proximity-induced effective *p*-wave superconductivity in atomic ferromagnetic chains on s-wave superconductors [15], as well as the quantum dots coupled through superconducting links considered in Ref. [47]. In the revised manuscript we have briefly mentioned the mechanism for creating inter-site *p*-wave superconductivity pairing when introducing the Kitaev triangle model below Eq. (2):

The minimal model may be realized as an effective low-energy model of carefully engineered mesoscopic superconductor devices, such as that made by quantum dots connected by superconducting islands [47].

About the second question, we were referring to the angular component of the 2D polar coordinates of the nearest-neighbor bond vector $\mathbf{r}_{jl}$. Having the phase angle of the complex pairing potential Δ locked to the nearest-neighbor bond angle in the pairing term $|\Delta| \exp(i\theta_{jl})\, c_j c_l$ leads to the desired $p_x + ip_y$ pairing near the Brillouin zone center after Fourier transform. To avoid confusion and to be consistent with other places where the in-plane angle is mentioned in the manuscript, we have changed “polar angle” to “azimuthal angle”.

Comment #2: *For both the toy model and the "hollow triangles", the authors assume that vector potential only couples to electron hopping, but not the superconducting coupling. In usual superconductors, the U(1) gauge symmetry is broken but here in this paper, vector potential plays important roles in tuning the phases. In my opinion, more physical discussions are needed to explain the coupling to vector potential in this case.*

Reply: We thank the referee for this suggestion. Although the superconductivity order parameter appears to break U(1) symmetry, all physical observables calculated from the BdG formalism are still gauge invariant. Upon a gauge transformation $\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla\chi$, the creation operator for an electron becomes

$$c_{i\alpha}^{\dagger} \to c_{i\alpha}^{\dagger} e^{-\frac{ie}{\hbar}\chi_i}$$

where i, α label position and internal degrees of freedom, respectively. Such a transformation amounts to a unitary transformation of the BdG Hamiltonian matrix under the ansatz that the pairing potential Δ is unchanged. Therefore the BdG eigenenergies as well as all physical observables stay unchanged, which also means Δ from the gap equation is unchanged, consistent with the ansatz (c.f. de Gennes, *Superconductivity of Metals and Alloys*). As a result, a divergence-free vector potential $\mathbf{A}$ coupled to the normal part of the BdG Hamiltonian can be transformed to that coupled to the pairing part and vice versa, which does not affect any physical observables. In this sense, gauge transformations can change the distribution of $\mathbf{A}$ between the normal and the pairing parts of the BdG Hamiltonian. However, the *net* $\mathbf{A}$ has physical meaning even if it is divergence-free, since it is equivalent to a finite supercurrent density which is a physical observable. In writing down the model BdG Hamiltonians in the main text, we have essentially chosen a gauge so that the vector potential only appears in the normal part. Additionally, the pairing potential Δ is assumed to be unchanged by the supercurrent or the vector potential. This is justified by the fact that the spinless *p*-wave pairing in the model system is an effective one, due to the coupling between the fermions in the model with another, supposedly much larger, superconductor. The influence of the vector potential near the fermions in the model system on the gap equation of the larger superconductor is negligible as a first approximation.

In the revised manuscript we have added the following sentences to the paragraph following Eq. (1) to incorporate the key points explained above.

We have chosen a gauge so that the vector potential only appears in the normal part of the Hamiltonian [59], and the *p*-wave gap Δ is assumed to be an effective one induced by proximity to a neighboring superconductor, on which the vector potential has negligible influence.

Question #3: *A lot of interesting developments in this field are not cited, including: Annals of Physics 432, 168564 (2021), Phys. Rev. B 107, 115418, Phys. Rev. B 99, 245416, Phys. Rev. B 106, L161412, etc.*

Reply: We thank the referee for bringing these papers to our attention and have cited the relevant ones in the revised manuscript.

Question #4: *In the section "hollow triangles", it seems that the authors talk about two geometries, but provide no figure for the "1D ribbon" structure, it may cause some confusion for the readers.*

Reply: We have added a schematic drawing of a finite-width triangular lattice ribbon as Fig. 3 (a) in the revision.

Question #5: *The structure of the article is not balanced in my opinion, the part for the toy model is long while the important parts like the "design for braiding" and "experimental realization" are short, the authors may consider adjusting that for publishing it as a Letter.*

Reply: We thank the referee for this suggestion. We have shortened the formalism part and have moved different material around for better balance of the contents in the revision.

Report of the Second Referee -- BJR1430/Winblad

Comment: *In this work, the authors present a platform to study Majorana zero-modes using triangular islands of Kitaev chains where the topological phase is controlled through the amplitude and orientation of a uniform vector potential. While the idea of using a vector potential to control the topological phase was previously discussed in the literature (see e.g. Ref. [52] of the manuscript), the novelty of this contribution is the use of a triangular structure that could allow to move the Majorana zero-modes by controlling which segments of the triangle are topological.*

I believe the idea is potentially interesting and could be of interest to the specialized research community. However, given the prior literature on using the vector potential (Ref. [52]) or magnetic fluxes to control Majorana zero-modes [see e.g. Hyart et al. Phys. Rev. B 88, 035121 (2013)], I do not believe that the manuscript reaches the bar set forth by APS to justify a Letter format manuscript instead of a Regular PRB Article. Before recommending publication as a Regular Article in PRB, I believe the following questions and comments should be addressed:

Reply: We thank the reviewer for their overall positive assessment of our work. We acknowledge that using a vector potential or supercurrent to manipulate superconducting phases for realizing MZM has been investigated in previous literature, upon which our work is indeed based. However, we emphasize that our paper clearly advances beyond previous work in the following aspects, warranting its recognition by the community through the publication of a Letter in PRB.

(1) Our proposal of the exactly solvable Kitaev triangle offers an alternative strategy towards MZM-based topological quantum computing (TQC) that is not based on bulk-boundary correspondence. While it is certainly ideal to build MZM-based quantum circuits exploiting the robustness of nonlocal MZM qubits in superconducting wires, such designs remain practically challenging in the near term, particularly due to materials engineering-related uncertainties in mesoscopic nanowire-based devices. However, with recent advancements in constructing minimal Kitaev chains using a few quantum dots coupled through superconductors, it is equally compelling to demonstrate braiding-based MZM logic gate operations in such well-controlled prototypical systems. In small systems with only a few fermion degrees of freedom, discussing the emergence of MZM due to bulk-boundary correspondence is less meaningful. (Indeed, for the vector potential considered in our Kitaev triangle model, the three edges are all in the topologically nontrivial phase.) Instead, it is easier to fine-tune system parameters based on exactly solvable models to realize well-behaved MZM. The 3-site Kitaev triangle in our work not only provides such a minimal model, which, to our knowledge, has not been discussed in previous literature, but it also points to an alternative route towards MZM-based TQC that does not rely on bulk-boundary correspondence. We also kindly remind the referee that Ref. 52 and PRB 88, 035121 (2013), as mentioned, are still limited to the existing architecture of wire-based T-junctions.

(2) Our proposal of a uniform vector potential coupled to hollow triangles explores the utility of geometry rather than the individual control of superconducting nanowires. We agree that previous literature has studied the effect of vector potential or supercurrent in tuning topological phases. However, these studies have not combined such manipulations with unique geometries for more efficient MZM manipulations. The only other similar designs, to our knowledge, are the ring-based geometry in Ref. [50], and those based on higher-order topological superconductors [51-53]. We do not argue which geometry is superior but wish to emphasize the importance of actively exploring alternative, theoretically established geometries. This

approach allows experimentalists familiar with different materials systems to choose the most appropriate architecture for their platforms. The hollow triangles considered in our work naturally arise from epitaxially-formed triangular islands in crystal growth, making them attractive to experts in this field.

Finally, we would like to highlight that triangles, as a geometry, are unique compared to other quasi-2D structures such as wires, squares, or circles. Triangles naturally break 2D inversion symmetry and do not present a straightforward strategy for morphing into either 1D or 2D structures with periodic boundary conditions. Therefore, we believe triangles can host fundamentally different bulk-boundary correspondences than those inferred from other geometries. We hope our work can serve as an initial exploration in this area.

In the revised manuscript we have integrated the key elements of our reply above into the introduction and discussion parts to better convey the importance of work to the readers.

Comment #1*: In the evolution of the 3-site Kitaev triangle, what sets the scale of the first state above the zero modes? (~0.2 energy scale in Fig. 2a). Some discussions on what controls that scale would strengthen the manuscript given that it sets the protection of the zero modes.*

Reply: We thank the referee for this useful question. Briefly speaking, the first excited state involves hybridization between the "bulk" states of the bottom 1-2 bond and site 3. In the revised manuscript we have added a new Sec. 1 to the supplemental material with more analytic results of the Kitaev triangle. Among them, the first excited states with the above-mentioned structure have the exact eigenenergy $\pm\left(1-\frac{\sqrt{2}}{2}\right)t \approx \pm 0.29t$. Moreover, we have proved the exact degeneracy of the two MZM at zero energy throughout the parameter path $\boldsymbol{\phi}_1 \to \boldsymbol{\phi}_2 \to \boldsymbol{\phi}_3 \to \boldsymbol{\phi}_1$ and have given their explicit wavefunctions. We kindly remind the referee that such a parameter path is different from prior literature based on quantum wires since the topology of the individual bonds is not changed throughout the path. It is the fine-tuned coupling among the MZM in a finite system that leads to such a surprising and useful behavior.

Question #2: *The superimposed phase diagrams (Fig 3a of main text and 1a of SM) can be confusing. It would be clarifying to use an additional color to indicate correctly the four different possible states (e.g. trivial phase for both vector potential orientation, trivial phase for y-orientation, but topological phase for the other orientation, etc.).*

Reply: We thank the referee for this suggestion and have updated both figures in the revision accordingly. The phase diagrams now have four colors corresponding to all four possible combinations of topological phases of the side and the bottom edges: purple—(trivial, trivial), yellow— (topological, topological), red—(trivial, topological), orange— (topological, trivial).

Question #3: *Some more discussion of the evolution of the MZMs described in Fig. 4 would be helpful. Based on the model, I would have naively expected the figures b-d to look the same up to a rotation. However, the zero-mode spatial overlap appears larger in Fig. 4c. What sets this direction apart from the other two? More generally, some discussion of the zero-mode overlap along the full evolution path would be helpful. The energy splitting of the MZMs does seem to increase periodically in Fig 4a (a zoomed in inset could be helpful here). What are the constraints on parameters, coherence lengths, etc. to ensure that this evolution scheme preserves quantum information (MZMs remain well defined and separated throughout the evolution)? For example, the splitting energy of the MZMs appear large in Fig. 2a of the SM.*

Reply: Firstly, we would like to remind the referee that Figs. 4 (b-d) [(c), (e), (f) in the revision, to which we refer below] correspond to $\varphi = 0, \frac{\pi}{6}, \frac{\pi}{3}$, respectively. Therefore, in (e) the vector potential is parallel to the upper right edge, which is different from being perpendicular to the edge hosting two MZM in either (c) or (f). As a result, although in (e) only one (upper-right) edge is nontrivial, similar to the situation in (c) and (f), the gap in each chain is different, hence the different MZM profiles. We have added the zoomed-in spectral flow near zero energy in the region of $\varphi \in [0, \frac{\pi}{3})$ as an inset to Fig. 4 (a).

To help the readers better understand the evolution of the MZM in Fig. 4, we have plotted the bulk (i.e., periodic boundary condition) band gap of the three edges for $\varphi \in [0, \frac{\pi}{3})$ in Fig. 4 (b). One can see that near the middle of the $\varphi \in [0, \frac{\pi}{6})$, where the bottom and the upper-right edges would have undergone topological phase transitions if they were infinitely long, the gap closing is avoided due to the finite length of the edges.

In addition, we have made an animation of the spatial profile of the MZM through the $\varphi \in [0, \frac{\pi}{3})$ evolution as a separate supplemental material and have added the MZM profile at $\varphi = \frac{\pi}{12}$ as the new Fig. 4 (d). Although the MZM at this critical point become less localized, which is potentially harmful to the fidelity of MZM qubits, we note that it is mostly a consequence of the simplified parameter path using a rotating, constant-size vector potential. This is also the case for the more pronounced MZM hybridization in the supplemental Fig. 2 (a) for the $W = 3$ hollow triangle. Optimization of the parameter path, which is beyond the scope of the present work, can be done by either choosing triangles of appropriate sizes and/or controlling the vector potential, including its size, on three edges independently. For example, one can implement the following two-step process using edge-dependent vector potentials: the nontrivial bottom edge first grows to twice its length into the upper-right edge, and then shrinks to the upper-right edge completely. As long as the edge length L enables the finite-size quantization gap $E_g \sim \frac{\hbar v_F}{L}$, where v_F is the renormalized Fermi velocity at a bulk gap-closing point, comparable to the p-wave gap Δ at the ends of a parameter path, as discussed in Ref. [4], the localization and separation of the MZM are well protected.

In the revised manuscript we have added an abbreviated version of the above discussion below Fig. 4.

Question #4: *Finally, to improve clarity of the manuscript and figures, here are a few additional comments and suggestions:*

1) It would be helpful to readers to indicate clearly the parameters used in the legend of figures. Are all figures done for the case t=delta=1?

2) A definition of the x,y axis in Fig. 4 b-d would be appreciated.

Reply: We thank the referee for these suggestions and have made the corresponding updates in the revision:

1) Yes—we have added this information in Fig. 3 caption.
2) The horizontal and vertical axes are now labeled as *x* and *y* and defined in the caption.