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Kyoto University
Reentrant topological transitions in a quantum wire/superconductor system with quasiperiodic lattice modulation

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We study the condition for a topological superconductor (TS) phase with end Majorana fermions to appear when a quasiperiodic lattice modulation is applied to a one-dimensional quantum wire with strong spin-orbit interaction situated under a magnetic field and in proximity to a superconductor. By density-matrix renormalization group analysis, we find that multiple topological phases with Majorana end modes are realized in finite ranges of the filling factor, showing a sequence of reentrant transitions as the chemical potential is tuned. The locations of these phases reflect the structure of bands in the noninteracting case, which exhibits a distinct self-similar structure. The stability of the TS in the presence of an on-site interaction or a harmonic trap potential is also discussed.

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Edge states of topologically nontrivial systems have attracted attention because they are topologically protected, that is, they are stable against weak perturbations that do not change the topology of their quantum state. Majorana surface states are observed in several regions with finite widths with that of the quantum wire. We find that TSs with Majorana end states are broadened by proximity-induced superconducting gap on a quantum wire, while an on-site electron-electron interaction has the lattice (or superlattice) constant incommensurate with the Zeeman energy, and \( \alpha \) is the chemical potential. In the noninteracting case, which exhibits a distinct self-similar structure. The locations of these phases reflect the structure of bands in the noninteracting case, which exhibits a distinct self-similar structure. The stability of the TS in the presence of an on-site interaction or a harmonic trap potential is also discussed.

Setup. We study a tight-binding 1D fermion model by the density-matrix renormalization group (DMRG). Up to 160 eigenstates of the reduced density matrix \( \rho \), with the sum of discarded eigenvalues of \( \rho \) at each step in the last finite-size system loop being typically less than \( 10^{-7} \), have been retained in the DMRG calculation.

We adopt the following Hamiltonian:

\[
\mathcal{H} = -\frac{t}{2} \sum_{l=0}^{L-2} \sum_{\sigma=\uparrow, \downarrow} (\epsilon_{\sigma,l} c_{\sigma,l+1}^\dagger + \text{h.c.}) + U \sum_{l=0}^{L-1} \hat{n}_{\uparrow,l} \hat{n}_{\downarrow,l} + \Delta \sum_{l=0}^{L-1} (\hat{c}_{\uparrow,l}^\dagger \hat{c}_{\downarrow,l} + \text{h.c.}) + \sum_{l=0}^{L-1} \left[ V_z (\hat{n}_{\uparrow,l} - \hat{n}_{\downarrow,l}) + \sum_{\sigma=\uparrow, \downarrow} (\mu - \epsilon_{\sigma,l}) \hat{n}_{\sigma,l} \right] + \frac{\Delta}{2} \sum_{l=0}^{L-2} (\hat{c}_{\downarrow,l+1}^\dagger \hat{c}_{\uparrow,l}^\dagger - \hat{c}_{\downarrow,l}^\dagger \hat{c}_{\uparrow,l+1} + \text{h.c.}). \tag{1}
\]

Here, \( \hat{c}_{\sigma,l} \) annihilates a fermion with spin \( \sigma (= \uparrow, \downarrow) \) at site \( l (=0, 1, \ldots, L-1) \), \( \hat{n}_{\sigma,l} \equiv \hat{c}_{\sigma,l}^\dagger \hat{c}_{\sigma,l} \), \( t \) is the nearest-neighbor hopping, \( U \) is the on-site interaction, \( \Delta \) is the coupling to the bulk superconductor, \( \alpha \) is the Rashba-type SOI, \( V_z \) is the Zeeman energy, and \( \mu \) is the chemical potential. In the following, we set \( L = 200 \) and \( t = 1 \). We take \( (\Delta, \alpha, V_z) = (0.1, 0.3, 0.3) \) unless noted otherwise, as in Figs. 2, 3, and 6 of Ref. 20. \( \epsilon_{\sigma,l} = \epsilon_l \) is the site energy for spin \( \sigma \) on site \( l \).

For an infinite-size system with \( U = \Delta = 0 \) and \( \epsilon_{\uparrow,0} = 0 \), it is straightforward to obtain the single-particle dispersion relation as a function of the quasimomentum \( k \):

\[
E_{\pm}(k) = t [1 - \cos(k)] \pm \sqrt{\alpha^2 \sin^2(k) + V_z^2}. \tag{2}
\]

In this Rapid Communication, we call them the upper and lower Rashba–Zeebra (RZ) bands.

If the Hamiltonian can be mapped to that of a spinless system, the TS state is realized by the introduction of the pairing \( \Delta \). When \( \Delta \ll V_z \), such mapping is possible if \( \mu \) is in only one of the RZ bands. For a more general discussion on the origin of the topological states, we refer to Ref. 29. Note that even when \( U = 0 \), while only quadratic terms of annihilation and creation operators appear in the Hamiltonian,
Δ ≠ 0 introduces nonzero matrix elements between states whose number of fermions differs by two. The dimension of the Hilbert space grows exponentially as the number of lattice sites \( L \) is increased, strongly limiting the availability of the exact diagonalization approach.

Suppose that we have a lattice system having two Majorana end modes \( \gamma_1, \gamma_2 \) such that \( \eta^\pm \equiv \gamma_1 \pm i \gamma_2 \) is a fermionic operator satisfying \( \{ \eta^\pm \} = (\gamma_1 + i \gamma_2)^\dagger = \gamma_1 - i \gamma_2 = \eta^- \). If the Majorana operators can be approximated by linear combinations of the single-particle annihilation and creation operators, \( \gamma_j = \sum_{\sigma} \langle a_{\sigma,j}^\dagger | \gamma_{\sigma} | a_{\sigma,j} \rangle \) (\( j = 1, 2 \)), then we can think of two single-particle wave functions, \( | \gamma_j \rangle = \sum_{\sigma} \langle a_{\sigma,j}^\dagger | \gamma_{\sigma} | a_{\sigma,j} \rangle \), in which \( | \rangle \) is the empty state, as the “Majorana wave functions.” For the ground-state many-body wave functions in the sectors of total number of fermions being even (e) and odd (o), \( \{ | \gamma_e,o \rangle \} \) with energies \( E_{e,o} \), we can obtain the values of \( a_{\sigma,j}^\dagger \) as follows:20

\[
\begin{align*}
\langle \gamma_e | a_{\sigma,j}^\dagger | \gamma_e \rangle &= \langle \gamma_e | a_{\sigma,j}^\dagger | \gamma_o \rangle, \\
\langle \gamma_o | a_{\sigma,j}^\dagger | \gamma_e \rangle &= \langle \gamma_o | a_{\sigma,j}^\dagger | \gamma_o \rangle.
\end{align*}
\]

In Ref. 20, the phase diagrams for \( U > 0 \) and \( U = 0 \) are obtained by calculating \( | \gamma_e,o \rangle \) and checking if the following three conditions are met: (i) \( \Delta E = E_e - E_o \) vanishes; (ii) the left reduced density matrices of the system, obtained from the density matrices \( | \gamma_{e,o} \rangle \langle \gamma_{e,o} | \) by tracing out all sites in the right half, have degenerate eigenvalue spectrum; and (iii) \( \{ a_{\sigma,j} \} \) and \( \{ a_{\sigma,j}^\dagger \} \) are spatially localized to the different ends. Now we apply these conditions to the case with spatial inhomogeneity.

**Quasiperiodic site potential.** We study the effect of a quasiperiodic site potential, which is given by

\[ \epsilon_{\sigma,j} = V_Q \cos[k(l - l_0) + \delta], \]

in which \( V_Q ≥ 0, l_0 \equiv (L - 1)/2 \), and the phase is \( \delta = 0 \) unless noted. We choose \( k = 2 \pi g \), in which \( g = \sqrt{5} - 2 \).

In the noninteracting case \( (U = Δ = 0) \), we can consider a periodic lattice with \( g_n = F_{n-3}/F_n \), in which \( F_n \) is the \( n \)th Fibonacci number, to obtain the approximate eigenenergy distribution. The Fourier transform of the site potential then has only components with \( k = ±2\pi g, ±2\pi (1 - g_n) \) but mixes states between the upper and lower RZ bands because the spin composition of the states in the RZ bands depends on the wave number, \( g_n \) rapidly converges to \( g \) as \( n \) is increased, as does the eigenvalue distribution. As \( V_Q \) is increased, the number and widths of the gaps in the eigenvalue distribution both increase. For \( V_Q \sim t \), the spectrum exhibits a distinct self-similar structure when \( k \) is changed, which resembles two Hofstadter butterflies30,31 shifted in energy and overlapping each other, as shown in the inset of Fig. 1(a). We note that for \( \alpha = V_Q = 0 \), all single-body wave functions are extended for \( V_Q < t \) and localized for \( V_Q > t \) in the limit of large system \( (L \rightarrow \infty) \).

In Fig. 1, we plot \( \Delta E \) against \( \mu \) for several values of \( V_Q \) for \( L = 200 \) sites, as well as the eigenenergies of the noninteracting case with the quasiperiodic potential. The slope of \( \Delta E \) as a function of \( \mu \) is often close to \( ±1 \) outside the TS phase, which corresponds to the fact that \( N_e - N_o \) is close to \( ±1 \) in such regions of \( \mu \). The two regions with \( \Delta E = 0 \) for \( V_Q = 0 \) correspond to the ranges of \( \mu \) crossing only one of the two RZ bands. The RZ bands are gradually mixed and split into several minibands as \( V_Q \) is increased also for the open boundary condition. While the locations and widths of some of the regions with vanishing \( \Delta E \) resemble those of the minibands, not all of the regions of the chemical potential overlapping with one of the minibands have \( \Delta E = 0 \). While the value of \( \Delta E \) outside of the plateaus at \( \Delta E \) depends on the choice of \( \delta \), the locations and widths of the plateaus almost do not change when \( \delta \) is changed.

We have observed that the other two conditions of Ref. 20, namely, (i) the localized end states and (iii) the degeneracy of reduced density-matrix eigenvalues, are satisfied in the regions in which \( \Delta E \) vanishes, and they are not satisfied when \( |\Delta E| ≥ 10^{-4} \). The amplitude distribution of the wave function of the end Majorana modes for \( (V_Q, \mu) = (0.2, 0.5) \) is shown in Fig. 2(a). The distributions of \( |a_{\sigma,j}^\dagger|^2 \) and \( |a_{\sigma,j}^\dagger|^2 \) are, respectively, localized to the right and left ends of the
system. While for $V_Q \gtrsim 1$, the plots of $\Delta E(\mu, U = 0)$ exhibit significantly shorter plateaus at $\Delta E = 0$, the two Majorana modes localized at the two ends are observed inside such plateaus, as shown for $(V_Q, \mu) = (1.2, 1.36)$ in Fig. 2(b). This is a nontrivial observation because for $|V_Q| > 1$ we expect localized single-particle states for $\Delta = 0$, and localized states would not support global TSs. The reduced density-matrix eigenvalues are also degenerate, therefore we conclude that a TS with end Majorana fermions is realized in the $\Delta E = 0$ plateau. We have also observed that the dependence of the regions with Majorana end states on the initial phase $\delta$ is weak in our system, which is similar to the noninteracting case,\textsuperscript{15} while the sign of $\Delta E$ between these regions depends on the choice of $\delta$.

While we easily obtain the Bogoliubov quasiparticle energies by retaining the value of $\Delta$ and diagonalizing the Hamiltonian in the Nambu spinor space,\textsuperscript{11} the correspondence between the degenerate region and the single band region in the quasiparticle spectrum has been observed to be comparable at best to the correspondence between the former and the single band region of the minibands without $\Delta$. We believe that not only the energy spectrum but also the spatial distribution of the states is important in the realization of the TS states.

In the studies of 1D topological phases of free fermions in bichromatic superlattices,\textsuperscript{15,16} the topological phases appear only at special filling factors between the bulk bands. Here we emphasize that in our system of the 1D quantum wire with strong SOI, placed under a magnetic field and having a proximity-induced pairing, the topological phases are realized in several finite ranges of $\mu$ that correspond to finite ranges of the filling factor, as observed in Figs. 1 and 3 ($U = 0$), with some of them much closer to half filling compared to the $V_Q = 0$ case. This is the main result of this Rapid Communication.

\textbf{Effect of fermion-fermion interaction.} Next we study the effect of an on-site fermion-fermion interaction coexisting with the quasiperiodic site potential modulation. In Fig. 3, the values of $\Delta E(\mu, U)$ for $U = 0, 0.2$, and 0.5 are plotted against the number of fermions $N_e$ in the system, as well as against $\mu$.

When $U$ is larger, the amount of increase in $\mu$ required for adding the same number of fermions at the same filling factor becomes larger because of the stronger repulsive interaction. The $\Delta E(\mu) = 0$ plateaus in the inset of Fig. 3 are observed in broader ranges of the chemical potential, as expected from Ref. 20, with $V_Q = 0$. Furthermore, we observe that the plateaus are broader for larger $U$ also in terms of the number of fermions.\textsuperscript{32}

For a fixed $N_e$, chosen so that $\Delta E$ approaches zero as $U$ is increased, in Figs. 2(c)–2(e) we observe that the distributions of $|a^{(j)}_{\eta \sigma}|$ become localized toward the ends. We also observe that the difference between the eigenstate spectra of the reduced density matrices for $\Psi_e$ and $\Psi_\sigma$, plotted in the bottom part of Fig. 2, becomes smaller as $\Delta E$ becomes smaller. Similar behavior of the distributions of $|a_{\eta \sigma}^{(j)}|$ and the eigenstate spectra of the reduced density matrices are observed in other plateaus of $\Delta E(\mu, U)$.

\textbf{Effect of a trapping potential.} In many cold-atom experiments, atom clouds are trapped in the vacuum by (magneto)optical potentials that are better approximated by a harmonic or Gaussian potential rather than a flat, boxlike potential. Also, in condensed-matter systems, the shape of the potential for electrons in the quantum wire would depend on how it is fabricated. Studying the effect of an additional trapping potential on the realization of the Majorana end fermions is therefore important and has already been conducted for noninteracting cases.\textsuperscript{15,16} To complete this Rapid Communication, we study the effect of a harmonic potential, $V_{\text{tr}}[(l - l_c)/l_c]^2$ ($l = 0, 1, \ldots, L - 1 = 2l_c$), added to the site potential (5).

![FIG. 2. (Color online) Top: The values of $\sum_{\eta \sigma} |a^{(j)}_{\eta \sigma}|^2$ are plotted against the site $l$ for (a) $(U, V_Q, \mu) = (0, 0, 2, 0.6)$, (b) $(U, V_Q, \mu) = (0.1, 2, 1.36)$, (c) $(U, V_Q, \mu) = (0.2, 0, 0.6)$, (d) $(U, V_Q, \mu) = (0.2, 0.2, 0.75743)$, and (e) $(U, V_Q, \mu) = (0.5, 0.2, 0.85472)$. In (c)–(e), the value of $\mu$ has been chosen so that $N_e = 155.000$. Bottom: The eigenvalue spectra of the reduced density matrix for the left half of the system in states $\Psi_e$ and $\Psi_\sigma$ are plotted for the parameter sets used in (c)–(e).](image1)

![FIG. 3. (Color online) The energy difference between ground states in the sectors with even and odd number of fermions plotted against the number of fermions for $U = 0, 0.2$, and 0.5. The other parameters are $(\Delta, \alpha, V_c) = (0.1, 0.3, 0.3)$ and $V_Q = 0$. Inset: the same plotted against the chemical potential $\mu$.](image2)
Figure 4 shows $\Delta E$ plotted against $\mu$ for $(V_Q, V_H) = (0,0)$, $(0,0,5)$, $(0,2,0)$, and $(0,2,0,5)$ with $(\Delta, \alpha, V_s, U) = (0,1,0,3,0,5)$. Inset: $\Delta E$ plotted against $\mu$ for $V_Q = 0$ and $V_H = 0, 0.1, 0.3, 0.5, 1$. We observe that between these plateaus, $\Delta E$ plotted for $(V_Q, V_H) = (0,2,0,5)$ shows repeated oscillations.

In the inset of Fig. 4 we have plotted $\Delta E$ for $V_Q = 0$ and several values of $V_H$. For increasing $V_H$, the first region of vanishing $\Delta E$ is broadened. The Majorana fermion states are localized close to the system boundary, where the harmonic trap decreases the effective chemical potential, measured from the local site potential, by almost the depth of the trap potential $V_H$. This explains the increase of the value of $\mu$ at the upper boundary.

On the other hand, our system with the quasiperiodic potential has the Majorana state broken down not only between the plateau for the system with $(V_Q, V_H) = (0,2,0)$, but also inside the second and third plateaus, when $V_H$ is introduced. We believe that this is because the values of the effective chemical potential at which the quasiperiodic potential destroys the TS is reached at some location even for greater values of $\mu$ for $V_H > 0$. This effect seems to compete with the decrease of the effective chemical potential at the edge of the fermion distribution and $\Delta E$ oscillates. While for simplicity we have shown here the results for the case with $U = 0.5$, the discussion above is also consistent with those for other values of $U \geq 0$.

In conclusion, we have studied the effect of spatial inhomogeneity realized by a quasiperiodic site potential modulation applied on a tight-binding model of a TS, which is a 1D conductor with SOI in the proximity of a bulk superconductor and under a magnetic field. When the modulation is induced, the topological phase appears not only when the band is almost empty or almost full, but also in several regions of the filling factor (or the chemical potential) with finite widths much closer to half filling, even when the modulation is strong enough to turn the system without SOI and pairing insulating.

We have also studied the effects of on-site fermion-fermion interaction and a harmonic trap. Without the trap, as the interaction becomes stronger, the TS phase becomes wider in the phase diagram, as in the case without the spatial inhomogeneity, in terms of both the chemical potential and the number of fermions in the system. Our results reveal the possibility of realizing Majorana end states in 1D systems such as cold-atom systems and superconductor-metal heterostructures with inherent or imposed inhomogeneities.

Recently, we became aware that the interplay of disorder and correlation in 1D TSs has also been investigated in Ref. 33.

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FIG. 4. (Color online) $\Delta E$ plotted against $\mu$ for $(V_Q, V_H) = (0,0)$, $(0,0,5)$, $(0,2,0)$, and $(0,2,0,5)$. The other parameters are $(\Delta, \alpha, V_s, U) = (0,1,0,3,0,5)$. Inset: $\Delta E$ plotted against $\mu$ for $V_Q = 0$ and $V_H = 0, 0.1, 0.3, 0.5, 1$. We observe that between these plateaus, $\Delta E$ plotted for $(V_Q, V_H) = (0,2,0,5)$ shows repeated oscillations.
REENTRANT TOPOLOGICAL TRANSITIONS IN A . . .


$N_e$ and $N_o$ are both increasing functions of $\mu$. While they are degenerate only inside the topological insulator phase, $|N_e - N_o|$ is observed to be at most unity. Therefore the widths of the $\Delta E = 0$ plateaus are not significantly changed if we choose to plot $\Delta E$ against $N_o$.