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Topological phase diagrams and Majorana zero modes of the Kitaev ladder and tube*

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In this paper, we study two quasi-one-dimensional (1D) Kitaev models with ladder-like and tube-like spatial structures, respectively. Our results provide the phase diagrams and explicit expressions of the Majorana zero modes. The topological phase diagrams are obtained by decomposing the topological invariants and the topological conditions for topologically nontrivial phases are given precisely. For systems which belongs to topological class BDI, we obtain the regions in the phase diagrams where the topological numbers show even-odd effect. For the Kitaev tube model a phase factor induced by the magnetic flux in the axial direction of the tube is introduced to alter the classification of the tube Hamiltonian from class BDI to D. The Kitaev tube of class D is characterized by the Z_2 index when the number of chains is odd while 0, 1, 2 when the number of chains is even. The phase diagrams show periodic behaviors with respect to the magnetic flux. The bulk-boundary correspondence is demonstrated by the observations that the topological conditions for the bulk topological invariant to take nontrivial values are precisely those for the existence of the Majorana zero modes.

Keywords: topological phase transition, Majorana zero modes, Kitaev model

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1. Introduction

In 2001, Kitaev proposed a one-dimensional (1D) spinless p-wave superconductor,[1] which is the first and simplest prototype to realize the long-sought Majorana fermions[2] in solid state systems. This so-called Kitaev chain was demonstrated theoretically to host an unpaired Majorana zero mode (MZM) at each of its ends.[1,3–10] These MZMs are exotic quasiparticle excitations which are their own antiparticles, each of which can be considered as half of a fermion. Topological superconductors supporting MZMs are candidate platforms to realize fault tolerant topological quantum computation and storage due to their non-Abelian statistics and immunity to local perturbations.[11–16] Intense research interest has been stimulated in the community of condensed matter physics since the seminal paper by Kitaev. Various 1D topological superconducting systems have been proposed theoretically[17–20] to realize effective p-wave pairing in real materials with spinful fermions and several experiments[21–24] reported signatures of observing the MZMs in the InSb or InAs nanowire systems based on the theoretical suggestions that the semiconductor nanowires with strong Rashba spin–orbit coupling in proximity to an s-wave superconductor can support MZMs in presence of a Zeeman field.

On the other hand there are also theoretical efforts[25–31] on generalizing the Kitaev chain model to quasi-1D spinless fermion systems to provide practical route to realize MZMs in thin-film microstructures[25,32] or to understand the signatures of MZMs observed in nanowire systems[30,33] which have finite width instead of a strict 1D atomic chain. A quasi-1D $p_x + \mathrm{i}p_y$-wave superconductor with strip geometry was first investigated[25] and robust Majorana ends states were found beyond the strict 1D limit. Later similar ideas based on the quasi-1D ladder model were also discussed by several authors.[28–31] The so-called Kitaev ladder is actually multiple Kitaev chains placed in parallel and coupled via inter-chain hopping or pairing with each other. People found that the Kitaev ladder system undergoes multiple topological phase transitions and the number of MZMs varies as a function of system parameters.

In this paper, we give some analytic results of the quasi-1D ladder-like and pipe-like Kitaev models. These so-called Kitaev ladder and Kitaev tube are generalization of the Kitaev chain model and can be used to simulate the thin-film microstructures[25,32] and nanowire systems,[21–24] which are commonly employed to implement topological superconductors experimentally. The topological phase diagrams and the MZMs are investigated analytically for these two types of quasi-1D topological superconductors. For both the Kitaev ladder belonging to class BDI and the Kitaev tube, we decompose the topological invariants of the system into sums of independent topological numbers by transformations in momentum space. The dependence of the phase diagrams on the parity of the number of chains is also examined for all the

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cases studied in this work. We confirm the bulk-boundary correspondence by combining the results of MZMs in real space with the topological properties in momentum space.

This paper is organized as follows. In Section 2, we discuss the Kitaev ladder model. The topological invariant and phase diagrams are studied. The MZMs are investigated. In Section 3, the Kitaev tube model is introduced. Both the class BDI and class D cases are discussed. Finally, We give the conclusion in Section 4.

2. Multi-leg Kitaev ladder

In this section we consider the multi-leg Kitaev ladder model that is a quasi-1D model of topological superconductors. The so-called Kitaev ladder is composed of identical Kitaev chains placed in parallel and coupled with each other as shown Fig. 1. The ladder Hamiltonian is given by

$$\begin{aligned} H = & -\sum_{m=1}^{M}\sum_{n=1}^{N-1}\left(t_x c_{m,n}^{\dagger}c_{m,n+1}+\Delta_x c_{m,n}^{\dagger}c_{m,n+1}^{\dagger}+\text{h.c.}\right) \\ & -\sum_{n=1}^{N}\sum_{m=1}^{M-1}\left(t_y c_{m,n}^{\dagger}c_{m+1,n}+\Delta_y c_{m,n}^{\dagger}c_{m+1,n}^{\dagger}+\text{h.c.}\right), \\ & -\sum_{m=1}^{M}\sum_{n=1}^{N}\mu c_{m,n}^{\dagger}c_{m,n}, \end{aligned} \tag{1}$$

where M is the number of legs of the ladder and N denotes the length of each chain. $c_{m,n}$ and $c_{m,n}^{\dagger}$ represent the annihilation and creation operators of spinless fermion on the n-th site of the m-th leg, respectively. Here $t_{x(y)}$ and $\Delta_{x(y)}$ are the intra(inter)-chain hopping integral and pairing potential, respectively. μ is the chemical potential. We consider the ladder Hamiltonian belonging to topological class BDI[34] which has time-reversal, particle-hole and chiral symmetries.[30] t_x, t_y, Δ_x, Δ_y, and μ are all real variables. Without loss of generality, we set $t_x > 0$. Furthermore Δ_x can also be set as positive under suitable gauge.

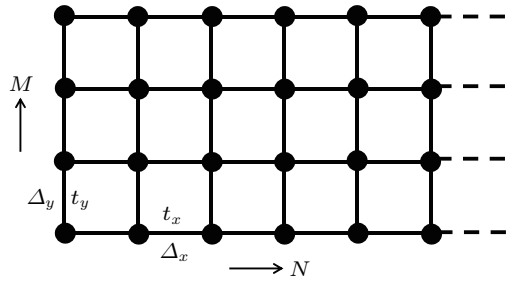


Fig. 1. Illustration of quasi-1D Kitaev ladder model, which is composed of M identical Kitaev chains of length N coupled with each other via nearest-neighbor inter-chain hopping t_y and pairing Δ_y. t_x and Δ_x denote the intra-chain hopping integral and pairing potential.

2.1. Topological invariant and phase diagrams

To show the topological properties of this system, we take a Fourier transformation as shown in Eq. (2) along the x direction

$$c_{m,k} = \frac{1}{\sqrt{N}}\sum_{n=1}^{N} c_{m,n}\,\mathrm{e}^{-\mathrm{i}kn} \tag{2}$$

and the Hamiltonian (1) can be expressed as

$$\hat{H} = -\sum_{k}\Psi_k^{\dagger}H_k\Psi_k \tag{3}$$

with $\Psi_k^{\dagger} = [c_{1,k}^{\dagger}, c_{2,k}^{\dagger}, \ldots, c_{M,k}^{\dagger}, c_{1,-k}, c_{2,-k}, \ldots, c_{M,-k}]$ and

$$H_k = \begin{bmatrix} \xi_k & \Delta_k \\ -\Delta_k & -\xi_k \end{bmatrix}, \tag{4}$$

where ξ_k and Δ_k are $M\times M$ tridiagonal matrix whose elements are

$$(\xi_k)_{i,j} = \left(t_x\cos k + \frac{\mu}{2}\right)\delta_{i,j} + t_y(\delta_{i+1,j}+\delta_{i,j+1}), \tag{5}$$

$$(\Delta_k)_{i,j} = \mathrm{i}\Delta_x\sin k\delta_{i,j} + \Delta_y(\delta_{i+1,j}-\delta_{i,j+1}) \tag{6}$$

The Bogoliubov–de-Gennes (BdG) Hamiltonian H_k has chiral symmetry $\tau_1 H_k \tau_1 = -H_k$ with τ_1 the Pauli matrix and therefore is converted into a block-off-diagonal form by the following unitary transformation, and we have

$$UH_kU^{\dagger} = \begin{bmatrix} 0 & Q_k \\ Q_k^{\dagger} & 0 \end{bmatrix}. \tag{7}$$

Here the unitary matrix U is

$$U = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}\otimes I_M \tag{8}$$

with I_M the $M\times M$ identity matrix. Q_k in Eq. (7) is given by $Q_k = \xi_k + \Delta_k$. The topological invariant of this quasi-1D BDI system[30,35] can be expressed as

$$\nu = \frac{1}{2\pi\mathrm{i}}\int_0^{2\pi}\frac{\partial \ln\det Q_k}{\partial k}\mathrm{d}k = \sum_{m=1}^{M}\nu_m, \tag{9}$$

where ν_m denotes the winding number calculated according to

$$\nu_m = \frac{1}{2\pi\mathrm{i}}\int_0^{2\pi}\frac{\mathrm{d}\lambda_m(k)}{\lambda_m(k)} \tag{10}$$

with $\lambda_m(k)$ the m-th eigenvalue of the tridiagonal matrix Q_k, which is written as

$$\lambda_m(k) = t_x\cos k + \frac{\mu}{2} + \mathrm{i}\Delta_x\sin k + \sqrt{t_y^2-\Delta_y^2}\cos\frac{m\pi}{M+1} \tag{11}$$

with $m = 1, 2, \ldots, M$. Equation (9) indicates that the topological invariant of the whole Kitaev ladder system is simply the sum of M individual topological numbers. Each ν_m as shown in Eq. (10) denotes the winding number of a closed curve formed by $\lambda_m(k)$ on the complex plane around the origin. And ν_m takes 0 or 1 according to Eqs. (10) and (11). The sum of the first three terms of the right hand side of Eq. (11) is the result of a strict 1D Kitaev chain, while the last term shows the renormalization effect resulting from the coupling among chains. In the following we will discuss two cases according to the sign of $t_y^2 - \Delta_y^2$.

The first case is $t_y^2 > \Delta_y^2$ where the real part of Eq. (11) is renormalized and consequently ν_m takes nontrivial value 1 under the following topological condition

$$\left| \frac{\mu}{2t_x} + \frac{\sqrt{t_y^2 - \Delta_y^2}}{t_x} \cos\frac{m\pi}{M+1} \right| < 1, \tag{12}$$

which is identical with the result of Ref. [30]. Hence there are totally $M+1$ topologically distinct phases depending on how many topological conditions (12) can be fulfilled when m ranges from 1 to M. According to Ref. [30], the topological index is Z regardless of the parity of the number of legs.

The second case is $t_y^2 < \Delta_y^2$, for which the topological condition of the class-BDI system is not given by the authors of Ref. [30], although they discussed the topological condition of the class-D system. In this case, the imaginary part of Eq. (11) is renormalized and accordingly we find that the topological condition becomes

$$\left(\frac{\mu}{2t_x}\right)^2 + \frac{\Delta_y^2 - t_y^2}{\Delta_x^2} \cos^2\frac{m\pi}{M+1} < 1, \tag{13}$$

which shows that topological conditions for m and $M+1-m$ are actually identical and therefore $\nu_m = \nu_{M+1-m}$. Equation (9) can then be further reduced to

$$\nu = \nu_{(M+1)/2} \times \mathrm{mod}_2(M) + 2\sum_{m=1}^{M/2} \nu_m. \tag{14}$$

One can see that there is no contribution from the first term on the right hand side of Eq. (14) to ν if M is even, and the topological invariant ν always changes by 2 due to the second term.

The topological phase diagrams of 4- and 5-leg Kitaev ladder models belonging to class BDI are shown in Fig. 2. The system is characterized by the Z index in the region $t_y^2 > \Delta_y^2$ as illustrated by Fig. 2, which is compatible with the results of Ref. [30]. However, in the region where $t_y^2 < \Delta_y^2$ there is an even-odd effect with respect to the number of legs of the ladder as indicated by Eq. (14). To be specific, for even M the topological number is $\nu = 0, 2, 4, \ldots, M$ and there are $M/2+1$ topologically distinct phases. Whereas for odd M the topological number is $\nu = 0, 1, 3, \ldots, M$ and there are $(M+1)/2+1$ topologically distinct phases. Accordingly, this even-odd effect leads to rich phase diagrams as illustrated in Fig. 2 for the Kitaev ladder belonging to class BDI in comparison with the simple phase diagrams of that belonging to class D in the region $t_y^2 < \Delta_y^2$.[30]

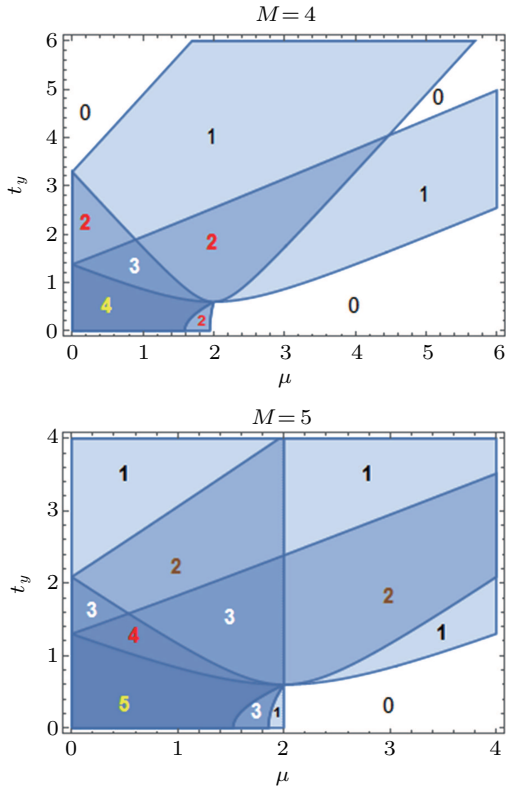


Fig. 2. (color online) Phase diagrams of the 4-leg and 5-leg Kitaev ladder models. t_x is chosen as energy unit. $\Delta_x = 0.8$ and $\Delta_y = 0.6$. The integer numbers in the figure represent the Z index. In the regions where $t_y < \Delta_y$, the topological indices are $0, 2, 4$ for $M = 4$ (upper panel) and $0, 1, 3, 5$ for $M = 5$ (lower panel).

2.2. Majorana zero modes

Here we study the presence of MZMs at the boundary of the Kitaev ladder. In the following basis of Majorana fermions,

$$a_{m,n} = c_{m,n} + c_{m,n}^\dagger, \quad b_{m,n} = -\mathrm{i}(c_{m,n} - c_{m,n}^\dagger), \tag{15}$$

which satisfy the algebra $a_{m,n}^\dagger = a_{m,n}$, $b_{m,n}^\dagger = b_{m,n}$, $\{a_{m,n}, a_{m',n'}\} = 2\delta_{m,m'}\delta_{n,n'}$, $\{b_{m,n}, b_{m',n'}\} = 2\delta_{m,m'}\delta_{n,n'}$, and $\{a_{m,n}, b_{m',n'}\} = 0$, the tight-binding Hamiltonian (1) is then rewritten as

$$\begin{aligned}\hat{H} = -\frac{\mathrm{i}}{2}\Bigg\{ &\sum_{m=1}^{M}\sum_{n=1}^{N-1}\left[(t_x - \Delta_x)a_{m,n}b_{m,n+1} - (t_x + \Delta_x)b_{m,n}a_{m,n+1}\right] \\ &+ \sum_{n=1}^{N}\sum_{m=1}^{M-1}\left[(t_y - \Delta_y)a_{m,n}b_{m+1,n} - (t_y + \Delta_y)b_{m,n}a_{m+1,n}\right] \\ &+ \mu\sum_{m=1}^{M}\sum_{n=1}^{N} a_{m,n}b_{m,n}\Bigg\}.\end{aligned} \tag{16}$$

For a very long (semi-infinite) ladder with $N \to \infty$, the MZMs of the system can be written in the following form

$$\gamma = \sum_{m=1}^{M}\sum_{n=1}^{N} f_{m,n}a_{m,n}, \tag{17}$$

where $f_{m,n}$ is the wave function of the Majorana fermion to be determined. As a Majorana fermion $\gamma^\dagger = \gamma$ and thus $f_{m,n}$ is

real. The wave function satisfies the boundary conditions

$$f_{m,0}=0, \lim_{n\to\infty} f_{m,n}=0, \tag{18}$$

in the x direction and

$$f_{0,n}=f_{M+1,n}=0 \tag{19}$$

in the y direction. Note that the second condition of Eq. (18) is due to the localized nature of MZMs around the left boundary of the ladder. From $[H,\gamma]=0$ since γ is a zero-energy mode, we obtain the following second-order difference equations,

$$\begin{aligned}&(t_x+\Delta_x)f_{m,n+1}+\mu f_{m,n}+(t_x-\Delta_x)f_{m,n-1}\\&+(t_y+\Delta_y)f_{m+1,n}+(t_y-\Delta_y)f_{m-1,n}=0\end{aligned} \tag{20}$$

for $m=1,2,\ldots M$, which forms one M-dimensional second-order difference equation system. We take a transformation along the y direction as follows:

$$f^q_{m,n}=F_{q,n}\left(\frac{t_y-\Delta_y}{t_y+\Delta_y}\right)^{m/2}\sin\left(\frac{qm\pi}{M+1}\right), \tag{21}$$

and then obtain M independent equations written as,

$$(t_x+\Delta_x)F_{q,n+1}+\mu_q F_{q,n}+(t_x-\Delta_x)F_{q,n-1}=0, \tag{22}$$

where

$$\mu_q=\mu+2\sqrt{t_y^2-\Delta_y^2}\cos[q\pi/(M+1)] \tag{23}$$

with $q=1,2,\ldots,M$. The above results show manifestly that the Kitaev ladder can be effectively decoupled into M independent Kitaev chains each of which has a renormalized chemical potential μ_q. The MZMs in the Kitaev ladder can be found from Eq. (22) for each q separately.

For the case of $t_y^2-\Delta_y^2>0$, we find that the solution $F_{q,n}$ of Eq. (22) exists iff q satisfies the topological condition (12) (see Appendix A for detail) and correspondingly there exists an MZM γ_q according to Eq. (17) after substituting $F_{q,n}$ into Eq. (21)

$$\gamma_q=\sum_{m,n} f^q_{m,n}a_{m,n} \tag{24}$$

with $f^q_{m,n}$ obviously obeying the boundary conditions (18) and (19).

For $t_y^2-\Delta_y^2<0$, the solution $F_{q,n}$ of Eq. (22) exists iff the topological condition Eq. (13) is satisfied for q. Furthermore $F_{q,n}$ is generally complex because μ_q may have an imaginary part. Considering that equation (13) is met simultaneously for q and $M+1-q$ and that $\mu_{M+1-q}=\mu_q^*$ and $F_{M+1-q,n}=F^*_{q,n}$, we have two complex fermions γ_q and γ_{M+1-q} with relation $\gamma_q=\gamma^\dagger_{M+1-q}$ according to Eqs. (21) and (24). Consequently, two Majorana fermions $\gamma_{1,q}=\gamma_q+\gamma_{M+1-q}$ and $\gamma_{2,q}=-\mathrm{i}(\gamma_q-\gamma_{M+1-q})$ are obtained pairwise. Note that there exists an exception with $q=M+1-q=(M+1)/2$ for odd M. In this case $\mu_{(M+1)/2}=\mu$ and one MZM is built according to Eq. (24).

From the above results of MZMs, it is demonstrated that the topological conditions for the bulk topological invariant to take nontrivial values are precisely those for the existence of boundary MZMs. Thus the topologically distinct phases are characterized by either the winding numbers obtained in momentum space or equivalently by the number of MZMs in real space. These observations obviously manifest the bulk-boundary correspondence in the Kitaev ladder system.

3. Kitaev tube

In this section we consider the Kitaev tube model as shown in Fig. 3. Similar to the ladder model, the Kitaev tube is also composed of M identical Kitaev chains that are coupled with each other. The significant difference between the tube and ladder is the boundary condition along the y direction, namely we have closed boundary condition for the former and open for the latter. The merit of the tube structure is that one can change the classification of the model by applying a magnetic field along its axial direction. The tube Hamiltonian is written as

$$\begin{aligned}\hat{H}=&-\sum_{m=1}^{M}\sum_{n=1}^{N-1}\left(t_x c^\dagger_{m,n}c_{m,n+1}+\Delta_x c^\dagger_{m,n}c^\dagger_{m,n+1}+\mathrm{h.c.}\right)\\&-\sum_{n=1}^{N}\sum_{m=1}^{M}\left(t_y\mathrm{e}^{\mathrm{i}\theta}c^\dagger_{m,n}c_{m+1,n}\right.\\&\left.+\Delta_y\mathrm{e}^{\mathrm{i}\phi}c^\dagger_{m,n}c^\dagger_{m+1,n}+\mathrm{h.c.}\right)-\sum_{m=1}^{M}\sum_{n=1}^{N}\mu c^\dagger_{m,n}c_{m,n},\end{aligned} \tag{25}$$

where the meanings of the operators and parameters are the same as those of the ladder model Eq. (1) except that there are two additional parameters θ and ϕ. θ denotes the relative phase between the intra- and inter-chain hopping integrals, which results from the magnetic field applied in the axial direction of the tube as shown in Fig. 3. ϕ denotes the relative phase between the intra- and inter-chain pairing potentials. If $\phi=0$ we have a p_x+p_y-wave pairing model and if $\phi=\pi/2$ we have a $p_x+\mathrm{i}p_y$-wave pairing model.

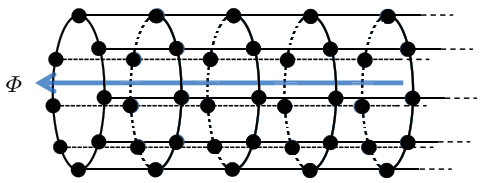


Fig. 3. (color online) Illustration of the Kitaev tube which can be viewed as the Kitaev ladder (see Fig. 1) rolled up in y dimension. Φ denotes the magnetic flux through the tube, which leads to a phase factor $\mathrm{e}^{\mathrm{i}\theta}$ in the inter-chain hopping integral as shown in Eq. (25). The relation of θ and Φ is $\theta=2\pi\Phi/(M\Phi_0)$ with Φ_0 being the magnetic flux quantum.

Taking the periodic boundary condition along y direction into account, the fermions are expressed in momentum space

by the Fourier transformation

$$c_{q,k} = \frac{1}{\sqrt{MN}} \sum_{m=1}^{M} \sum_{n=1}^{N} c_{m,n} \exp[-\mathrm{i}(kn + qm)], \tag{26}$$

where k and q represent the momenta along x and y directions, respectively. Then taking thermodynamic limit $N \to \infty$ while keeping M fixed, the Hamiltonian (25) is rewritten as

$$\hat{H} = -\frac{1}{2\pi} \sum_{q} \int_{0}^{2\pi} \Psi_q^{\dagger}(k) H_q(k) \Psi_q(k) \mathrm{d}k. \tag{27}$$

Here $\Psi_q^{\dagger}(k) = [c_q^{\dagger}(k), c_{-q}(-k)]$ and the above summation is taken over q in the following set

$$\left\{0, \frac{2\pi}{M}, \frac{4\pi}{M}, \ldots, \frac{2\pi(M-1)}{M}\right\}. \tag{28}$$

The BdG Hamiltonian is

$$H_q(k) = \begin{bmatrix} \xi_{q,+}(k) & \Delta_q(k) \\ \Delta_q^*(k) & -\xi_{q,-}(k) \end{bmatrix}, \tag{29}$$

where

$$\xi_{q,\pm}(k) = t_x \cos k + t_y \cos(q \pm \theta) + \frac{\mu}{2}, \tag{30}$$

$$\Delta_q(k) = \mathrm{i}(\Delta_x \sin k + \Delta_y \mathrm{e}^{\mathrm{i}\phi} \sin q). \tag{31}$$

The form of the Hamiltonian in momentum space as shown in Eq. (27) obviously indicates that the system can be viewed as stack of M independent Kitaev chains with renormalized chemical potential and gap function as shown in Eqs. (30) and (31). Therefore by calculating the topological invariant ν_q of the BdG Hamiltonian $H_q(k)$ for each given q, one can obtain the topological invariant of the whole tube system,

$$\nu = \sum_{q} \nu_q. \tag{32}$$

3.1. Class BDI

For $\theta = 0, \pi$ and $\phi = 0, \pi$, the system as shown in Eq. (25) belongs to class BDI, which has time-reversal, particle-hole, and chiral symmetries.[34] Since $\Delta_q^*(k) = -\Delta_q(k)$, $H_q(k)$ has chiral symmetry with $\tau_1 H_q(k) \tau_1 = -H_q(k)$ for each given q. And thus $H_q(k)$ can be transformed into off-diagonal form,

$$U H_q(k) U^{\dagger} = \begin{bmatrix} 0 & Q_q(k) \\ Q_q^*(k) & 0 \end{bmatrix}, \tag{33}$$

where

$$U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \tag{34}$$

and $Q_q(k) = \xi_q(k) + \Delta_q(k)$. For each q, a winding number ν_q is associated with $Q_q(k)$ by

$$\nu_q = \frac{1}{2\pi \mathrm{i}} \int_{-\pi}^{\pi} \frac{\partial \ln Q_q(k)}{\partial k} \mathrm{d}k = \frac{1}{2\pi \mathrm{i}} \int_{-\pi}^{\pi} \frac{\mathrm{d}Q_q(k)}{Q_q(k)}$$

$$= \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{d}\theta_q(k), \tag{35}$$

where $\theta_q(k) = \arg Q_q(k)$. ν_q equals 1 if the following topological condition

$$\left(\frac{\mu}{2t_x} + \frac{t_y}{t_x} \cos q\right)^2 + \left(\frac{\Delta_y}{\Delta_x} \sin q\right)^2 < 1 \tag{36}$$

is satisfied and 0 otherwise. Equation (36) shows that topological conditions for q and $2\pi - q$ are the same and therefore $\nu_q = \nu_{2\pi - q}$. Correspondingly equation (32) becomes

$$\nu = \nu_0 + \nu_\pi \times \mathrm{mod}_2(M+1) + 2 \sum_{0<q<\pi} \nu_q. \tag{37}$$

For odd M, π is not in the set of q's as shown in Eq. (28) and therefore there is no contribution to the topological invariant from ν_π as shown in Eq. (37).

The phase diagrams of the Kitaev tube models belonging to class BDI are illustrated in Fig. 4. The system is characterized by the Z index overall and the even–odd effect with respect to M is also manifested in the region where

$$|\mu + 2t_y| < 2t_x,$$

similar to the Kitaev ladder belonging to the same class. Specifically speaking, for odd M the topological number is $\nu = 1, 3, \ldots, M$, while for even M the topological number is $\nu = 2, 4, \ldots, M$ as dictated by Eq. (37).

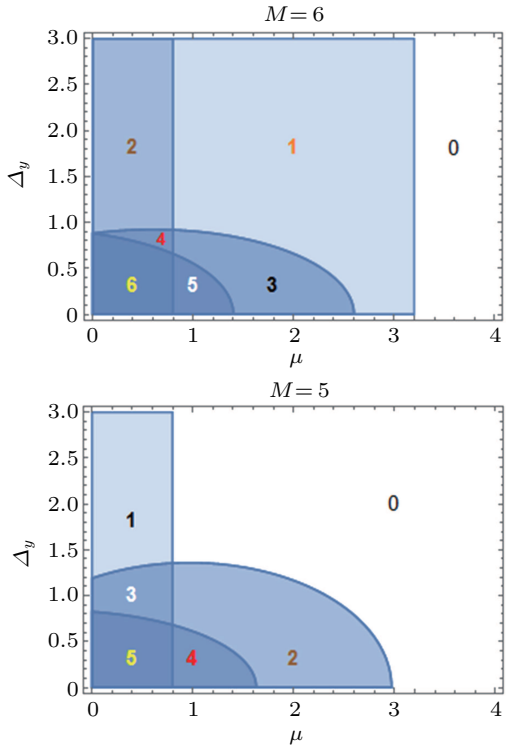


Fig. 4. (color online) Phase diagrams of the Kitaev tubes composed of even and odd number of chains, which belongs to class BDI. The tube is composed of 6 Kitaev chains for the upper panel, while 5 chains for the lower panel. t_x is chosen as energy unit. $\Delta_x = 0.8$ and $t_y = 0.6$. The integer numbers in the figure represent the Z index. In the regions where $\mu < 2(t_x - t_y) = 0.8$, the topological indices are $2, 4, 6$ for $M = 6$ (upper panel) and $1, 3, 5$ for $M = 5$ (lower panel).

Next we study the MZMs of the Kitaev tube system belonging to class BDI. For this purpose the Hamiltonian (25) is rewritten in the Majorana basis (15),

$$\begin{aligned}\hat{H} = -\frac{\mathrm{i}}{2}\sum_{m=1}^{M}\sum_{n=1}^{N}\{&(t_x-\Delta_x)a_{m,n}b_{m,n+1}-(t_x+\Delta_x)b_{m,n}a_{m,n+1}\\&+(t_y-\Delta_y)a_{m,n}b_{m+1,n}-(t_y+\Delta_y)b_{m,n}a_{m+1,n}\\&+\mu a_{m,n}b_{m,n}\}.\end{aligned} \tag{38}$$

The MZM has the same form as Eq. (17) and the wave function $f_{m,n}$ also satisfies Eq. (18). However, we emphasize that $f_{m,n}$ here for the tube structure satisfies the periodic boundary condition in the y direction

$$f_{m+M,n} = f_{m,n}, \tag{39}$$

instead of the open boundary condition as shown in Eq. (19) of the ladder structure. Therefore Fourier transformation is applied

$$f^{q}_{m,n} = F_{q,n}\,\mathrm{e}^{\mathrm{i}qm} \tag{40}$$

and we have

$$(t_x+\Delta_x)F_{q,n+1}+\mu_q F_{q,n}+(t_x-\Delta_x)F_{q,n-1}=0 \tag{41}$$

with

$$\mu_q = \mu + 2t_y\cos q + 2\mathrm{i}\Delta_y\sin q. \tag{42}$$

Similar to the ladder case, we find the correspondence of bulk topological invariant and boundary zero modes in the Kitaev tube of class BDI. Iff certain q satisfies the topological condition Eq. (36) the solution of Eq. (41) exists (See Appendix A for detail) which ensures the presence of the boundary zero modes. If q equals 0 (or $q=\pi$ if M is even), $F_{q,n}$ can give rise to an MZM considering that $\mu_{q=0,\pi}$ is real. Otherwise, $F_{q,n}$ is complex because μ_q takes complex value. However since q and $-q$ are counterparts of each other and $\mu_{-q}=\mu_q^*$, we have $F_{-q,n}=F_{q,n}^*$. From $F_{q,n}$ and $F_{-q,n}$, two complex fermions can be constructed according to $\alpha_q=\sum_{m,n}F_{q,n}\,\mathrm{e}^{\mathrm{i}qm}a_{m,n}$ and $\alpha_{-q}=\alpha_q^\dagger$ with relation $\{\alpha_q,\alpha_q^\dagger\}=1$. Consequently, two Majorana fermions $\gamma_{1,q}=\alpha_q+\alpha_{-q}$ and $\gamma_{2,q}=-\mathrm{i}(\alpha_q-\alpha_{-q})$ are obtained.

3.2. Class D

In this section, we consider the case $\theta\neq 0,\pi$ or $\phi\neq 0,\pi$ which results in that the system Hamiltonian Eq. (25) belongs to class D because the time-reversal and chiral symmetries are broken. For each given q which is not equal to the time-reversal-invariant momentum 0 or π, the topological invariant of the 1D BdG Hamiltonian $H_q(k)$ is zero because it belongs to symmetry class A[34] as known from Eqs. (29), (30), and (31). For $q=0,\pi$, the BdG Hamiltonian simply is

$$H_{q=0,\pi}(k) = \left(t_x\cos k \pm t_y\cos\theta+\frac{\mu}{2}\right)\tau_3-\Delta_x\sin k\,\tau_2, \tag{43}$$

which belongs to class BDI and accordingly $\nu_{q=0,\pi}=0,1$. Note that the Kitaev tube composed of odd number of chains has only one time-reversal-invariant momentum, i.e., $q=0$, and thus the topological number is $\nu=\nu_0$. Consequently there are two topologically distinct phases and the topological condition for $\nu_0=1$ is

$$\left|\frac{\mu}{2t_x}+\frac{t_y}{t_x}\cos\theta\right|<1. \tag{44}$$

On the other hand, the Kitaev tube composed of even number of chains has two time-reversal-invariant momenta, i.e., 0 and π, and thus the topological number is $\nu=\nu_0+\nu_\pi$. Three topologically distinct phases exist and in addition to Eq. (44) for ν_0 there is also a topological condition for $\nu_\pi=1$

$$\left|\frac{\mu}{2t_x}-\frac{t_y}{t_x}\cos\theta\right|<1. \tag{45}$$

From the above results, the topological invariant of the class D Kitaev tube can be written as

$$\nu=\nu_0+\nu_\pi\times\mathrm{mod}_2(M+1). \tag{46}$$

As a result, the topological index is Z_2 for odd M while $0,1,2$ for even M.

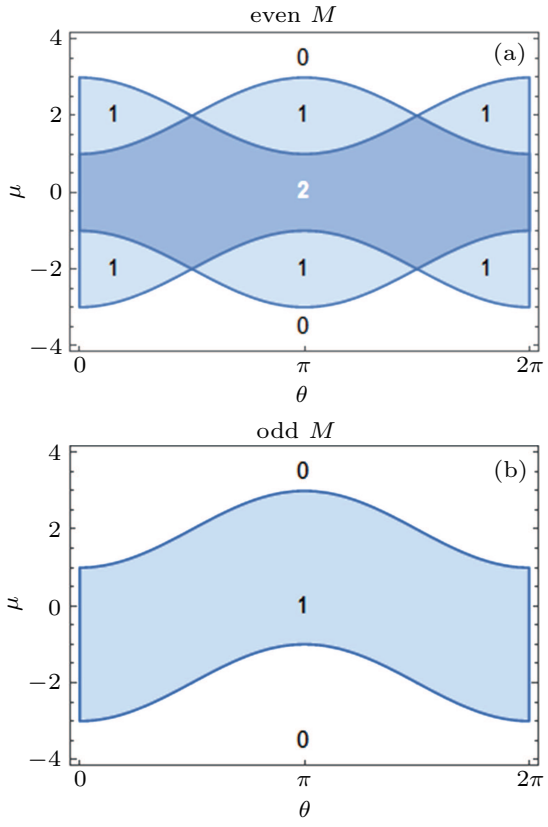


Fig. 5. (color online) Phase diagrams of the Kitaev tubes composed of even (a) and odd number (b) of chains, which belongs to class D. t_x is chosen as energy unit. $\Delta_x=0.8$, $t_y=0.5$, and $\Delta_y=0.6$. The integer numbers in panels (a) represent $0,1,2$ index, while those in panel (b) represent the Z_2 index.

The phase diagrams of the Kitaev tube models belonging to class D in the (θ,μ) plane are plotted in Fig. 5. One can see that the phase diagram of even M has a period of π instead of the trivial period 2π for odd M. This finding can be explained by $H_{q=0}(\theta+\pi)=H_{q=\pi}(\theta)$ derived from Eq. (43). Correspondingly we have $\nu_0(\theta+\pi)=\nu_\pi(\theta)$ and thus $\nu(\theta+\pi)=\nu(\theta)$ for even M, which is compatible with the fact that the topological conditions (44) and (45) are interchanged through $\theta\to\theta+\pi$. From the relation $\theta=2\pi\Phi/M\Phi_0$ and $\Phi=BS$ with B the magnetic field and S the sectional area of the tube, an oscillation of the topological properties as a function of the magnetic field B can be inferred with the period $B_p\propto M\Phi_0/S$, which depends on the number of chains M and the sectional area S of the tube.

At last we consider the MZMs of the Kitaev tube of class D. Two cases with odd and even chains are studied. In terms of Majorana basis, equation (38) reads

$$\begin{aligned}\hat{H} =& -\sum_{m=1}^{M}\sum_{n=1}^{N}(t_x-\Delta_x)a_{m,n}b_{m,n+1}-(t_x+\Delta_x)b_{m,n}a_{m,n+1}\\&+(t_y\cos\theta-\Delta_y\cos\phi)a_{m,n}b_{m+1,n}\\&-(t_y\cos\theta+\Delta_y\cos\phi)b_{m,n}a_{m+1,n}\\&+(t_y\sin\theta+\Delta_y\sin\phi)a_{m,n}a_{m+1,n}\\&+(t_y\sin\theta-\Delta_y\sin\phi)b_{m,n}b_{m+1,n}\\&+\mu a_{m,n}b_{m,n}.\end{aligned}\tag{47}$$

The results in momentum space suggest that the one solution of the MZM should be translation invariant along the y direction, namely $f_{m,n}=f_n$ corresponding to the time-reversal-invariant momentum $q=0$ in Eq. (43). Therefore

$$\gamma=\sum_n f_n\sum_m a_{m,n},\tag{48}$$

and from $[\hat{H},\gamma]=0$, we have

$$(t_x-\Delta_x)f_{n-1}+\mu' f_n+(t_x+\Delta_x)f_{n+1}=0.\tag{49}$$

The above equation is equivalent to that of the 1D Kitaev chain with an effective chemical potential

$$\mu'=\mu+2t_y\cos\theta\tag{50}$$

and there exists one MZM if the topological condition (44) is satisfied. (See Appendix A for detail)

If M is even, there may exist another MZM whose wave function is staggered along the y direction $f_{m,n}=(-1)^m f_n$ corresponding to the time-reversal-invariant momentum $q=\pi$ in Eq. (43), and accordingly

$$\gamma=\sum_n f_n\sum_m(-1)^m a_{m,n}.\tag{51}$$

Substituting Eq. (51) into $[\hat{H},\gamma]=0$, we have Eq. (49) with

$$\mu'=\mu-2t_y\cos\theta.\tag{52}$$

Accordingly the presence of MZM can be guaranteed iff the topological condition (45) is satisfied.

The bulk-boundary correspondence is reconfirmed in the Kitaev tube belonging to class D as in the cases of the Kitaev ladder and tube belonging to class BDI.

4. Conclusion

In this paper, we have studied two quasi-1D Kitaev models, namely the Kitaev ladder and tube, respectively. The topological phase diagrams and wave functions of the Majorana zero modes have been given explicitly. Under the condition that the amplitude of the interchain pairing potential is greater than that of the interchain hopping integral, we have revealed that the M-leg Kitaev ladder model of class BDI is characterized by the $0,1,3,\ldots,M$ index if M is odd, while by the $0,2,4,\ldots,M$ index if M is even. For the Kitaev tube model, the topological invariants have been given after taking Fourier transformation in the circumferential direction. The topological number of the Kitaev tube which belongs to class BDI also shows even–odd effect with respect to the number of chains in certain regions of the phase diagrams. For Kitaev tube of class D, the topological number is Z_2 when the number of chains is odd, while $0,1,2$ when the number of chains is even. For all the cases studied in this paper, we have shown that bulk topological invariant equals to the number of MZMs, which demonstrates the bulk-boundary correspondence in these systems.

Appendix A

In the study of MZMs, the Kitaev ladder or tube has a semi-infinite structure with an open boundary at the left-most lattice sites. As shown in the text of the paper, we find that the transformed wave function F_n satisfying the following second-order difference equation

$$(t+\Delta)F_{n+1}+\mu F_n+(t-\Delta)F_{n-1}=0.\tag{A1}$$

Here $t>0$, $\Delta>0$, and μ is generally a complex number. The general solution of Eq. (A1) is

$$F_n=C(\lambda_+^n-\lambda_-^n),\tag{A2}$$

where C is a constant to be determined by the normalization condition of the Majorana fermion $\gamma^2=1$ and λ_+ and λ_- are the roots of the following quadratic equation

$$(t+\Delta)\lambda^2+\mu\lambda+(t-\Delta)=0\tag{A3}$$

with

$$\lambda_\pm=\frac{-\mu\pm\sqrt{\mu^2+4\Delta^2-4t^2}}{2(t+\Delta)}.\tag{A4}$$

The form of solution as Eq. (A2) obviously gurrentees the open boundary condition $F_0 = 0$. Furthermore, as a boundary mode the MZM is localized around the left end of the semi-infinite ladder or tube, which demands that $\lim_{n\to\infty} F_n = 0$. To meet this, the following damping condition

$$|\lambda_{\pm}| < 1 \tag{A5}$$

should be fulfilled. After straightforward derivation one can easily find that the above damping condition is equivalent to

$$\left(\frac{\mu_{\mathrm{r}}}{2t}\right)^2 + \left(\frac{\mu_{\mathrm{i}}}{2\Delta}\right)^2 < 1, \tag{A6}$$

where μ_{r} and μ_{i} are the real and imaginary parts of μ, i.e. $\mu = \mu_{\mathrm{r}} + \mathrm{i}\mu_{\mathrm{i}}$. As we show in the main text of the paper, the topological conditions obtained by examining the Hamiltonian in momentum space, i.e. Eqs. (12), (13), (36), (44), and (45), are the same as those deduced from the condition Eq. (A6) for the existence of MZMs in real space with the renormalized chemical potential μ being equal to Eqs. (23), (42), (50), and (52). This observation is exactly the manifestation of the bulk-boundary correspondence.

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